Lecture Notes Package for

General, Organic, and Biochemistry

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Includes Worksheets

Chapter 1 Lecture Notes: Stuff and Energy

Educational Goals

1. Explain, compare, and contrast the terms **scientific method**, **hypothesis**, and **experiment**.
2. Compare and contrast scientific **theory** and **scientific law**.
3. Define the terms **matter** and **energy**. Describe the three phases (states) of matter and the two forms of energy.
4. Describe and give examples of **physical properties** and **physical change.**
5. Perform **unit conversion** calculations.
6. Express and interpret numbers in **scientific (exponential) notation**.
7. Explain the difference between the terms **accurate** and **precise**.
8. Know and use the rules for **significant figures**.
   - Given a value, determine the number of significant figures.
   - Use the correct number of significant figures to report the results of calculations involving measured quantities.

Science is a _____ for gaining knowledge and understanding of reality.

It produces *generalizations* with _____value.

The Scientific Method

There are two ways to do science: *scientific* _____ and *scientific* _____.

- It is important to note that *both* methods are used to acquire predictive power and both begin with _____

Scientific Theory

Other words for **theory** are _____ or _____.

- Scientific theory uses models/explanations to make sense of observables. Often, a first guess at a model is proposed.

- The first guess is called a _____.

The hypothesis can usually be tested by experiment or additional observations.

If the hypothesis continues to be validated by experiment or new observations, it becomes _____.

In the healthcare field, another word for theory or model is _____.

Scientific Law

A scientific law is simply *a _____ about something that generally occurs*.

Note that in using scientific law, _____ explanation (model) is given.

Scientific law can be contrasted with scientific theory that involves proposing a model or explanation for what is observed.

Chemistry

Chemistry is the study of matter and how it interacts with other _____ and/or _____.

Matter and Energy

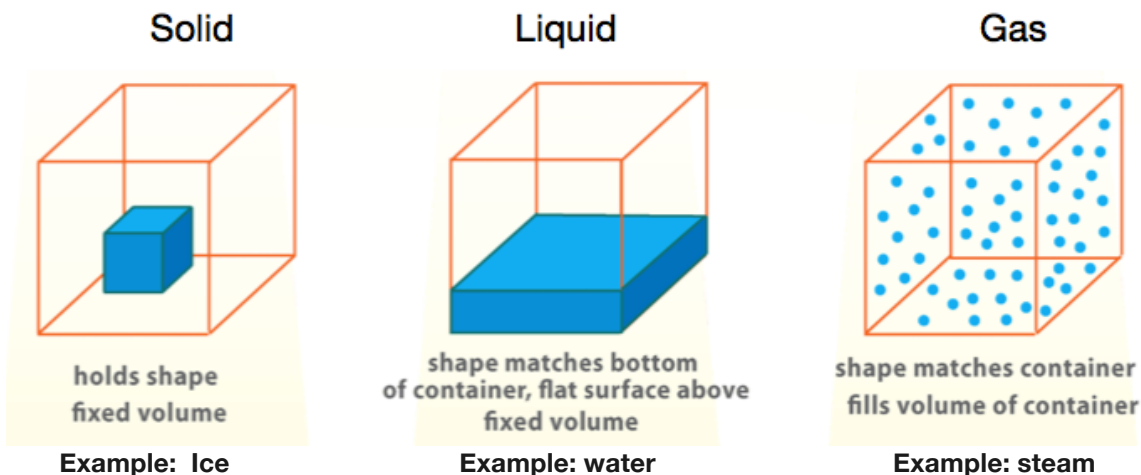Matter is anything that has _____ and occupies _____.

We can describe matter in terms of_____ _____, those characteristics that can be determined without changing it into a different substance.

- Example: Sugar is white, tastes sweet, and can be crushed into powder. Crushing sugar does not change sugar into something else.

Matter can also be described in terms of its _____ *properties*. Chemical properties of substances describe *how they are converted to new substances* in processes called chemical reactions.

- Example: Caramelization of sugar

Matter is typically found in one of three different physical _____ (sometimes called _____).

Solid	Liquid	Gas
holds shape fixed volume	shape matches bottom of container, flat surface above fixed volume	shape matches container fills volume of container
Example: Ice	**Example: water**	**Example: steam**

Changing the phase of matter, converting matter between solid, liquid, and gas is considered a *physical change* because the identity **does not** change.

- Examples of phase changes are: melting, boiling water to make steam, and melting an iron rod.

Energy

Energy is commonly defined as the ability to do _____.

Energy can be found in two forms, _____ *energy* and _____ *energy*.

Potential energy is _____ energy; it has the potential to do work.

- An example of potential energy is water stored in a dam. If a valve is opened, the water will flow downhill and turn a paddle connected to a generator to create electricity.

Kinetic energy is the energy of _____.

- Any time matter is moving, it has kinetic energy.

An important law that is central to understanding nature is: **matter will exist in the lowest possible energy state**. Another way to say this is "if matter can lose energy, it will always do so."

Units of Measurements

Measurements consist of two parts – a _____ and a_____.

SI Units and Their Symbols

Quantity	SI Unit Name	Symbol
Length	meter	m
Mass	kilogram	kg
Time	second	s
Temperature	Kelvin	K

Commonly Used Units and Their Symbols

Quantity	Unit Name	Symbol
Length	foot	ft
	inch	in
Mass	gram	g
	pound	lb.
Volume	Liter	L
Temperature	Fahrenheit	0F
	Celsius (or Centigrade)	0C

Scientific Notation and Metric Prefixes

Scientific Notation

When making measurements, particularly in science and in the health sciences, there are many times when you must deal with very large or very small numbers.

Example: a typical red blood cell has a diameter of about 0.0000075 m.

In _____ _____(exponential notation) this diameter is written 7.5×10^{-6} m.

Values expressed in scientific notation are written as a number between _____ and _____ multiplied by a power of 10.

The superscripted number to the right of the ten is called an *exponent*.

$$7.5 \times 10^{-6}$$

a number between 1 and 10   exponent
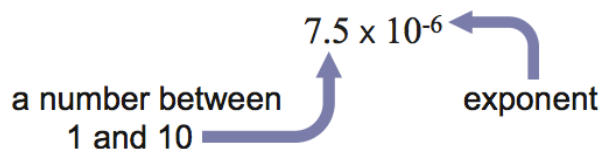
- An exponent with a positive value tells you how many times to **multiply** a number by 10.

$$3.5 \times 10^4 = 3.5 \times 10 \times 10 \times 10 \times 10 = 35000$$

- An exponent with a negative value tells you how many times to **divide** a number by 10.

$$3.5 \times 10^{-4} = \frac{3.5}{10 \times 10 \times 10 \times 10} = 0.00035$$

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Converting from Regular Notation to Scientific

1) Move the decimal point to the right of the first (right-most) non-zero number
   - The exponent will be equal to the number of decimal places moved.

2) When you move the decimal point to the left, the exponent is positive.

$$35000 = 3.5 \times 10^4$$

$$285.2 = 2.852 \times 10^2$$

$$8300000 = 8.3 \times 10^6$$

3) When you move the decimal point to the right, the exponent is negative.

$$0.00035 = 3.5 \times 10^{-4}$$

$$0.0445 = 4.45 \times 10^{-2}$$

$$0.00000003554 = 3.554 \times 10^{-8}$$

Understanding Check: Convert each number into scientific notation.

   a) 0.0144
   b) 144
   c) 36.32
   d) 0.0000098

Converting from Scientific Notation to Regular Notation
You just learned how to convert from regular numerical notation to scientific notation. Now let's do the reverse; convert from scientific notation to regular notation.

Step 1: Note the value of the *exponent*.

Step 2: The value of the exponent will tell you which direction **_and_** how many places to move the decimal point.

- If the value of the exponent is **positive**, remove the power of ten and move the decimal point that value of places to the *right*.

- If the value of the exponent is **negative**, remove the power of ten and move the decimal point that value of places to the *left*.

Example: Convert 3.7×10^5 into regular notation.

Step 1: Note the value of the *exponent*: The exponent is **positive 5**.

Step 2: The value of the exponent will tell you which direction <u>and</u> how many places to move the decimal point.
   - If the value of the exponent is **positive**, remove the power of ten and move the decimal point that value of places to the *right*.
      o We will move the decimal point 5 places to the *right*.

$$3.7 \longrightarrow 3.70000 \longrightarrow 370000$$

When the decimal point is **not shown** in a number, as in our answer, it is assumed to be *after the right-most digit*.

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Let's do another example: Convert 1.604×10^{-3} into regular notation.

Step 1: Note the value of the *exponent*: The exponent is *negative* **3**.

Step 2: The value of the exponent will tell you which direction <u>and</u> how many places to move the decimal point.

- If the value of the exponent is **negative**, remove the power of ten and move the decimal point that value of places to the *left*.
  - o We will move the decimal point 3 places to the *left*.

$$1.604 \longrightarrow 001.604 \longrightarrow .001604$$

$$\textit{or } 0.001604$$

Understanding Check: Convert the following numbers into regular notation.

      a) 5.2789×10^{2}
      b) 1.78538×10^{-3}
      c) 2.34×10^{6}
      d) 9.583×10^{-5}

Measurements and Significant Figures

There are three important factors to consider when making measurements:

    1) **accuracy**

    2) **precision**

    3) **significant figures**

_____ is related to how close a measured value is to a true value.

Example: Suppose that a patient's temperature is taken twice and values of 98 $^{\circ}$F and 102 $^{\circ}$F are obtained. If the patient's true temperature is 103 $^{\circ}$F, the second measurement is more *accurate*.

_____ is a measure of reproducibility.

Example: Suppose that a patient's temperature is taken three times and values of 98 $^{\circ}$F, 99 $^{\circ}$F, and 97 $^{\circ}$F are obtained. Another set of temperature measurements gives 90 $^{\circ}$F, 100 $^{\circ}$F, and 96 $^{\circ}$F.

- The values in the first set of measurements are closer to one another, so they are more precise than the second set.

The quality of the equipment used to make a measurement is one factor in obtaining accurate and precise results. The ability of the human operator to correctly use the measuring device is another factor.

Significant Figures

One way to include information on the _____ of a measured value (or a value that is calculated using measured values) is to report the value using the correct number of significant figures.

 The precision of a measured value can be determined by the _____ -most decimal place reported.

- The names and precision of the decimal places for the number **869.257** are shown below:

Digit in Number	8	6	9	2	5	7
Decimal Place Name	Hundreds (100's)	Tens (10's)	Ones (1's)	Tenths (1/10th's)	Hundredths (1/100th's)	Thousandths (1/1000th's)

Increasing Precision

A simple way to understand significant figures is to say that a digit is significant if we are _____ of its value.

Method for Counting Significant Figures

Measured and calculated values should be reported using significant figures. We can look at a numerical value and determine the number of significant figures as follows:

- If the decimal point is _____, starting from the *left*, count all numbers (including zeros) beginning with the first non zero number.

- If the decimal point is _____, starting from the *right*, count all numbers (including zeros) beginning with the first non zero number.

- When numbers are given in scientific notation, **do not** consider the power of 10, only the value before " $x\ 10^{n}$."

Example: If the botanist reported the age of the tree as **500 years**, how many significant figures are given?

Note that although the decimal point is implied to be after the right-most zero, it is **absent** (not shown explicitly), therefore we use the decimal point **absent** rule shown above; if the decimal point is **absent**, starting from the *right*, count all numbers (including zeros) beginning with the first non zero number.

- We will start inspecting each digit from right (to left) as shown by the arrow.
- We will start counting when we get to the first non zero number.

$$500 \leftarrow$$

We do not count the first two zeros, but start counting at the **5**. Therefore, there is **one** significant figure present.

Example: If the botanist reported the age of the tree as **500.** years (note the decimal point present), how many significant figures are given?

Note that in this case, the decimal point is **present** (shown), therefore we use the decimal point **present** rule shown above; if the decimal point is **present**, starting from the *left*, count all numbers (including zeros) beginning with the first non zero number. We will start inspecting each digit from left to right as shown by the arrow. We will start counting when we get to the first non zero number.

$$\rightarrow 500.$$

We begin with the **5**, then count <u>all</u> numbers ***including zeros***. In this case, the two zeros are also significant. Therefore there are **three** significant figures present.

Outside of the science fields, "**500**" and "**500.**" are generally thought of as equivalent, however, the use of significant figures tells us that when we write "**500.**" (with the decimal point present) we know that number one hundred times more precisely than when we write "**500**" (without the decimal point). We have precision to the "ones" decimal place in "**500.**" vs. precision to the "hundreds" place in "**500**".

Here are some other examples:

Example: How many significant figures are contained in 0.00045?

Note that in this case, the decimal point is **present** (shown). We will start inspecting each digit from left to right as shown by the arrow. We will start counting when we get to the first non zero number.

$$\longrightarrow \quad 0.00045$$

We begin with the **4**, then count <u>all</u> numbers *including zeros*. Therefore there are **two** significant figures present.

Example: How many significant figures are contained in 0.0002600?

Note that in this case, the decimal point is **present** (shown). We will start inspecting each digit from left to right as shown by the arrow. We will start counting when we get to the first non zero number.

$$\longrightarrow \quad 0.0002600$$

We begin with the **2**, then count <u>all</u> numbers *including zeros*. Therefore there are **four** significant figures present.

Example: How many significant figures are contained in 7080?

If the decimal point is **absent**, starting from the *right*, count all numbers (including zeros) beginning with the first non zero number. We will start inspecting each digit from right (to left) as shown by the arrow. We will start counting when we get to the first non zero number.

$$7080 \quad \longleftarrow$$

We do not count the first zero, but start counting at the **8,** and then count <u>***all***</u> *numbers (including zeros)*. Therefore, there are **three** significant figures present.

Understanding Check: Specify the number of significant figures in each of the values below.

a) 23.5

b) 0.0073000

c) 6.70

d) 48.50

e) 6200

f) 6200.

g) 6200.0

h) 0.6200

i) 0.62

j) 930

Significant Figures in Scientific Notation

When numbers are given in scientific notation, **do not** consider the power of 10, only the value before "**x 10^n.**"

Examples: How many significant figures are contained in each of the values shown below?

a) $\boxed{5}$ x 10^2 **one** significant figure

b) $\boxed{5.0}$ x 10^2 **two** significant figures

c) $\boxed{5.00}$ x 10^2 **three** significant figures

When converting back and forth from standard numerical notation to scientific notation, the number of significant figures used **should not change**.

Understanding Check: Write each measured value in *scientific notation*, being sure to use *the correct number of significant figures*.

    a)   5047
    b)   87629.0
    c)   0.00008
    d)   0.07460

Calculations Involving Significant Figures

When doing _____ ____ _____with measured values, the answer should have *the same number of significant figures* as the measured value with the least number of significant figures.

When doing _____ ____ _____with measured values, the answer should have the same *precision* as the least precise measurement (value) used in the calculation.

Example for Multiplication or Division:

- When doing *multiplication or division* with measured values, the answer should have *the same number of significant figures* as the measured value with the least number of significant figures.

- **Example:** If an object has a mass of 5.324 grams and a volume of 7.9 ml, what is its density?

$$\text{density} = \frac{\text{mass}}{\text{volume}} = \frac{5.324 \text{ g}}{7.9 \text{ ml}} = 0.67 \text{ g/ml}$$

4 sig figs   2 sig figs   2 sig figs

Example for Addition or Subtraction:

- When doing *addition or subtraction* with measured values, the answer should have the same *precision* as the least precise measurement (number) used in the calculation.

- **Example:** A book 50.85 mm thick, a box 168.3 mm thick and a piece of paper 0.037 mm thick are stacked on top of each other. What is the height of the stack?

   50.85 mm
 168.3   mm ← Least precise: precise to tenths
+   0.037 mm
219.187 mm Round to tenths → 219.2 mm

> **Understanding Check:** Each of the numbers below is measured. Solve the calculations and give the correct number of significant figures.
>
> a) 0.12×1.77
> b) $690.4 \div 12$
> c) $5.444 - 0.44$
> d) $16.5 + 0.114 + 3.55$

Unit Conversions

Typical Unit Conversion Problems:
- A package weighs 3.50 kg (kilograms), what is the weight in lbs. (pounds)
- A student is 60.0 inches tall, what is the student's height in cm?
- The temperature in Cabo San Lucas, Mexico is $30^{\circ}C$, what is the temperature in $^{\circ}F$?

To convert from one unit to another, we must know the _____ between the two units of measure.

- Examples:
  - A package weighs 3.50 kg (kilograms), what is the weight in lbs. (pounds)
    - 1kg = 2.20 lb
  - A student is 60.0 inches tall, what is the student's height in cm?
    - 1 inch = 2.54 cm

Unit Relationships to Know:

- 1 milliliter (mL) = 1 cubic centimeter (cm^3)
- 1 inch (in) = 2.54 centimeters (cm)
- 1 kilogram (kg) = 2.20 pounds (lb)
- 4.184 Joule (J) = 1 calorie (cal)

The *relationships* between units are called _____ _____.

Unit Conversion Calculations: The Factor Label Method

A package weighs 3.50 kg (kilograms), what is the weight in lbs. (pounds)?

Equivalence statement: 1kg = 2.20 lb

$$\left(\frac{1\ kg}{2.20\ lb} \right) \quad \text{Conversion Factors} \quad \left(\frac{2.20\ lb}{1\ kg} \right)$$
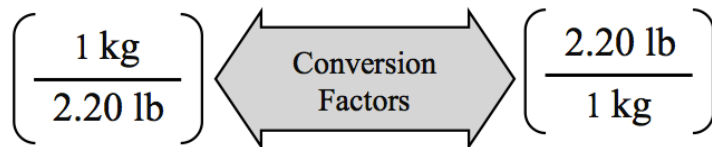
Equivalence statements can be written as _____ _____.

> **Take notes here:**
>
> $$\underline{\quad\quad\quad}\underline{\quad\quad\quad}\underline{\quad\quad\quad} =$$
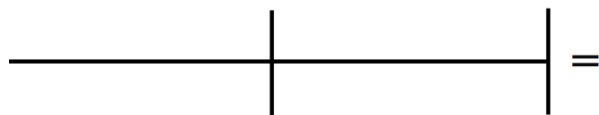
Some conversion factors have an _____ number of significant figures.

_____ (**defined or agreed upon**) conversion factors have an *infinite* number of significant figures.

•Examples of exact/defined conversion factors
- 1 lb = 0.45359237 kg
- 1 inch = 2.54 cm
- 1 cg = 10^{-2}g
- 1 ft = 12 inches
- 1 ml = $1cm^3$

A student is 60.0 inches tall, what is the student's height in cm?
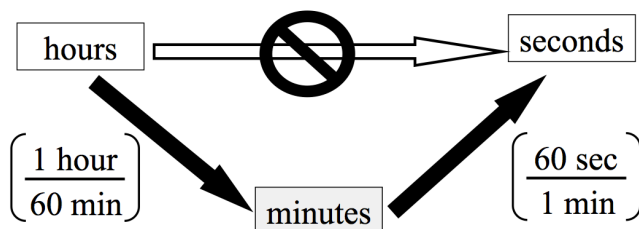
Equivalence statement: 1 inch = 2.54 cm

$$\left(\frac{1\ in}{2.54\ cm} \right) \Longleftrightarrow \text{Conversion Factors} \Longrightarrow \left(\frac{2.54\ cm}{1\ in} \right)$$

$$60.0\ in \left(\frac{2.54\ cm}{1\ in} \right) = 152\ cm$$

three significant figures

an **infinite** number of significant figures

Take notes here:

—————|—————| =
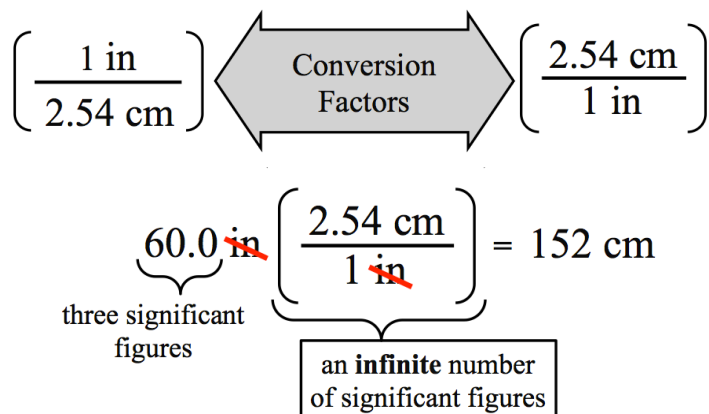
Understanding Check:

1) How many ft. (feet) in 379.3 in. (inches)?
   - 1 ft = 12 inches

2) How many eggs in 7.5 dozen?
   - 12 eggs = 1 dozen

3) How many calories in 514 joules?
   - 1 calorie = 4.184 joules

Sometimes it takes more than one step!

•Example: How many seconds in 33.0 hours?

$$\boxed{\text{hours}} \Longrightarrow \bigcirc\!\!\!\!/ \Longrightarrow \boxed{\text{seconds}}$$

$$\left(\frac{1 \text{ hour}}{60 \text{ min}}\right) \qquad \boxed{\text{minutes}} \qquad \left(\frac{60 \text{ sec}}{1 \text{ min}}\right)$$

Take notes here:

$$\underline{\qquad\qquad} \Big| \underline{\qquad\qquad} \Big| \quad =$$

$$\underline{\qquad\qquad} \Big| \underline{\qquad\qquad} \Big| \quad =$$

Take notes here:

$$\underline{\qquad\qquad} \Big| \underline{\qquad\qquad} \Big| \underline{\qquad\qquad} \Big| \quad =$$

Now you try a two-step conversion: How many inches in 5.5 meters given that:

- 1 inch = 2.54 cm
- 100 cm = 1 m

Metric Prefixes

Earlier, we used scientific notation to simplify working with very large or very small numbers.

Another way to simplify working with large or small numbers is to use metric _____.

Example: The volume of blood required for diabetics to measure blood glucose levels in modern glucometers is about 0.0000005 L.

It is much more practical to use and say:

$$0.5 \, \mu\text{L}$$

The Metric Prefix	The Base Unit
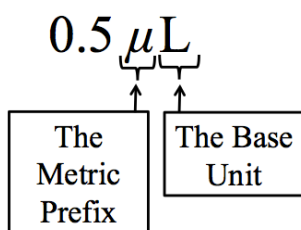
The metric **prefix** tells the **_fraction_** or **_multiple_** of the **base unit(s)**.
- For example, $1 \times 10^{6} \, \mu\text{L} = 1 \text{ L}$

The base unit can be _____ metric unit:
- liter (L), gram (g), meter (m), joule (J), second (s), calorie (cal)…etc.

Unit Conversions Within The Metric System

Example: The volume of blood required to measure blood glucose levels in modern glucometers is about 0.0000005 L.

- Question: How can we convert that to μL?
- Answer: We need the relationship between L and μL to get the conversion factor.

We will use the "Equality Table":

1 base unit =	
10 d (deci-)	0.1 da (deca-)
100 c (centi-)	.01 h (hecto)
1000 m (milli-)	.001 k (kilo)
$1 \times 10^6 \mu$ (micro-)	1×10^{-6} M (mega-)
1×10^9 n (nano)	1×10^{-9} G (giga)

All these quantities in the table are equal; any pair can be used as a conversion factor!!!

Example: What is the relationship between L (microliters) and liters (L)?

1 base unit (Liters in this problem) =	
10 d (deci-)	0.1 da (deca-)
100 c (centi-)	.01 h (hecto)
1000 m (milli-)	.001 k (kilo)
$1 \times 10^6 \mu$ (micro-)	1×10^{-6} M (mega-)
1×10^9 n (nano)	1×10^{-9} G (giga)

Equivalence statement: $1 \text{ L} = 1 \times 10^6 \ \mu$L

This table works for **any** units!

The _____ _____ could be gram (g), meter (m), liter (L), joule (J), second (s), mole (mol), calorie (cal)… etc.

Understanding Check: Find the relationships between the following:

_____ L = _____ mL

_____ kg = _____ mg

_____ nm = _____ m

_____ cm = _____ mm

Example: How many µL (microliters) in 0.0000005 L?

$$\left(\dfrac{1 \times 10^6\ \mu L}{1\ L}\right) \overset{\text{Conversion}}{\underset{\text{Factors}}{\Longleftrightarrow}} \left(\dfrac{1\ L}{1 \times 10^6\ \mu L}\right)$$

Equivalence statement: $1\ L = 1 \times 10^6\ \mu L$

1 base unit (Liters in this problem) =	
10 d (deci-)	0.1 da (deca-)
100 c (centi-)	.01 h (hecto)
1000 m (milli-)	.001 k (kilo)
1 x 10⁶ µ (micro-)	1 x 10⁻⁶ M (mega-)
1 x 10⁹ n (nano)	1 x 10⁻⁹ G (giga)

Take notes here:
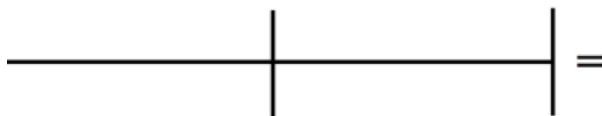
You try one: How many mL (milliliters) in 0.0345 (kL) kiloliters?

Equivalence statement: _____ mL = _____ kL
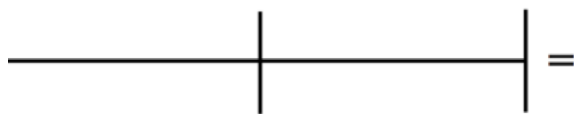
1 base unit (Liters in this problem) =	
10 d (deci-)	0.1 da (deca-)
100 c (centi-)	.01 h (hecto)
1000 m (milli-)	.001 k (kilo)
1 x 10⁶ µ (micro-)	1 x 10⁻⁶ M (mega-)
1 x 10⁹ n (nano)	1 x 10⁻⁹ G (giga)

You try another one: A vial contains 9758 mg of blood serum. Convert this into grams (g).

Equivalence statement: _____ g = _____ mg

Temperature Unit Conversions

$$°F = (1.8 × °C) + 32$$

$$°C = \frac{(°F - 32)}{1.8}$$

$$K = °C + 273.15$$

- Note: The 273.15, 32, and 1.8 in the temperature conversion equations are *exact*.

When doing a calculation that involves **only** multiplication and/or division, you can do the entire calculation then round the answer to the correct number of significant figures at the end. The same is true for a calculation that involves **only** addition and/or subtraction. But what about a calculation that involves mixed operations: **both** multiplication or division **_and_** addition or subtraction?

When doing calculations that involve **both** multiplication or division **_and_** addition or subtraction, first do a calculation for the operation *shown in parenthesis* and round that value to the correct number of significant figures, **then** use the rounded number to carry out the next operation.

Example: On a warm summer day, the temperature reaches 85 °F. What is this temperature in °C?

The relationship between °F and °C is:

$$°C = \frac{(°F - 32)}{1.8}$$

First, we do the subtraction (operation in parenthesis) and round the calculated value to the correct number of significant figures based on the rule for addition/subtraction.

Next, we divide that rounded number by 1.8 (exactly 1.8 = 1.80000....) then round the calculated value to the correct number of significant figures using the rule for multiplication/division.

Take notes here:

Significant Figures, Scientific Notation, and Rounding
1) Determine the number of significant figures in the following values:

Value	# of sig. figures	Value	# of sig. figures
140.74		4	
0.0041		3.70×10^{14}	
31.00		1.05×10^{12}	
1300		7.0400×10^{3}	
847.040		2495	

2) Round the following values to 3 significant figures.

3.76411 →	0.0411984 →
3.76811 →	150.6142 →
3.76511 →	0.013877 →
11.048176 →	4.88223×10^{9} →
8.75510 →	2.0097×10^{-12} →

3) Perform the following calculations and round the final answer to the correct number of significant figures.

Calculation	Rounded Answer	Calculation	Rounded Answer
18.7644 - 3.472 + 0.4101	=	0.87 + 4.061 + 10.4	=
17.441 ÷ 3	=	16 x 841.1 ÷ 16.300	=
14.044 + 8.11 + 3.4	=	21.01 x 2.0	=
3.41 − 0.086652	=	18.4 +12.99 +13.772 + 9.704	=

4. Convert the following into scientific notation or standard notation

Standard notation	Scientific notation
47,000	
0.0008	
675,000,000	
157,000,000,000,000,000,000,000	
0.0000003407	
	7.66×10^{-2}
	7.8×10^{5}
	4.75×10^{-4}
	6×10^{-3}
	9×10^{8}

Conversions Within the Metric System:

Perform the following metric conversions. Show your conversion factors. Use correct number of significant figures. If you need more room, do calculations on separate page(s.

0.50 m = _____mm	2.00 km = _____m	0.4000 L = _____mL
1.00 g = _____kg	01.00 cm = _____m	8.00 mm = _____cm
22.4 L = _____mL	5.00 g = _____kg	4.245 L = _____ mL
345 g = _____kg	10.0 nm = _____m	3.22 Gg = _____kg
3.001 cg = _____mg	1.2 m = _____µm	455 nm = _____m

English-Metric Conversions (show your work)

10.0 cm = _____in	15.0 lb = _____kg (1kg=2.205 lb)
1.00 yd = _____ cm (1 yard = exactly 36 in)	16.9 fl. oz = _____L (0.0338 fl oz.= 1 mL)
1.00 qt = _____ L(1qt = 946 mL)	6.00 in = _____cm
0.800 kg = _____oz (16 oz = exactly 1 lb and 1kg=2.205 lb)	1.83 kg = _____lb (1kg=2.205 lb)
25.00 mL = _____qt (1qt = .946L)	1.40 L = _____ = cm^3 note: 1 mL = exactly $1cm^3$

<u>Temperature Conversions</u>

Recall the Temperature Conversions from Chapter 1 lecture notes:

- $°F = (1.8 \text{ x } °C) + 32$

- $°C = (°F - 32) / 1.8$

- $K = °C + 273.15$

NOTE: In temperature conversion equations, the 273.15, 32 and 1.8 are ***exact.***

IMPORTANT: When doing a calculation that involves **only** multiplication and/or division, you can do the entire calculation then round the answer to the correct number of significant figures at the end. The same is true for a calculation that involves **only** addition and/or subtraction.

But what about a calculation that involves mixed operations: **both** multiplication or division ***and*** addition or subtraction?

When doing calculations that involve **<u>both</u>** multiplication or division ***and*** addition or subtraction, first do a calculation for the operation *shown in parenthesis* and round that value to the correct number of significant figures, **then** use the rounded number to carry out the next operation.

Perform the following temperature conversions (show your calculation)

$75^{o}C =$ _____ K
$-15^{o}C =$ _____ K
$0.00 K$ =   _____ ^{o}C =   _____ ^{o}F
$25^{o}C$ (room temperature) = _____ K
98.6 ^{o}F (body temperature) = _____ ^{o}C
$25^{o}C =$ _____ ^{o}F
-40.0 $^{o}C =$ _____ ^{o}F
412 K = _____ ^{o}F

Chapter 1 Worksheet 1 and KEY

Significant Figures, Scientific Notation, and Rounding

1) Determine the number of significant figures in the following values:

Value	# of sig. figures	Value	# of sig. figures
140.74	5	4	1
0.0041	2	3.70×10^{14}	3
31.00	4	1.05×10^{12}	3
1300	2	7.0400×10^{3}	5
847.040	6	2495	4

2) Round the following values to 3 significant figures.

3.76411 →3.76	0.0411984 →0.0412
3.76811 →3.77	150.6142 → 151
3.76511 →3.77	0.013877 → 0.0139
11.048176 →11.0	4.88223×10^{9} →4.88×10^{9}
8.75510 →8.76	2.0097×10^{-12} →2.01×10^{-12}

3) Perform the following calculations and round the final answer to the correct number of significant figures.

Calculation	Rounded Answer	Calculation	Rounded Answer
18.7644 - 3.472 + 0.4101	= 15.703	0.87 + 4.061 + 10.4	= 15.3
17.441 ÷ 3	= 6	16 x 841.1 ÷ 16.300	= 830
14.044 + 8.11 + 3.4	= 25.6	21.01 x 2.0	= 42
3.41 – 0.086652	= 3.32	18.4 +12.99 +13.772 + 9.704	= 54.9

4. Convert the following into scientific notation or standard notation

Standard notation	Scientific notation
47,000	4.7×10^{4}
0.0008	8×10^{-4}
675,000,000	6.75×10^{8}
157,000,000,000,000,000,000,000	1.57×10^{23}
0.0000003407	3.407×10^{-7}
0.0766	7.66×10^{-2}
780,000	7.8×10^{5}
0.000475	4.75×10^{-4}
0.006	6×10^{-3}
900,000,000	9×10^{8}

Metric System:
Perform the following metric conversions. Show your conversion factors. Use correct number of significant figures. If you need more room, do calculations on separate page(s).

0.50 m = _5.0 x 10^2___ mm	2.00 km = __2.00 x 10^3__ m	0.4000 L = 4.000 x 10^2 mL or 400.0 mL
1.00 g = _1.00 x 10^{-3}_kg or .00100 kg	01.00 cm = __0.0100__ m or 1.00 x 10^{-2} m	8.00 mm = __0.800___ cm or 8.00 x 10^{-1} cm
22.4 L = 2.24 x 10^4 mL or 22400 mL	5.00 g = 5.00 x 10^{-3}_kg or .00500 kg	4.245 L = __4245__ mL or 4.245 x 10^3 mL
345 g = _0.345_kg or 3.45 x 10^{-1} kg	10.0 nm = 1.00 x 10^{-8}_m or .0000000100 m	3.22 Gg = 3.22x 10^6 kg or 3220000 kg
3.001 cg = _30.01_mg or 3.001 x 10^1 mg	1.2 m = _1.2 x 10^6_ μm or 1200000 μm	455 nm = _4.55 x 10^{-7} m or .000000455 m

English-Metric Conversions (show your work)

10.0 cm = 3.94_in	15.0 lb = ___6.80__ kg
1.00 yd = __91.4____ cm	16.9 fl. oz = __0.500___ L (0.0338 fl oz.= 1 mL)
1.00 qt = ___0.946___ L	6.00 in = ___15.2___ cm
0.800 kg = ___28.2___ oz (16 oz = 1 lb)	1.83 kg = ___4.04___ lb
25.00 mL = ___0.0264___qt (1qt = .946L)	1.40 L = __1.40 x 10^3___ = cm^3 note: 1 mL = 1cm^3

Temperature Conversions
Perform the following temperature conversions (show your calculation)

75°C = __348___ K
-15°C = ___258___ K
0.00 K = __-273.15_ °C = __-459.67__ °F
25°C (room temperature) = ____298___ K
98.6 °F (body temperature) = ___37.0___ °C
25°C = ___77____ °F
-40.0 °C = __-40.0___ °F
412 K = __282____ °F

Significant Figures Worksheet

1. Indicate how many significant figures there are in each of the following measured values.

246.32 _____   1.008 _____   700000 _____

107.854 _____   0.00340 _____   350.670 _____

100.3 _____   14.600 _____   1.0000 _____

0.678 _____   0.0001 _____   320001 _____

2. Calculate the answers to the appropriate number of significant figures.

32.567	246.24	658.0
135.0	238.278	23.5478
+ 1.4567	+ 98.3__	+ 1345.29__

3. Calculate the answers to the appropriate number of significant figures.

a) 23.7 x 3.8   = _____   e) 43.678 x 64.1   = _____

b) 45.76 x 0.25   = _____   f) 1.678 / 0.42   = _____

c) 81.04 x 0.010   = _____   g) 28.367 / 3.74   = _____

d) 6.47 x 64.5   = _____   h) 4278 / 1.006   = _____

Significant Figures Worksheet Key

1. Indicate how many significant figures there are in each of the following measured values.

246.32	5 sig figs	1.008	4 sig figs	700000	1 sig fig
107.854	6 sig figs	0.00340	3 sig figs	350.670	6 sig figs
100.3	4 sig figs	14.600	5 sig figs	1.0000	5 sig figs
0.678	3 sig figs	0.0001	1 sig fig	320001	6 sig figs

2. Calculate the answers to the appropriate number of significant figures.

32.567	246.24	658.0
135.0	238.278	23.5478
+ 1.4567	+ 98.3__	+ 1345.29__
169.0	**582.8**	**2026.8**

3. Calculate the answers to the appropriate number of significant figures.

a) 23.7 x 3.8   = **90.**

b) 45.76 x 0.25   = **11**

c) 81.04 x 0.010   = **0.81**

d) 6.47 x 64.5   **= 417**

e) 43.678 x 64.1   = **2.80×10^3**

f) 1.678 / 0.42   = **4.0**

g) 28.367 / 3.74   = **7.58**

h) 4278 / 1.006   = **4252**

Unit Conversions Worksheet

Complete each of the following conversions to the proper number of significant figures; clearly show your set-up with units in the set-up and the answer.

1) 0.30 m   =   _____ mm

2) 5.00 mm   =   _____ cm

3) 10.0 cm   =   _____ in

4) 2.00 km   =   _____ m

5) 33.4 L   =   _____ mL

6) 15.0 lb   =   _____ kg
(use 2.20 lb = 1 kg)

7) 0.400 L   =   _____ mL

8) 5.00 g   =   _____ kg

9) 1.00 yd   =   _____ cm
(3 ft = 1 yard, exactly)

10) 6.35 g   =   _____ kg

11) 8.245 L =   _____ mL

12) 16.9 fl. oz=   _____ L
(0.0338 fl oz.= 1 mL)

13) 1.00 cm =   _____ m

14) 345 g   =   _____ kg

See next page for Key

Unit Conversion Worksheet Key

1) 0.30 m = 3.0 x 10^2 mm

2) 5.00 mm = 0.500 cm <u>or</u> 5.00 x 10^{-1} cm

3) 10.0 cm = 3.94 in

4) 2.00 km = 2.00 x 10^3 m

5) 33.4 L = 3.34 x 10^4 mL <u>or</u> 33400 mL

6) 15.0 lb = 6.82 kg

7) 0.400 L = 400. mL <u>or</u> 4.00 x 10^2 mL

8) 5.00 g = 5.00 x 10^{-3} kg <u>or</u> 0.00500 kg

9) 1.00 yd = 91.4 cm

10) 6.35 g = 0.00635 kg <u>or</u> 6.35 x 10^{-3} kg

11) 8.245 L = 8245 mL <u>or</u> 8.245 x 10^3 mL

12) 16.9 fl. oz = 0.500 L <u>or</u> 5.00 x 10^{-1} L

13) 1.00 cm = 0.0100 m <u>or</u> 1.00 x 10^{-2} m

14) 345 g = 0.345 kg <u>or</u> 3.45 x 10^{-1} kg

Chapter 2 Lecture Notes: Atoms

Educational Goals

1. Describe the subatomic structure of an atom.

2. Define the terms **element** and **atomic symbol.**

3. Understand how elements are arranged in the periodic table based on the number of protons they contain.

4. Understand how **atomic number** and **mass number** are used to indicate details of an atom's nucleus.

5. Know how **isotopes** of an element differ from one another.

6. Define the term **mole** and describe the relationship between **moles** and **molar mass**.

7. Given the **molar mass** of an element, convert between number of atoms, number of moles, and mass (grams).

An Introduction to Atoms

Matter (stuff) is made of _____.

Model of the Atom

> **Check your current model: Draw a carbon atom.**

Atoms are made of _____ *particles*.

There are *three* types of subatomic particles that will make up our atomic model:

1. _____
2. _____
3. _____

Protons and neutrons are compacted together in what we call the _____ of an atom. Electrons are distributed in space around the nucleus.

- They are moving very fast in a volume surrounding the nucleus.

Atoms are mostly empty space.

1

Electrical Charge

There are a few fundamental properties of nature.

- Examples: Gravity, magnetism, and mass.

Another fundamental property in nature is _____ _____.

Particles *may or may not* have electrical charge.

There are two types of electrical charge; we arbitrarily call one type _____ and the other type

_____.

Every thing we discuss in this course ultimately occurs because of the interaction of these two types of charges.

Particles with *opposite charges attract* each other.

The natural attraction is called

_____ _____ force.
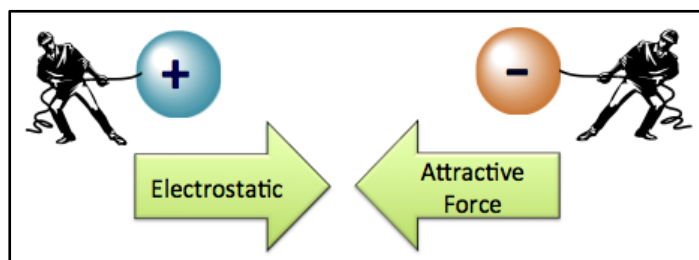
Oppositely charged particles will accelerate **toward** one another if not held apart.
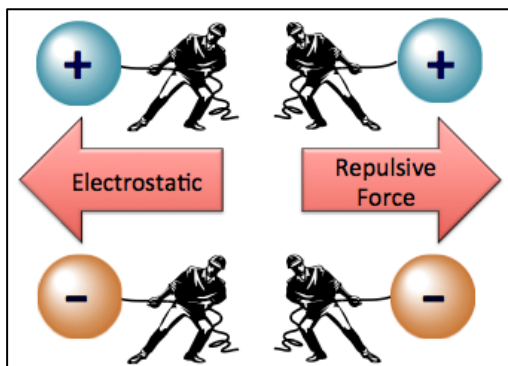
Particles with *like charges repel* each other.

The natural repulsion is called

_____ _____ force.

Like charged particles will accelerate **away** from one another if not held together.

Subatomic Particles

1) Protons

Protons are _____ *charged* particles located in the _____ of an atom.

The number of protons a particular atom contains determines that atom's identity.

- For example, any atom that contains just **one proton** is called *hydrogen*. An atom with **two protons** is called *helium*. An atom with **six protons** is called *carbon*.

Historically, matter with different numbers of protons, such as hydrogen, helium, and carbon were called the _____.

There are 92 elements that occur in nature. About 25 others have been man-made by slamming two atoms together causing their nuclei to combine, however these new atoms do not last long (fractions of a second up to one year), they break apart into smaller atoms.

A modern periodic table of the elements is shown on the next page.

- You can download a copy of this periodic table at:
  http://www.zovallearning.com/GOBlinks/ch2/periodictablezovalbasic.pdf

Periodic Table of the Elements

I Alkali Metals	II Alkaline Earth Metals											III	IV	V	VI	VII Halogens	VIII Noble Gases
1 **H** Hydrogen 1.0079																	2 **He** Helium 4.003
3 **Li** Lithium 6.941	4 **Be** Beryllium 9.012183											5 **B** Boron 10.811	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.0067	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.998403	10 **Ne** Neon 20.1797
11 **Na** Sodium 22.989770	12 **Mg** Magnesium 24.3050											13 **Al** Aluminum 26.9815	14 **Si** Silicon 28.0855	15 **P** Phosphorus 30.973762	16 **S** Sulfur 32.066	17 **Cl** Chlorine 35.4527	18 **Ar** Argon 39.948
19 **K** Potassium 39.0983	20 **Ca** Calcium 40.078	21 **Sc** Scandium 44.955908	22 **Ti** Titanium 47.867	23 **V** Vanadium 50.9415	24 **Cr** Chromium 51.9961	25 **Mn** Manganese 54.938044	26 **Fe** Iron 55.845	27 **Co** Cobalt 58.933194	28 **Ni** Nickel 58.6934	29 **Cu** Copper 63.546	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92160	34 **Se** Selenium 78.971	35 **Br** Bromine 79.904	36 **Kr** Krypton 83.80
37 **Rb** Rubidium 85.4678	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.90584	40 **Zr** Zirconium 91.224	41 **Nb** Niobium 92.90637	42 **Mo** Molybdenum 95.95	43 **Tc** Technetium (98)	44 **Ru** Ruthenium 101.07	45 **Rh** Rhodium 102.90550	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.8682	48 **Cd** Cadmium 112.414	49 **In** Indium 114.818	50 **Sn** Tin 118.710	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447	54 **Xe** Xenon 131.29
55 **Cs** Cesium 132.90545	56 **Ba** Barium 137.327	57 **La** Lanthanum 138.90545	72 **Hf** Hafnium 178.49	73 **Ta** Tantalum 180.9479	74 **W** Tungsten 183.84	75 **Re** Rhenium 186.207	76 **Os** Osmium 190.23	77 **Ir** Iridium 192.217	78 **Pt** Platinum 195.078	79 **Au** Gold 196.96657	80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98038	84 **Po** Polonium (209)	85 **At** Astatine (210)	86 **Rn** Radon (222)
87 **Fr** Francium (223)	88 **Ra** Radium (226)	89 **Ac** Actinium (227)	104 **Rf** Rutherfordium (261)	105 **Db** Dubnium (262)	106 **Sg** Seaborgium (263)	107 **Bh** Bohrium (262)	108 **Hs** Hassium (265)	109 **Mt** Meitnerium (266)									

58 **Ce** Cerium 140.116	59 **Pr** Praseodymium 140.90766	60 **Nd** Neodymium 144.24	61 **Pm** Promethium (145)	62 **Sm** Samarium 150.36	63 **Eu** Europium 151.964	64 **Gd** Gadolinium 157.25	65 **Tb** Terbium 158.92534	66 **Dy** Dysprosium 162.50	67 **Ho** Holmium 164.93033	68 **Er** Erbium 167.26	69 **Tm** Thulium 168.93422	70 **Yb** Ytterbium 173.04	71 **Lu** Lutetium 174.967
90 **Th** Thorium 232.0377	91 **Pa** Protactinium 231.03588	92 **U** Uranium 238.0289	93 **Np** Neptunium (237)	94 **Pu** Plutonium (244)	95 **Am** Americium (243)	96 **Cm** Curium (247)	97 **Bk** Berkelium (247)	98 **Cf** Californium (251)	99 **Es** Einsteinium (252)	100 **Fm** Fermium (257)	101 **Md** Mendelevium (258)	102 **No** Nobelium (259)	103 **Lr** Lawrencium (262)

Note that each element is represented by its **atomic** _____ (a one- or two-letter name abbreviation) and occupies a box in the table.

Above each element's symbol is the _____ _____.

The **atomic number** tells us the _____ *of* _____ in an atom of that particular element.

- Example: Look at carbon, symbol C, atomic number 6. Carbon has an atomic number of *six* because an atom with six protons is called carbon. If it had *seven* protons, it would not be carbon - it would be nitrogen and have an atomic number of 7.

- Atomic number can be abbreviated using "**Z**."
  - o For example, with carbon, **Z** = 6, with hydrogen, **Z** = 1.

- Elements are ordered in the periodic table by *increasing* atomic number.

2) Electrons

Electrons are ***negatively charged*** subatomic particles.

They are light-weight particles that move extremely fast.

- For the remainder of chapter 2 we can visualize the electrons as bees flying around a beehive (the bee hive represents the nucleus). In chapter 3 you will learn more details about the regions around the nucleus that the electrons can occupy.

- Electrons are very light compared to protons and neutrons.

- Protons and neutrons are about 2000 times **heavier** than electrons and therefore compose most of an atom's mass.

3) Neutrons

Neutrons are located in the _____ (with the protons).

Neutrons **do not** have electrical charge; we say they are ***electrically*** _____.

The names, charges, and symbols for the three types of subatomic particles are shown below:

SUBATOMIC PARTICLE	SYMBOL	CHARGE
PROTON	p	positive (1+)
NEUTRON	n	none
ELECTRON	e or e^-	negative (1-)

How many neutrons are in an atom?

We ***cannot determine*** the number of neutrons in an atom based on the number of protons.

- This is because atoms of a particular element ***do not all have the same number of neutrons***.

Example: Some carbon atoms have *six neutrons*, some have *seven neutrons*, and some have *eight neutrons*.

- These three different forms of carbon are called _____ of carbon.

Isotopes are defined as atoms with the *same* number of protons (same element), but a *different* number of neutrons.

You learned that an atom's *"atomic number (Z)"* is the *number of protons* it contains.

When considering the number of neutrons in an isotope of a particular atom, it is useful to learn a new term called "**mass number**."

The _____ _____ of an atom is defined as *the number of protons plus the number of neutrons*.

$$mass\ number = number\ of\ \textbf{protons} + number\ of\ \textbf{neutrons}$$

Mass number can be abbreviated using "A."

	SYMBOL	DEFINITION
ATOMIC NUMBER	Z	number of protons
MASS NUMBER	A	number of protons + number of neutrons

Example: How many neutrons are in a sodium (Na) atom that has a *mass number* of **23**?

> **Take notes here:**

> **Understanding Check:** How many neutrons are in a **carbon (C)** atom that has a *mass number* of **14**?

You will often see one of two "shorthand notation" methods used to differentiate the various isotopes:

Method 1: Write the *element symbol*, a dash, then the *mass number* (A)

Let's use our three isotopes of carbon for examples:

NUMBER OF NEUTRONS IN THE CARBON ATOM	SHORTHAND NOTATION
6	C-12
7	C-13
8	C-14

Method 2: Write the *element symbol*, we superscript the *mass number* (A) to the left of the symbol.

NUMBER OF NEUTRONS IN THE CARBON ATOM	SHORTHAND NOTATION
6	^{12}C
7	^{13}C
8	^{14}C

- Although redundant, sometimes the atomic number (Z) is also subscripted to the left of the symbol.
    - For example:

$$^{12}_{6}C$$

Understanding Check: Fill in the blanks for the following isotopes:

    a. ^{14}N number of protons ___   number of neutrons ___   atomic number ___   mass number ___

    b. ^{15}N number of protons ___   number of neutrons ___   atomic number ___   mass number ___

    c. ^{42}Ca number of protons ___   number of neutrons ___   atomic number ___   mass number ___

    d. ^{1}H number of protons ___   number of neutrons ___   atomic number ___   mass number

Atoms are *electrically neutral*; their **total charge** is equal to **zero**.

- They have the same number of electrons (-) as protons (+), so the positive and negative charges add up to zero (cancel).

The Mole

Atoms are so tiny and small in mass that it is more convenient to do calculations with a large number of atoms

- Just like bakers and chefs use eggs by the dozen, chemists use atoms and molecules by the mole.

  - A _____ is a counting unit used for atoms and molecules.

  - A _____ _____ is any term that refers to a specific number of things.

    – a couple = 2 items (e.g. people)
    – a dozen = 12 items (e.g. eggs, donuts)
    – a mole = 6.022 x 10^{23} (e.g. atoms, molecules)

The Chemist's Mole

- **One mole** of anything represents 6.022 x 10^{23} of the things.
- This is referred to as **Avogadro's number**.
- 1 mole = 6.022 x 10^{23}

Understanding Check: How many atoms are in *1 mole* of helium (He)? _____

Because the mole is the standard counting unit used to indicate the number of atoms present in a sample, it is useful to **convert** back and forth from *moles* to *atoms*.

- Use our *conversion factor* method.
- The *relationship* between # of atoms and moles is:
  - 1 mole = 6.022 x 10^{23}

$$\left(\frac{1 \text{ mol}}{6.022 \text{ x } 10^{23} \text{ atoms}}\right) \quad \text{Conversion Factors} \quad \left(\frac{6.022 \text{ x } 10^{23} \text{ atoms}}{1 \text{ mol}}\right)$$

Conversion Map

Atoms

$$\left(\frac{1 \text{ mol}}{6.022 \text{ x } 10^{23} \text{ atoms}}\right) \quad \boxed{\text{Use Avogadro's Number}} \quad \left(\frac{6.022 \text{ x } 10^{23} \text{ atoms}}{1 \text{ mol}}\right)$$
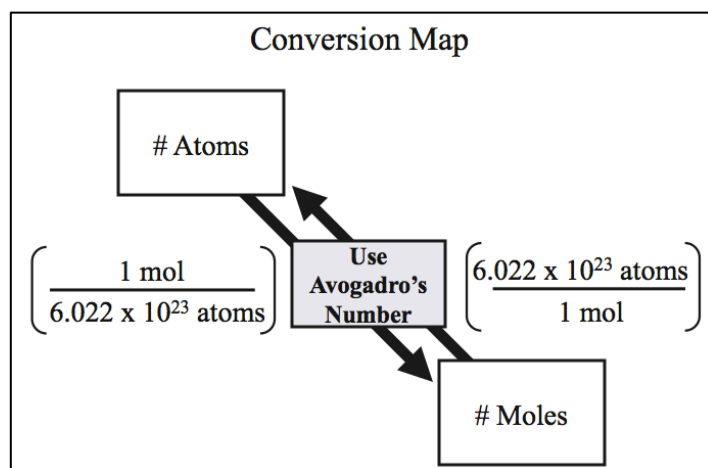
Moles

Example: How many carbon atoms are there in 0.100 mole of carbon?

Take notes here:

You try one: How many moles are 2.9×10^{12} F atoms?

The Mole and Mass

- The _____ _____ of an element is equivalent to the mass (in grams) of one mole of the element.
- Molar mass is given in the ***periodic table*** _____ the symbol of the element.
  - Molar mass units: _____
  - Example: Carbon – molar mass is _____
  - Another example:
    - 1 mole of argon (Ar) = 39.95 g
    - Molar mass of argon is 39.95 g/mole

Understanding Check:
1 mole of C = _____ grams of carbon (C) = _____ atoms of C
1 mole of Al = _____ grams of aluminum (Al) = _____ atoms of Al

Because the molar mass gives us the _____ between the number of moles and the mass of an element, it can be used to _____ back and forth between moles and mass (in grams).

   - Use our conversion factor method

Conversion Map

Mass (grams)

$\left(\dfrac{1 \text{ mole}}{\# \text{ grams}} \right)$ **Use Molar Mass** $\left(\dfrac{\# \text{ grams}}{1 \text{ mole}} \right)$
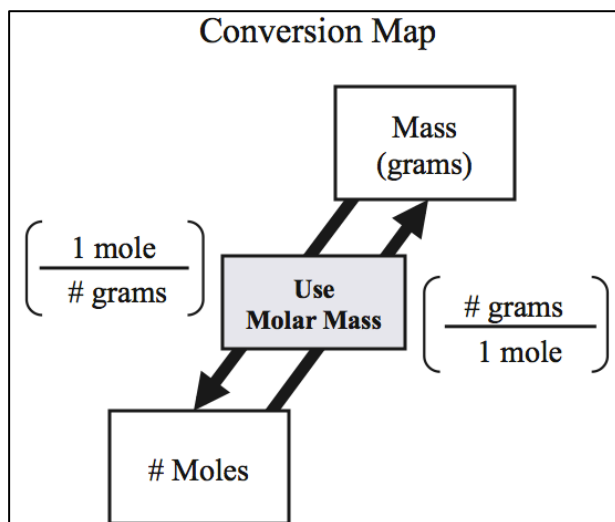
Moles

Example: **Carbon**

- The relationship between # of moles of carbon and grams of carbon is:
  - 1 mole Carbon = 12.01 g
- This can be written as conversion factors:

$$\left(\frac{1 \text{ mole C}}{12.01 \text{ grams C}} \right) \quad \boxed{\begin{array}{c} \text{Conversion} \\ \text{Factors} \end{array}} \quad \left(\frac{12.01 \text{ grams C}}{1 \text{ mole C}} \right)$$

Example Problem: What is the mass of 0.770 moles of carbon?

Take notes here:

You try one: How many moles are there in 50.0 g of lead?

Converting Between the Number of Atoms and Grams
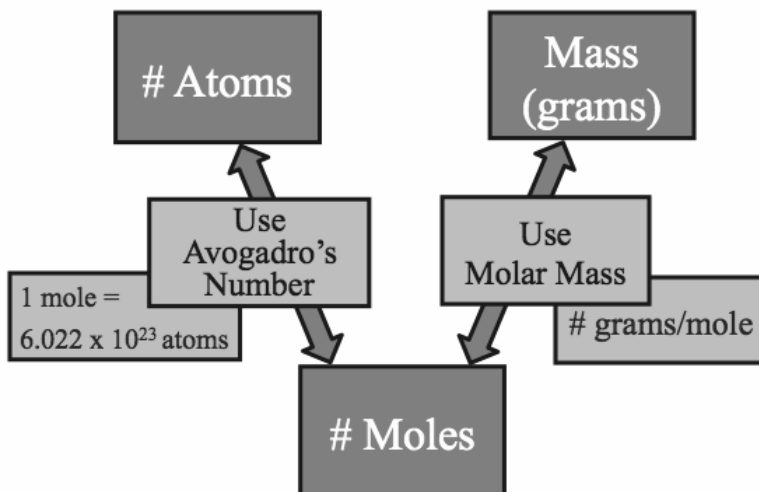
Example: (atoms to grams) What is the mass of 2.50×10^{21} Lead (Pb) atoms?

Take notes here:

You try one: (grams to atoms) Compute the number atoms in 10.0 g of Aluminum (Al)?

The Periodic Table

As we continue to build our model of atoms and matter in later chapters, we will gain more understanding of why the elements are arranged as they are in the periodic table and how the periodic table can be very useful in predicting the chemical and physical properties of matter.

Classification of Elements Based on Electrical and Heat Conduction

CATEGORY	PROPERTIES
Metals	•Good conductors of heat and electricity •Ductile (can be pulled into wires and pounded flat) •Have a luster
Nonmetals	•Poor conductors of heat and electricity •Brittle (break or shatter if bent or hammered)
Metalloids **(sometimes called Semimetals)**	Intermediate conductors of heat and electricity

1 H		Metals (Green)		Nonmetals (Blue)		Metalloids (Red)											2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt									

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Elements in the periodic table are arranged in columns called _____ (sometimes, but much less often, called **Families)**.

- Sometimes these groups are shown with **group numbers** in Roman numerals above the column.

I														III	IV	V	VI	VII	VIII
1 1 **H**	II	s-Block		p-Block															2 2 **He**
2 3 **Li**	4 **Be**	d-Block		f-Block										III 5 **B**	IV 6 **C**	V 7 **N**	VI 8 **O**	VII 9 **F**	10 **Ne**
3 11 **Na**	12 **Mg**			Transition Metals										13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**

	I												III	IV	V	VI	VII	VIII
4	19 **K**	20 **Ca**	21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
5	37 **Rb**	38 **Sr**	39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
6	55 **Cs**	56 **Ba**	57 **La**	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
7	87 **Fr**	88 **Ra**	89 **Ac**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**									

(Inner) Transition Metals

6 Lanthanides	58 **Ce**	59 **Pr**	60 **Nd**	61 **Pm**	62 **Sm**	63 **Eu**	64 **Gd**	65 **Tb**	66 **Dy**	67 **Ho**	68 **Er**	69 **Tm**	70 **Yb**	71 **Lu**
7 Actinides	90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**

The elements in **Group I** (also called Group 1A) are called the _____ *metals*.

- Although it is not a metal, note that hydrogen is in this group *for reasons that I will discuss in chapter 3*.

The elements in **Group II** (also called group 2A) are called the _____ *earth metals*.

The elements in **Group VII** (also called group 7A) are called the _____.

The elements in **Group VIII** (also called group 8A) are called the _____**.**

The elements in **Group I** and **Group II** are in what is called the _____ **-Block**.

The elements in Groups **III - VIII** are in the _____ **-Block**.

The _____ _____, *located between the s- and p-Blocks*, are in the ___ **-Block**.

The **Inner Transition Metals**, located in the bottom two rows of the periodic table are in the ___ **-Block**.

- They are called *lanthanides* (top row of the *f-Block*) and *actinides* (bottom row of the *f-Block*).

The *rows* in the periodic table are called _____.

- The periods are often numbered to the left of each row.

Chapter 2: Atomic Molar Mass Worksheet and Key

1. Complete the following table:

Symbol	Symbol-Mass Number	Atomic #	Mass #	# protons	# neutrons	# electrons
^7_3Li						
	Mo-96					
				49	53	
			72			35
$^{238}_{92}U$						

Answer the following questions. ***Be sure to write units with every number and to use the correct number of significant figures***. Use **two digits to the right of the decimal place for molar masses when possible**, then your final answer will match the key exactly.

1. What is the molar mass of the following elements?

      a) B _____   b) Zn _____   c) He _____

2. What is the mass (grams) of one mole of Xenon?_____

3. How many atoms are in one mole of Xenon?   _____

Use the conversion map below to solve the following problems

4. How many moles of oxygen (O) contain 1.65×10^{27} oxygen atoms?

$$\frac{1.65 \times 10^{27} \text{ O atoms}}{} \left| \frac{\underline{\quad} \text{ mole O}}{\underline{\qquad} \text{ O atoms}} \right. = \underline{\qquad} \text{ mole O}$$

5. How many moles of K contain 3.50×10^{19} K atoms?

$$\frac{3.50 \times 10^{19} \text{ K atoms}}{} \left| \frac{\qquad}{\qquad} \right. = \underline{\qquad} \text{ mole K}$$

6. How many moles of fluorine (F) contain 8.27×10^{24} F atoms?

$$\frac{\qquad}{} \left| \frac{\qquad}{\qquad} \right. =$$

7. How many carbon atoms are contained in 5.45 moles of carbon?

$$\frac{5.45 \text{ moles C}}{} \left| \frac{\underline{\qquad} \text{ C atoms}}{\underline{\quad} \text{ mole C}} \right. = \underline{\qquad\qquad} \text{ C atoms}$$

8. How many Neon (Ne) atoms are contained in 0.75 moles of Ne?

$$\frac{\qquad}{} \left| \frac{\qquad}{\qquad} \right. = \underline{\quad}$$

9. How many moles of oxygen (O) is contained 2.65 grams of oxygen?

$$\frac{2.65 \text{ g O}}{} \left| \frac{1 \text{ mole O}}{\underline{\qquad} \text{ g O}} \right. = \underline{\quad} \text{ mole O}$$

10. How many moles of potassium (K) is contained 8.44 grams of potassium?

$$\frac{8.44 \text{ g K}}{} \left| \frac{\qquad}{\qquad} \right. = \underline{\quad} \text{ mole K}$$

11. How many g of Xe is contained in 0.054 moles of Xe?

$$\frac{0.054 \text{ moles Xe}}{} \left| \frac{\underline{\qquad} \text{ g Xe}}{\underline{\quad} \text{ mole Xe}} \right. = \underline{\quad}$$

12. How many g of C is contained in 39.5 moles of C?

$$\frac{\quad\quad\quad}{\quad\quad\quad} \bigg| \frac{\quad\quad\quad}{\quad\quad\quad} \bigg| = \underline{\quad}$$

13. What is the mass (grams) of 5.00×10^{24} oxygen atoms?

$$\frac{5.00 \times 10^{24} \text{ atoms O}}{\quad\quad} \bigg| \frac{\underline{\quad\quad} \text{ mole O}}{\underline{\quad\quad} \text{atoms O}} \bigg| \frac{\underline{\quad\quad} \text{ g O}}{\underline{\quad\quad} \text{ mole O}} = \underline{\quad\quad} \text{ g O}$$

14. What is the mass (grams) of 1.00×10^6 sodium (Na) atoms?

$$\frac{1.00 \times 10^6 \text{ Na atoms}}{\quad\quad} \bigg| \frac{\quad\quad}{\quad\quad} \bigg| \frac{\quad\quad}{\quad\quad} = \underline{\quad\quad} \text{ g Na}$$

15. How many iron atoms are in 10.0 grams of iron (Fe) ?

$$\frac{10.0 \text{ g Fe}}{\quad\quad} \bigg| \frac{\underline{\quad\quad} \text{ mole Fe}}{\underline{\quad\quad} \text{ g Fe}} \bigg| \frac{\underline{\quad\quad} \text{ Fe atoms}}{\underline{\quad\quad} \text{ mole Fe}} = \underline{\quad\quad} \text{Fe atoms}$$

16. How many copper (Cu) atoms are in a 257 gram copper pipe?

$$\frac{\quad\quad\quad}{\quad\quad\quad} \bigg| \frac{\quad\quad\quad}{\quad\quad\quad} \bigg| \frac{\quad\quad\quad}{\quad\quad\quad} = \underline{\quad\quad} \text{Cu atoms}$$

See next page for KEY

KEY

1. Complete the following table:

Symbol	Symbol- Mass Number	Atomic #	Mass #	# protons	# neutrons	# electrons
$^{7}_{3}Li$	Li-7	3	7	3	4	3
$^{96}_{42}Mo$	Mo-96	42	96	42	54	42
$^{102}_{49}In$	In-102	49	102	49	53	49
$^{72}_{35}Br$	Br-72	35	72	35	37	35
$^{238}_{92}U$	U-238	92	238	92	146	92

Answer the following questions. ***Be sure to write units with every number and to use the correct number of significant figures***.   Use **two digits to the right of the decimal place for molar masses when possible**, then your final answer will match the key exactly.

1. What is the molar mass of the following elements?

       a) B   10.81g/mole   b) Zn 65.39 g/mole   c) He   4.00 g/mole

2. What is the mass (grams) of one mole of Xenon? _____ 131.29 g _____

3. How many atoms are in one mole of Xenon? _____ 6.022×10^{23} _____

4. How many moles of oxygen (O) contain 1.65×10^{27} oxygen atoms?

$$\dfrac{1.65 \times 10^{27} \text{ O atoms}}{} \quad \Bigg| \quad \dfrac{1 \ \text{ mole O}}{6.022 \times 10^{23} \ \text{ O atoms}} \quad = 2740 \ \text{ mole O } \textbf{or } 2.74 \times 10^{3} \text{ mole O}$$

Note: 3 significant figures!!!

5. How many moles of K contain 3.50×10^{19} K atoms?

$$\dfrac{3.50 \times 10^{19} \text{ K atoms}}{} \quad \Bigg| \quad \dfrac{1 \ \text{ mole K}}{6.022 \times 10^{23} \text{ K atoms}} \quad = 5.81 \times 10^{-5} \text{ mole K}$$

6. How many moles of fluorine (F) contain 8.27×10^{24} F atoms?

$$\dfrac{8.27 \times 10^{24} \text{ F atoms}}{} \quad \Bigg| \quad \dfrac{1 \ \text{ mole F}}{6.022 \times 10^{23} \text{ F atoms}} \quad = 13.7 \text{ mole F}$$

7. How many carbon atoms are contained in 5.45 moles of carbon?

$$\frac{5.45 \text{ moles C}}{} \left| \frac{6.022 \times 10^{23}\text{C atoms}}{1 \text{ mole C}} \right. = 3.28 \times 10^{24} \text{ C atoms}$$

8. How many Neon (Ne) atoms are contained in 0.75 moles of Ne?

$$\frac{0.75 \text{ moles Ne}}{} \left| \frac{6.022 \times 10^{23}\text{Ne atoms}}{1 \text{ mole Ne}} \right. = 4.5 \times 10^{23} \text{ Ne atoms}$$

9. How many moles of oxygen (O) is contained 2.65 grams of oxygen?

$$\frac{2.65 \text{ g O}}{} \left| \frac{1 \text{ mole O}}{16.00 \text{ g O}} \right. = 0.166 \text{ mole O}$$

Molar Mass of Oxygen
1 mole O = 16.00 grams O
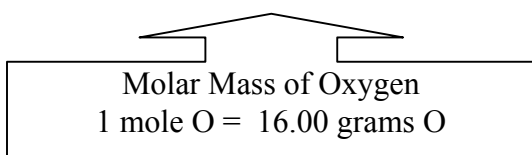
10. How many moles of potassium (K) is contained 8.44 grams of potassium?

$$\frac{8.44 \text{ g K}}{} \left| \frac{1 \text{ mole K}}{39.10 \text{ g K}} \right. = 0.216 \text{ mole K}$$

11. How many g of Xe is contained in 0.054 moles of Xe?

$$\frac{0.054 \text{ moles Xe}}{} \left| \frac{131.29 \text{ g Xe}}{1 \text{ mole Xe}} \right. = 7.1 \text{ g Xe (NOTE: 2 significant figures)}$$

12. How many g of C is contained in 39.5 moles of C?

$$\frac{39.5 \text{ mole C}}{} \left| \frac{12.01 \text{ g C}}{1 \text{ mole C}} \right. = 474 \text{ g C}$$

13. What is the mass (grams) of 5.00×10^{24} oxygen atoms?

$$\frac{5.00 \times 10^{24} \text{ atoms O}}{} \left| \frac{1 \text{ mole O}}{6.022 \times 10^{23} \text{ O atoms}} \right| \frac{16.00 \text{ g O}}{1 \text{ mole O}} = 133 \text{ g O}$$

14. What is the mass (grams) of 1.00×10^6 sodium (Na) atoms?

$$\frac{1.00 \times 10^6 \ \text{Na atoms}}{} \ \left| \ \frac{1 \ \text{mole Na}}{6.022 \times 10^{23} \ \text{Na atoms}} \ \right| \ \frac{22.99 \ \text{g Na}}{1 \ \text{mole Na}} \ \right| = 3.82 \times 10^{-17} \ \text{g Na}$$

15. How many iron atoms are in 10.0 grams of iron (Fe) ?

$$\frac{10.0 \ \text{g Fe}}{} \ \left| \ \frac{1 \ \text{mole Fe}}{55.85 \ \text{g Fe}} \ \right| \ \frac{6.022 \times 10^{23} \ \text{Fe atoms}}{1 \ \text{mole Fe}} \ \right| = 1.08 \times 10^{23} \ \text{Fe atoms}$$

16. How many copper (Cu) atoms are in a 257 gram copper pipe?

$$\frac{257 \ \text{g Cu}}{} \ \left| \ \frac{1 \ \text{mole Cu}}{63.55 \ \text{g Cu}} \ \right| \ \frac{6.022 \times 10^{23} \ \text{Cu atoms}}{1 \ \text{mole Cu}} \ \right| = 2.44 \times 10^{24} \ \text{Cu atoms}$$

CHAPTER 2 REVIEW WORKSHEET AND KEY

The Mole

1) How many zinc (Zn) atoms are contained in 5.16 moles of Zn?

2) How many moles of He are 221,000 He atoms?

3) How many atoms are contained in 0.98 moles of iron (Fe)?

4) How many moles of cesium are in 66.45 g Cs?

5) What is the mass (grams) of 2500. carbon atoms?

6) What is the mass (grams) of 6.52×10^{18} atoms of gold (Au)?

Isotopes

(IMPORTANT NOTE: X = Symbol, A=mass number, Z = atomic number)

Name	Atomic number	Mass number	# of protons	# of neutrons	X-A form	$^A_Z X$ notation
Cobalt		60				
					I-131	
						$^3_1 H$
	26	59				
						$^{99}_{42} Mo$
			11	24		
Strontium				52		
					U-235	
		134	55			
		19	9			
	79			118		
Copper				36		
			56	81		
					K-40	

KEY
The Mole
1) How many zinc (Zn) atoms in 5.16 moles of Zn?
3.11×10^{24} Zn atoms

2) How many moles of He are 221,000 He atoms?

3.67×10^{-19} moles He

3) How many atoms are contained in 0.98 moles of iron (Fe)?

5.9×10^{23} Fe atoms

4) How many moles of cesium are in 66.45 g Cs?

0.5000 moles Cs

5) What is the mass (grams) of 2500. carbon atoms?

4.986×10^{-20} g C

6) What is the mass (grams) of 6.52×10^{18} atoms of gold (Au)?

0.00213 g Au

Isotopes

Name	Atomic number	Mass number	# of protons	# of neutrons	X-A form	$^{A}_{Z}X$ notation
Cobalt	27	60	27	33	Co-60	$^{60}_{27}Co$
Iodine	53	131	53	78	I-131	$^{131}_{53}I$
Hydrogen	1	3	1	2	H-3	$^{3}_{1}H$
Iron	26	59	26	33	Fe-59	$^{59}_{26}Fe$
Molybdenum	42	99	42	57	Mo-99	$^{99}_{42}Mo$
Sodium	11	35	11	24	Na-35	$^{35}_{11}Na$
Strontium	38	90	38	52	Sr-90	$^{90}_{38}Sr$
Uranium	92	235	92	143	U-235	$^{235}_{92}U$
Cesium	55	134	55	79	Cs-134	$^{134}_{55}Cs$
Fluorine	9	19	9	10	F-19	$^{19}_{9}F$
Gold	79	197	79	118	Au-197	$^{197}_{79}Au$
Copper	29	65	29	36	Cu-65	$^{65}_{29}Cu$
Barium	56	137	56	81	Ba-137	$^{137}_{56}Ba$
Potassium	19	40	19	21	K-40	$^{40}_{19}K$

Chapter 3 Lecture Notes: Compounds

Educational Goals

1. Understand where electrons are located in atoms and how the locations of electrons affect the energy of the atom.

2. Define the term **valence electron** and draw the **electron dot structure** of an atom or ion.

3. Define the term **ion** and explain how the electron dot structure of a s- or p-block element can be used to predict the charge of the monoatomic ion.

4. Given the symbol, be able to name monoatomic **cations** and **anions** (and vice versa).

5. Explain the difference between an **ionic bond** and a **covalent bond**.

6. Understand the structural difference between ionic and covalent compounds.

7. Given the name, be able to write the formulas of ionic compounds and binary covalent compounds (and vice versa).

8. Define the terms **molar mass**, **formula mass,** and **molecular mass** and use these values in unit conversions involving moles and mass.

9. Given the formula, draw the **line bond structures** of diatomic molecules.

The Arrangement of Electrons

Before we learn about compound, we must build on our understanding of atoms and electrons.

Specifically, in the beginning of chapter 3 you will learn:

1) **Where electrons are located in atoms.**

2) **How the location of electrons effect the energy of the atom.**

Scientists used *light* to study how electrons are arranged around the nucleus.

Energy, in the form of light or heat, can be _____by atoms.

Energy is **absorbed** by _____an electron to a *new* area.

Atoms release energy when electrons move *back* to _____ _____areas.

*   This can happen when an atom collides with another particle.

*   Another way this can happen is by an atom emitting _____.

The Modern Model of the Atom

New scientific laws and models of nature were needed to explain the pattern of light that was emitted by atoms.

Another word for *light* is **electromagnetic radiation**.
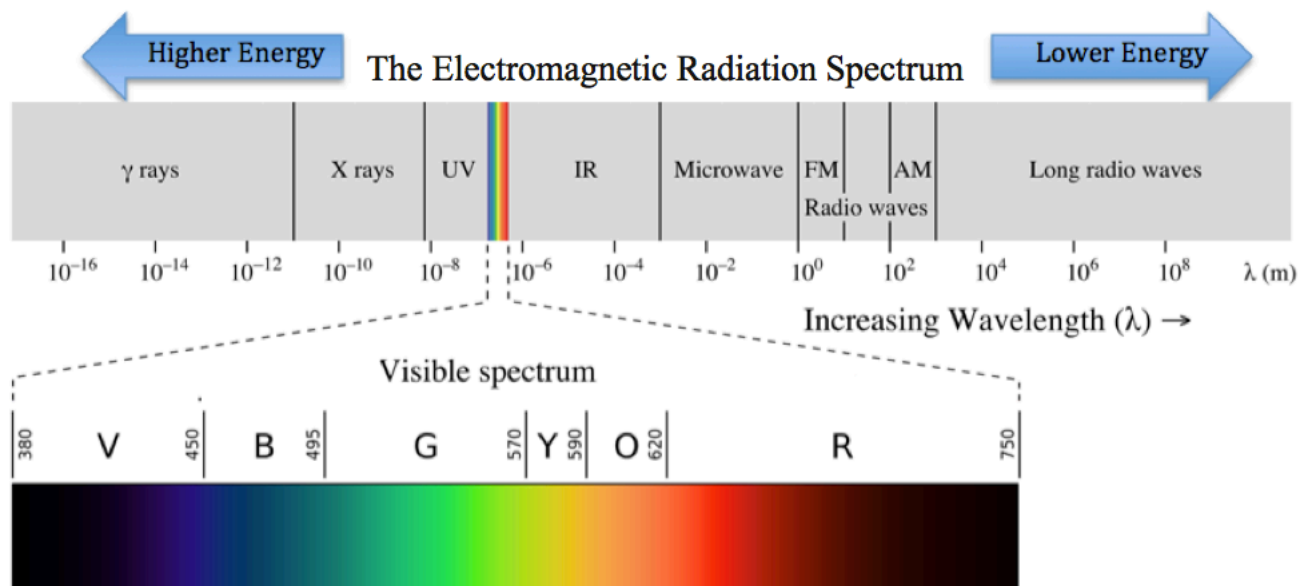
Visible light, the part of the electromagnetic spectrum that can be detected with the human eye, is a small part of the electromagnetic radiation spectrum (see the textbook for colored spectrum).

Short wavelengths correspond to higher energy; longer wavelengths correspond to lower energy light.

If **all energies** of light could be released from excited atoms, then we would expect the pattern of emitted light to look like this:

However, only light with **discrete** (distinct) energies is emitted. For example, the pattern of light emitted from excited hydrogen atoms is:

Our understanding of nature was dramatically changed when Max Planck and Albert Einstein introduced "_____ _____."

They proposed that energy is absorbed and emitted by atoms *only* in _____ amounts called **quanta**.

- Another word for "*discrete*" is "*distinct*."

Recall that the light emitted from excited atoms is generated by electrons losing energy as they move from areas further from the nucleus (high energy) to areas nearer the nucleus (low energy). To lose the energy in this process, atoms emit light.

The observation that only discrete energies are emitted from excited atoms is explained using an atomic model that says that the *electrons can only exist in certain areas and therefore atoms have discrete energies*.

- We say that the energy of atoms is "_____."
- The first scientist to propose a model of the atom where electrons existed in specific regions that had discrete energies was Niels Bohr.

2

Illustration of the "Quantized" Energy of Hydrogen
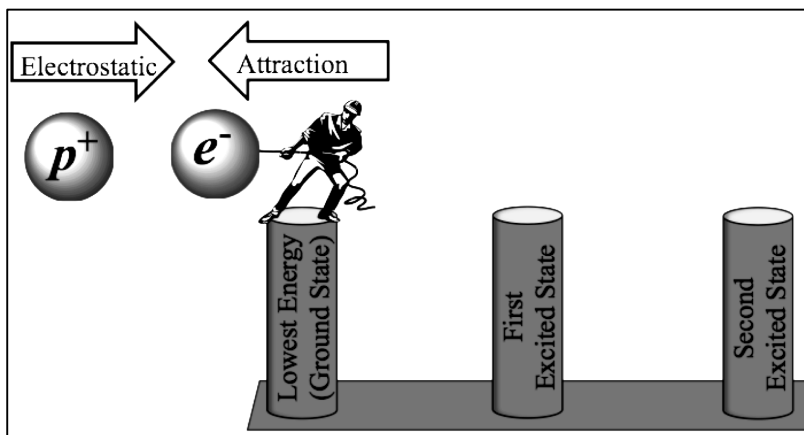
When an atom's electron(s) are in the lowest possible energy area, we call this the _____ _____.

- At room temperature, all atoms will exist in their ground state unless *temporarily* excited to a higher energy area by absorbing light.

Absorption of a discrete amount of energy corresponds to the worker **only** being able to move to ***particular areas*** (represented by posts in the illustration above).

When hydrogen's electron is in any other region than the ground state (lowest energy), we call that an _____ _____ of hydrogen.

The excited atom will soon lose energy as the electron moves back to the ground state position. When the energy lost is in the form of light, that light will be the color (wavelength) corresponding to the energy difference between the initial "excited" region and the final, lower energy region.

The Modern Model of the Atom: The Quantum Mechanical Model

You can ***avoid getting lost*** in the detail (and wonder) of nature by focusing on the following two educational goals:

1) Understand where electrons are _____ in atoms.

2) Understand how the location of electrons affect the _____ of the atom.

The Hydrogen Atom

Hydrogen is unique because it has only _____ electron.

Electrons exist in certain **three-dimensional regions** called _____.

Orbitals can be described by these properties:

1. **The _____ _____ an electron in a particular orbital is from the nucleus.**

    - Since orbitals are three-dimensional and the electrons move (very quickly) within the orbitals, the distance an electron is from the nucleus is not constant (as it would be in a circular two-dimensional path). Therefore, we talk about the electron's ***average distance*** from the nucleus.

  - As hydrogen's orbitals get larger, the average distance of an electron from the nucleus increases, therefore the _____ ***the orbital*** occupied by an electron, the _____ ***the energy***. (As described in the illustration at the top of this page).

3

2. **The three-dimensional _____ of the orbital.**

- Not only do the sizes of orbitals vary, the shapes of orbitals vary as well.

- When the shapes of orbitals are shown as three-dimensional representations, the shapes represent the region that would contain the electron _____ of the time. The remaining 10% of the time, the electron would be outside of the shape that is shown in the graphic representation.

The Language of Quantum Mechanics

The orbitals are *centered on the* _____, and are labeled by a _____.

In a hydrogen atom:
- This number is related to the orbital **size** and the **energy** of an electron in the orbital.
- The orbitals are numbered from **lowest** energy (smallest size) to **higher** energy (larger size).

These numbers are referred to as "energy level," or "quantum number," or "quantum level," or "shell."
- We will use the term "_____" or "_____ _____" and abbreviate it by using "__."

In the lowest energy state of a hydrogen atom (the *ground state*), the electron occupies the **n=1** quantum level.

The **n=1** quantum level has _____ orbital.
- It is called an _____ orbital.
- **"s"** represents the *shape* **of the orbital**, we use **1s** because **n=1**).
- **s** orbitals are _____ in shape.

An Illustration of a 1s Orbital

- The _____ is in the **center** of the orbital.

The **n=2** quantum level has _____ orbitals.
- There is **one 2s** orbital
  - *All* **s** orbitals are spherically shaped.
  - We use **2s** because **n=2**.
  - The major difference between the **2s** orbital and the **1s** orbital is that the **2s** orbital is **larger**.
- There are **three 2p** orbitals.
  - **p** represents the shape; we use **2p** because **n=2**.
  - The **p** orbitals all have the **same shape** and only differ in *how they are* _____ around the nucleus.

2s   2p_z   2p_x   2p_y
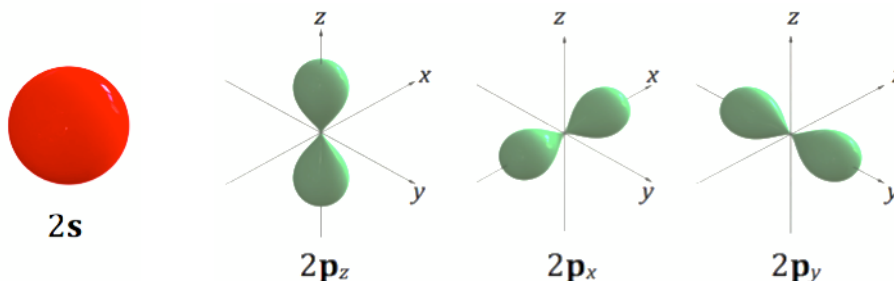
The **n=3** quantum level has _____ orbitals.

- There is **one 3s** orbital, **three 3p** orbitals, and **five 3d** orbitals.
- The shapes of the **3s** and **3p** orbitals are similar to those of the **2s** and **2p** orbitals, respectively, but they are *larger*.
- The **five 3d** orbital are illustrated below:
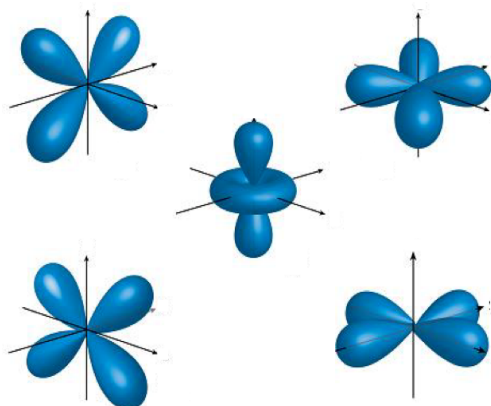
As is the case for all orbitals, the **d** orbitals are centered on the nucleus.

The **n=4** quantum level has _____ orbitals.
- There is **one 4s** orbital, **three 4p** orbitals, **five 4d** orbitals, and **seven 4f** orbitals.
- The **f** orbitals have shapes that are even more complicated then the **d** orbitals.
- The shapes of the **4s**, **4p**, and **4d** orbitals are similar to those of the **3s, 3p**, and **3d** orbitals, respectively, but they are *larger*.

The **n=5** level has **twenty-five** orbitals.

This just keeps going, **n= 6**, **7**, **8**, etc.

Although quantum levels with **n > 4** contain orbitals other than **s**, **p**, **d**, and **f**, these other orbitals are n*ever occupied by electrons of any element in its ground state*.
- The only time an electron can occupy any of those orbitals will be if the atom absorbs energy.

Energy Level Diagram for Hydrogen

We can organize the various atomic orbitals according to their energy in an illustration called an **energy level diagram**. The energy level diagram for the first five quantum levels (**n = 1-5**) of a **hydrogen atom** is shown below.
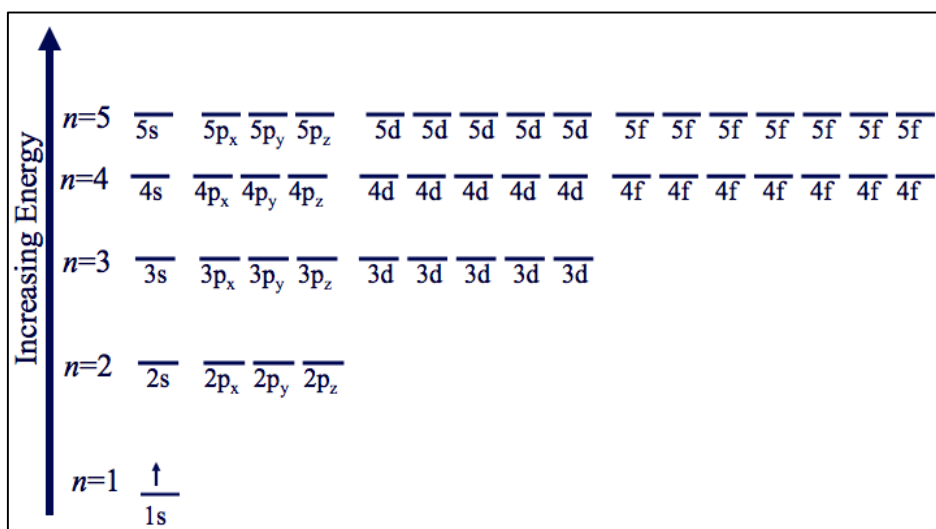
In an **energy level diagram,** we draw a short horizontal line that is labeled for each _____.

The orbitals are arranged, from bottom to top, in order of increasing _____.

An electron is depicted as an _____ above the line that represents the orbital occupied by it.

Let's compare the *energy level diagram* to a *skyscraper*, we will call this our **skyscraper model**.
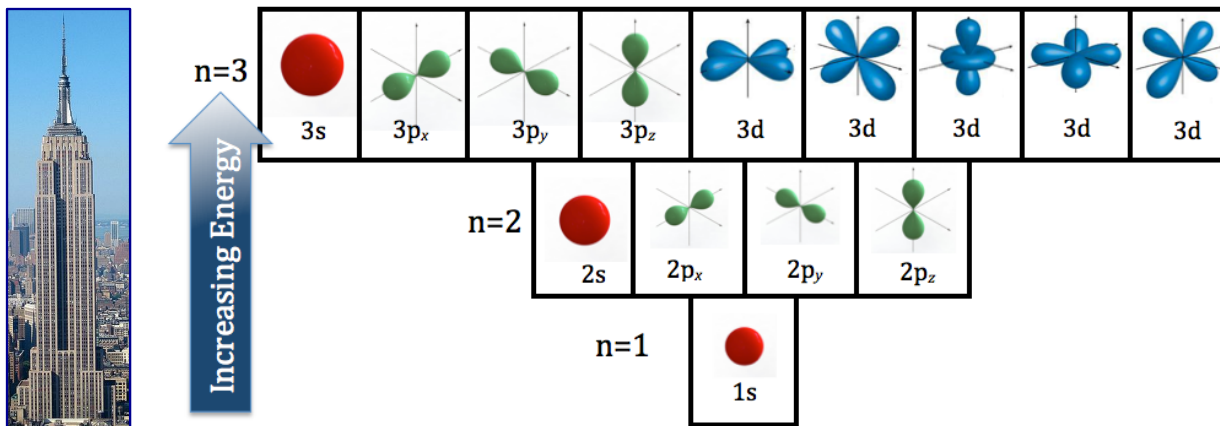
Skyscraper photo source: Wikimedia Commons, Author: Avala, CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcode

The different _____ of the skyscraper represent the quantum levels (**n**).

- The first floor is the lowest energy floor so it would correlate with **n**=1, the ground state.

_____ on a particular floor are analogous to the various orbitals in a particular *quantum level*.

Model of a Hydrogen Atom
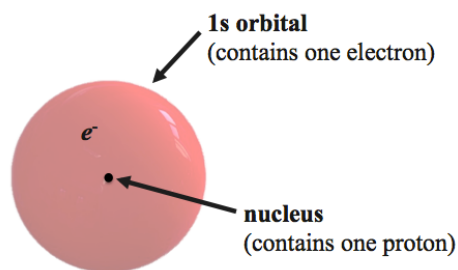
Atomic Model for Multi-Electron Atoms

Energy Level Diagram for Multi-Electron Atoms
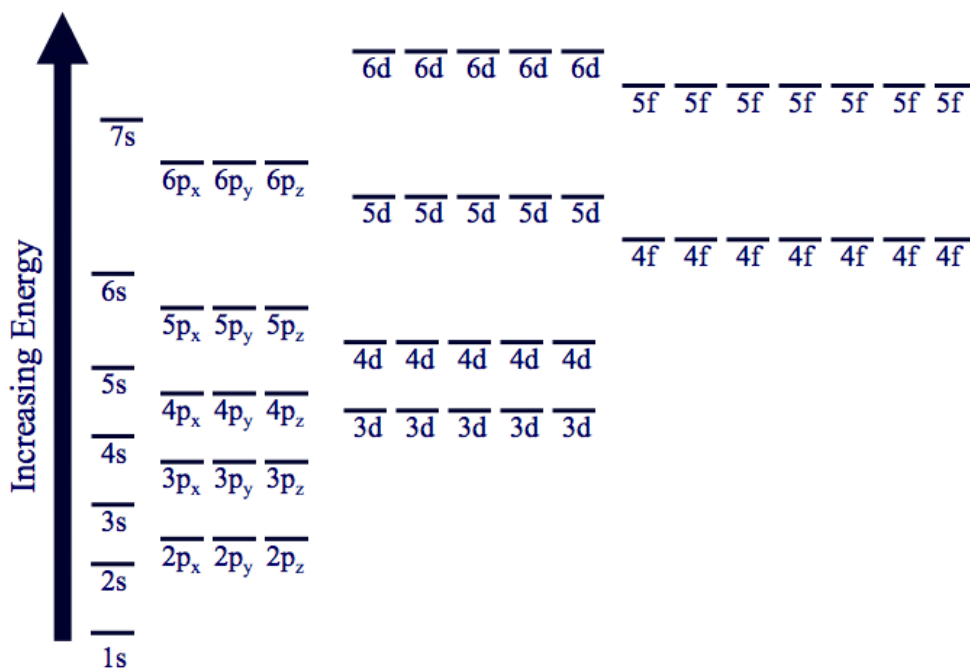
Skyscraper Model for Multi-Electron Atoms
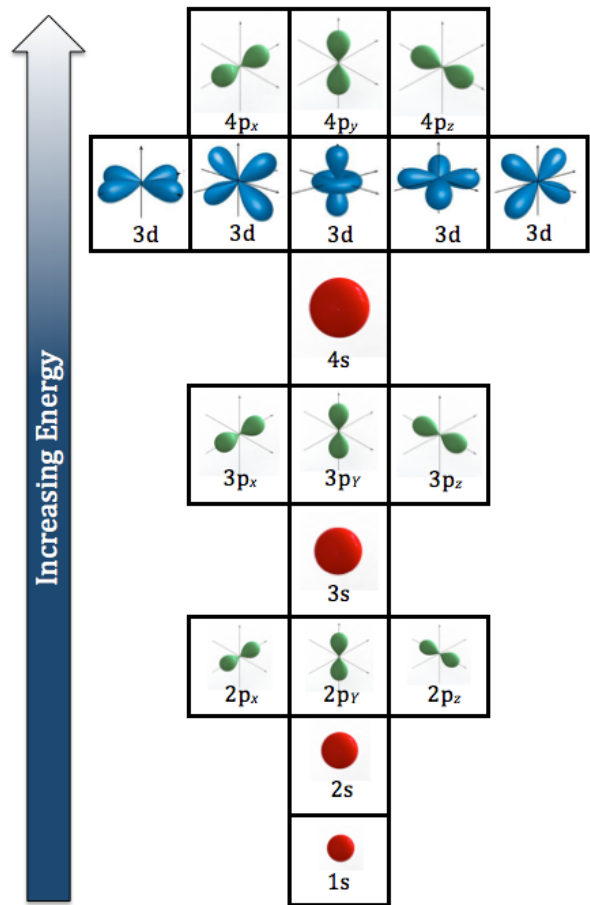
We live in a universe where matter tends to exist in the *lowest possible energy state*.

An informal way to state this is:

Nature wants everything to be at the _____ possible energy.

Electrons are arranged (configured) into the orbitals of multi-electron atoms in the way that results in the **lowest** possible energy.

Nature does this by obeying the following principles:

1) **The Aufbau Principle**

   "Aufbau" (German) means *build-up* or *construct*.
   The *aufbau principle* states that an electron occupies the *lowest energy orbital that can receive it*.

2) **The Pauli Exclusion Principle**

   An orbital can hold a maximum of _____ electrons.

   Electrons have a quantum mechanical property called **spin**.

   We call the spin states "**up**" or "**down**."

   - *When two electrons occupy the same orbital, one electron has spin "**up**" the other has spin "**down**."*

   This is all that you need to know about spin to understand all of the concepts covered in this textbook. You may find it interesting that spin is responsible for magnetic properties of matter. In fact, spin is the reason that electrons behave as tiny magnets!

Example:
Energy Level Diagram for a
Helium Atom

Model of a Helium Atom

1s orbital
(contains two electrons)

nucleus
(two protons)
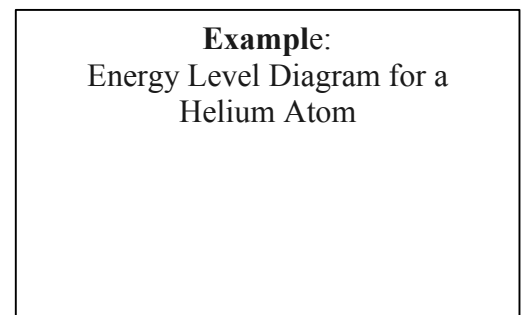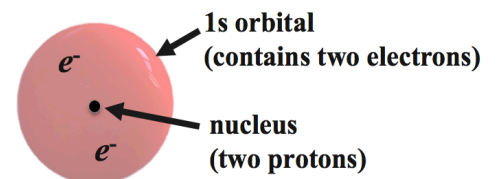
3) Hund's Rules

When electrons are configured into orbitals that all have the *same energy,* a ***single electron*** is placed into **each** of the equal-energy orbitals before a second electron is added to an occupied orbital.

When electrons are configured into a *set of orbitals* that all have the same energy, the spins of the first electrons to be placed into each orbital are all in the same state (for example all "up").

Example: Energy Level Diagram for a Carbon Atom	**Drawing of a Carbon-12 Atom**
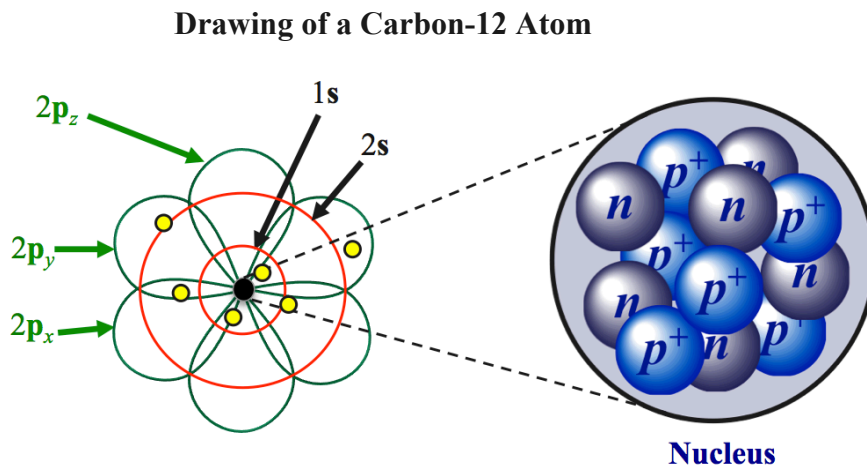
Understanding Check:
Energy Level Diagram for a Neon (Ne) Atom

Understanding Check:
Energy Level Diagram for an Iodine (I) Atom

Valence Electrons

Valence electrons are the electrons held in the _____ *shell* (largest "**n**").

> **Language Reminder:** *"shell" = "quantum level" = "energy level"*

- Valence electrons are furthest away from the _____.

• It is important to know how many valence electrons are in an atom because:

- These are the electrons that are involved in _____

_____ to other elements to form _____.

- These are the electrons that elements lose to become _____.

Example: How many valence electrons do **carbon** (C) atoms have?

$$\overline{3d}\ \overline{3d}\ \overline{3d}\ \overline{3d}\ \overline{3d}$$

$$\overline{4s}$$

$$\overline{3p_x}\ \overline{3p_y}\ \overline{3p_z}$$

$$\overline{3s}$$

$$\uparrow\ \uparrow$$
$$\overline{2p_x}\ \overline{2p_y}\ \overline{2p_z}$$
$$\uparrow\downarrow$$
$$\overline{2s}$$

→ four valence electrons

$$\uparrow\downarrow$$
$$\overline{1s}$$
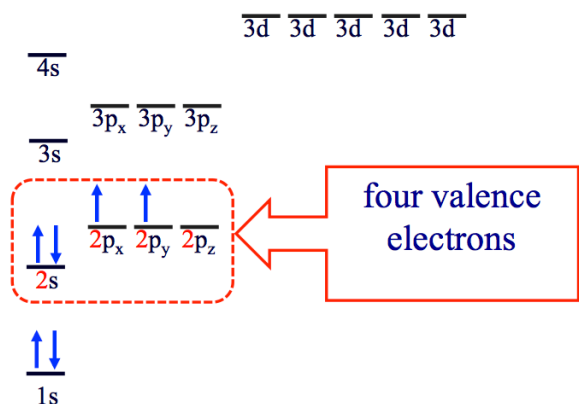
> **Understanding Check**: How many valence electrons do **oxygen** (O) atoms have?

Short-Cut for Determining the Number of Valence Electrons

Elements are arranged in the periodic table according to the number of valence electrons.

For **s-** and **p-block** elements, all elements in the same periodic _____ (group) have the *same number of valence electrons* as all others in that column.

The group numbers for the columns *represent* the number of valence electrons contained in those atoms.

Different elements with the same number of valence electrons are said to be _____.

Example of isoelectric elements: oxygen and sulfur

Isoelectric atoms often behave in similar ways. For example, oxygen atoms often chemically "bond" to two hydrogen atoms to form water (H_2O); sulfur atoms, also often "bond" with two hydrogen atoms to form hydrogen sulfide (H_2S).

9

Electron Dot Structures

Electron dot structures show the number of *valence electrons* that an atom carries.

- In these structures, *valence electrons are represented by* _____ drawn next to an element's symbol.

I													III	IV	V	VI	VII	VIII
H•	II																	He:
Li•	Be:												•Ḃ•	•Ċ•	•N̈•	•Ö•	•F̈:	:N̈e:
Na•	Mg:												•Al•	•Si•	•P̈•	•S̈•	•C̈l:	:Ar:
K•	Ca:												•Ga•	•Ge•	•As•	•Se•	•Br:	:Kr:
Rb•	Sr:												•In•	•Sn•	•Sb•	•Te•	•I:	:Xe:
Cs•	Ba:												•Tl•	•Pb•	•Bi•	•Po•	•At:	:Rn:
Fr•	Ra:																	

Noble Gases and the Octet Rule

The group VIII elements (He, Ne, Ar, Kr, Xe, and Rn) are called _____ *gases.*

He, Ne, Ar, Kr, Xe, and Rn belong to the **noble gas family**, which gets it's name from the fact that these elements are resistant to change and, with few exceptions, do not lose or gain electrons.

The resistance to change (stability) of the noble gases is related to having their outermost quantum level (***shell***) completely _____ with electrons
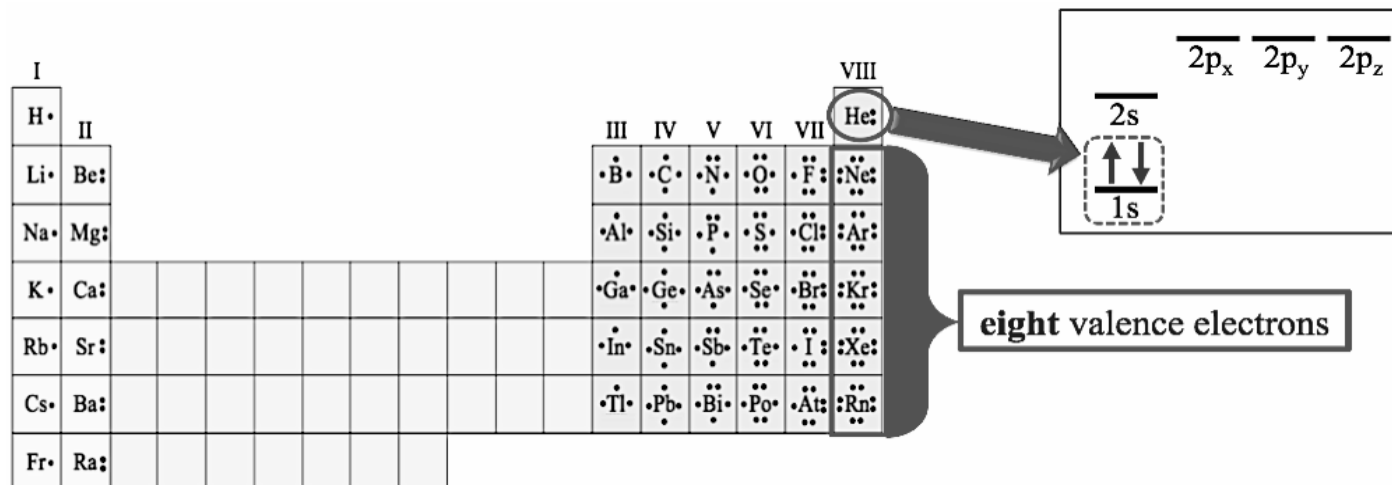
Helium's outermost shell (the n=1 quantum level) is completely filled with its ***two*** electrons.

All of the other noble gas elements have completely filled outermost shells with _____ electrons.

This stability of the noble gas elements that have ***eight electrons*** in their outermost shell led to what chemists call the _____ _____.

Most substances around us do not exist as individual atoms. Atoms will "bond" with other atoms to form compounds such as water (H_2O), carbon dioxide (CO_2), and table salt (sodium chloride). In the remainder of chapter 3, we will discuss the nature of this "bonding" of atoms to other atoms.

The Octet Rule is quite useful in predicting and understanding bonding patterns in chemical compounds.

The Octet Rule

Chemical compounds tend to form so that each atom, by gaining, losing, or sharing electrons, has an *octet* (eight) of electrons in its outermost shell.

There are exceptions to the octet rule. An important exception that we will always use is for ***hydrogen*** and ***helium***.

- Hydrogen and helium have filled outer shells (are stable) with just ***two*** electrons because their outermost level (**n**=1) has only one orbital.

Ions

Atoms have the same number of electrons as protons and are therefore ***electrically neutral***.

An _____ is a small particle that has an ***electrical charge***.

Atoms can ***gain or lose*** _____ to become **ions**.

Metal atoms can _____ electrons to form ***positive ions***.

If an atom *loses* one or more electrons, it will then have more protons than electrons and have an overall *positive charge*.

- *Positive ions* are called _____.

Nonmetal atoms can _____ electrons to form ***negative ions***.

If an atom *gains* one or more electrons, it will then have more electrons than protons and have an overall *negative charge*.

- *Negative ions* are called _____.

The Octet Rule in the Formation of Ions

The ***Octet Rule*** can be used to predict the formation of ions.

Very often, ions are formed such that the ***ion*** has an _____ in its outermost shell.

This tendency will allow us to predict the _____ of the ion that is formed for particular elements.

Example: Let's do a Cation - Sodium (Na)

- A sodium atom has _____ protons and _____ electrons.
- How many valence electrons does the sodium atom have? _____
- How many valence electrons does sodium want? _____

Fill the energy level diagrams with electrons:

Na **atom**

3s   3p

2s   2p

1s

Na **ion**   +

3s   3p

2s   2p

1s
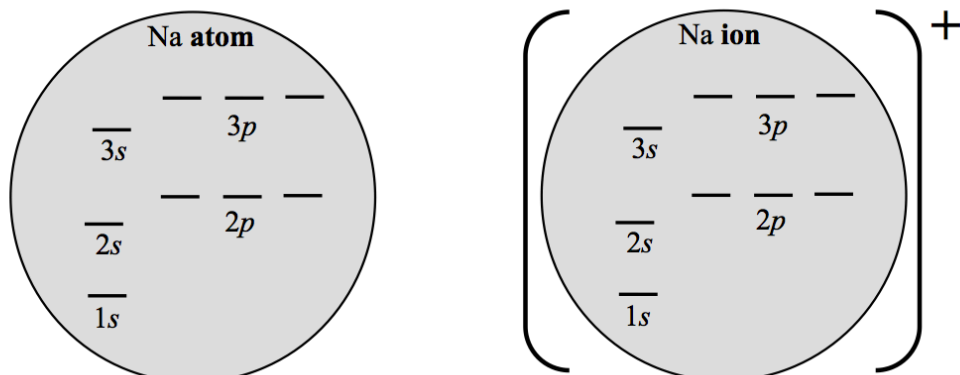
When sodium loses an electron, it has an octet of electrons in its outer shell.

Sodium will lose_____ electron to become a sodium ion (Na^+).

- Sodium has one valence electron
- There are two ways to have a filled octet:
    - 1) Add 7 electrons
    - 2) Remove one electron
- It is easier to remove one electron!

Na•

lose one electron

$(Na)^+$

electron dot structure for a **Sodium Atom**

electron dot structure for a **Sodium Ion**
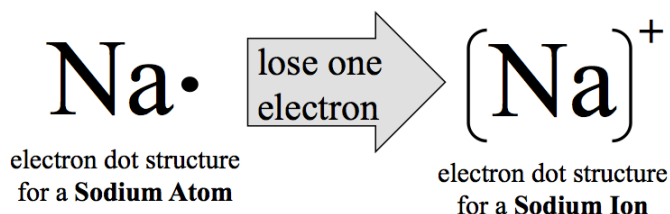
Example: Let's do Another Cation - Magnesium (Mg)

- A magnesium atom has _____ protons and _____ electrons.

- How many valence electrons does the magnesium atom have? _____

- How many valence electrons does magnesium "want?" _____

Fill the energy level diagrams with electrons:

Mg atom

___ ___ ___
3s   3p

___ ___ ___
2s   2p

___
1s

Mg ion

___ ___ ___
3s   3p

___ ___ ___
2s   2p

___
1s

2+
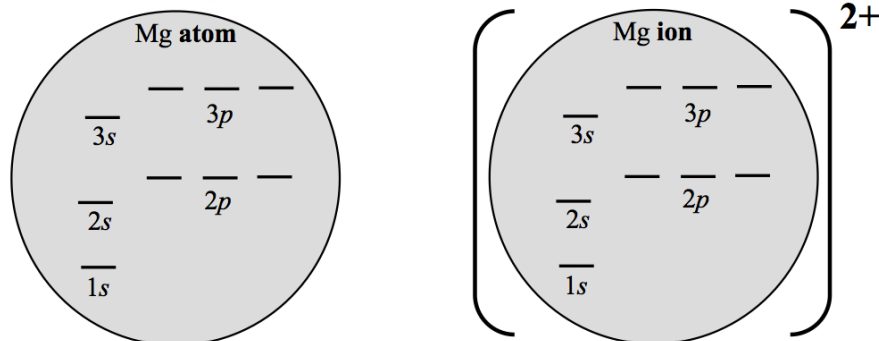
When magnesium loses two electrons, it has an octet of electrons in its outer shell.

Magnesium will lose _____ electrons to become a magnesium ion (Mg^{2+}).

Understanding Check: Based on the octet rule, what would be the charge of an aluminum ion?

HINT: Begin with the energy level diagram (or the number of valence electrons) for an aluminum atom.

Example: Let's do an Anion - Oxygen (O)

- An oxygen atom has _____ protons and _____ electrons.

- How many valence electrons does the oxygen atom have? _____

- How many valence electrons does oxygen want? _____

Fill the energy level diagrams with electrons:

O atom

___ ___ ___
3s   3p

___ ___ ___
2s   2p

___
1s

O ion

___ ___ ___
3s   3p

___ ___ ___
2s   2p

___
1s

2-
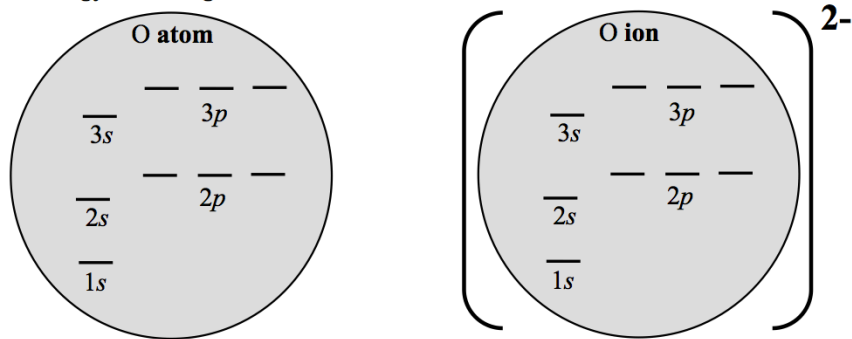
When oxygen gains two electrons, it has an octet of electrons in its outer shell.

Oxygen will gain_____ electrons to become an oxide ion (0^{2-}).

The *electron dot structure* can give us the same conclusion!

Draw an electron dot structure for an **Oxygen Atom**:

gain two electrons

Draw an electron dot structure for an **Oxide Ion**:

Oxygen has 6 valence electrons, if we add two electrons; its outer shell will have an octet.

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We can determine the charge of an ion formed from **s-block elements** and **p-block nonmetals** from the number of valence electrons in those elements, and therefore by their _location_ on the periodic table.

Periodic Group	Number of Valence Electrons of the Element	Number of Electrons Gained or Lost in Ion Formation	Charge of Ion Formed
s-Block Elements			
Group I	1	Lose 1 electron	1+
Group II	2	Lose 2 electrons	2+
p-Block Nonmetal Elements			
Group III		There are no Group III nonmetals (only metals and metalloids)	
Group IV	4	Do not form ions, high energy to gain **or** lose 4 electrons!	
Group V	5	Gain 3 electrons	3-
Group VI	6	Gain 2 electrons	2-
Group VII	7	Gain 1 electron	1-
Group VIII	8	Do not form ions, noble gas atoms have filled outer shells.	

The charge of the ions formed from the **transition metals** and **p-block metals** _cannot_ always be predicted by their position in the periodic table.

I																	VIII
1+																	
H^+	II										III	IV	V	VI	VII		
	2+												3-	2-	1-		
Li^+	Be^{2+}												N^{3-}	O^{2-}	F^-		
Na^+	Mg^{2+}		transition metals										P^{3-}	S^{2-}	Cl^-		
K^+	Ca^{2+}													Se^{2-}	Br^-		
Rb^+	Sr^{2+}														I^-		
Cs^+	Ba^{2+}																
Fr^+	Ra^{2+}																Do Not Form Ions

Many of these elements can form **_more than one_** type (charge) of ion.

Example: Iron (Fe):

Iron (Fe) ions can come as Fe^{2+} or Fe^{3+}

Fe^{2+} Fe^{3+}
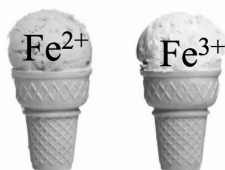
Example: Copper (Cu):

Copper (Cu) ions can come as Cu^{1+} or Cu^{2+}

To differentiate the various charge states of ions when reading or writing their names, we use _____ numerals corresponding to the **charge** after the element name.

Copper(I) ⇨ Cu^{1+} Cu^{2+} ⇦ Copper(II)
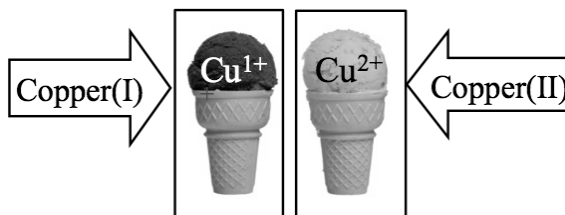
- When saying the ion's name, one would say "copper one" for Cu^{1+} and "copper two" for Cu^{2+}.

We **_only_** use the Roman numeral for ions that can **_exist in more than one charge state_**.

Some of the **transition metals** and **p-block metals** only exist in **one** charge state.

- For example, **cadmium ions** only exist as **Cd^{2+}**.

Cd^{2+}

Roman numerals **_are not used_** when the metal cations _have just one charge state_.

Since the charges of many of the transition metal and p-block metal ions *cannot* be easily predicted from their positions on the periodic table, and many can have more than one charge, we must refer to tabulated list for the charges.

The table below lists the charges for some transition metals and p-block ions.   **You do not need to memorize the metal names and charges in this table**; I will give you this table for with your exams.

Charges for Some Transition Metal and p-Block Metal Ions

Ions that occur with only <u>one</u> charge			
Name	Charge	Name	Charge
aluminum ion	Al^{3+}	cadmium ion	Cd^{2+}
silver ion	Ag^+	zinc ion	Zn^{2+}
Ions that occur with <u>multiple</u> charges			
Name	Charge	Name	Charge
copper(I) ion	Cu^+	tin(II) ion	Sn^{2+}
copper(II) ion	Cu^{2+}	tin(IV) ion	Sn^{4+}
iron(II) ion	Fe^{2+}	lead(II) ion	Pb^{2+}
iron(III) ion	Fe^{3+}	lead(IV) ion	Pb^{4+}
cobalt(II) ion	Co^{2+}	mercury(I) ion	Hg^+
cobalt(III) ion	Co^{3+}	mercury(II) ion	Hg^{2+}

This table does not contain data for the all ions formed by *all* of the transition and **p**-block metal cations, however it includes the ions that you will need in order to solve and understand any of the examples and problems in this course.

Naming Monatomic Ions

A ***monatomic ion*** is an ion that is made when a _____ **atom** gains or loses electron(s).

<div align="center">

Naming Monatomic *Cations*

</div>

Cations use the name of the element, followed by the word "ion."
- **Examples:**
    Na^+ is referred to as a sodium ion.
    Mg^{2+} is referred to as a magnesium ion.

For monatomic cations that can occur *with multiple charges,* indicate the charge using Roman numerals *after* the element's name.
- **Examples:**
    Fe^{2+} is referred to as an iron(II) ion
    Fe^{3+} is referred to as an iron(III) ion

<div align="center">

Naming Monatomic *Anions*

</div>

Anions are named by changing the *suffix* (ending) of the name to "-_____."
- **Examples:**
    F^- is referred to as a fluor**ide** ion.
    O^{2-} is referred to as an ox**ide** ion.

Polyatomic Ions

Several atoms often "*stick*" (bond) together to form a small particle.

If the resulting particle has the s*ame number of protons as electrons*, then it will be ***electrically neutral***, and we call the particle a _____.

If, on the other hand, there is an *excess of protons or an excess of electrons* in the particle, then it will have an ***overall electrical charge***, and we call the particle a _____ **ion**.

Example of a Polyatomic Ion: Nitrate Ion
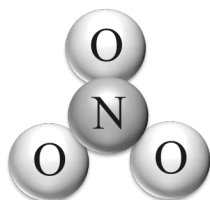
Nitrogen   (7 electrons, 7 protons)
Oxygen   (8 electrons, 8 protons)
Oxygen   (8 electrons, 8 protons)   Nitrate Ion
Oxygen   (8 electrons, 8 protons) NO_3^-
             + one extra electron

The table below lists the names and charges for some polyatomic ions. **You do not need to memorize this table**; I will give you this table for with your exams.

Some Polyatomic Ion Names and Charges

POLYATOMIC CATIONS	
H_3O^+ hydronium ion	NH_4^+ ammonium ion
POLYATOMIC ANIONS	
OH^- hydroxide ion	HSO_4^- hydrogen sulfate (or bisulfate) ion
CO_3^{2-} carbonate ion	PO_4^{3-} phosphate ion
HCO_3^- bicarbonate (also called hydrogen carbonate) ion	HPO_4^{2-} hydrogen phosphate ion
NO_2^- nitrite ion	$H_2PO_4^-$ dihydrogen phosphate ion
NO_3^- nitrate ion	CrO_4^{2-} chromate ion
SO_3^{2-} sulfite ion	$Cr_2O_7^{2-}$ dichromate ion
SO_4^{2-} sulfate ion	$C_2H_3O_2^-$ acetate ion (sometimes written as $CH_3CO_2^-$)
	CN^- cyanide ion

Chemical Compounds

Compounds: _____

_____

Each compound has the same _____ of the same elements.

- Example: Water = 2 hydrogen atoms and 1 oxygen atom (Ratio H:O = 2:1)

Chemical bonds

Atoms can **bond** with other atoms, and ions can **bond** with other ions to form **compounds** such as water (H_2O), carbon dioxide (CO_2), and table salt (sodium chloride).

Chemical bonds are the **electrical attractive** _____ that hold atoms or ions together in a compound.

There are *three types* of **chemical bonding**:

1) **Covalent Bonding**
2) **Ionic Bonding**
3) **Metallic Bonding**

In this chapter, you will learn about the first two types, *covalent bonding* and *ionic bonding*. You will learn about *metallic bonding* in chapter 5.

Some Terminology

All matter can be classified as either **mixtures** or **pure substances**. You will learn about mixtures in chapter 6. **Pure substances** are described in the chart *on the right*:

Chemistry is the study of matter and the *changes* it undergoes.

_____ *changes*, such as *melting* or *boiling*, result in changes in *physical properties* and **do not** involve the formation of new *pure substances*.

- For example, the melting of ice is simply H_2O being changed from the *solid* phase to the *liquid* phase. The chemical bonds between oxygen and hydrogen atoms do not change in that process.

_____ *changes*, on the other hand, result in the formation of **new** *pure substances*.

- To make a **new** pure substance, **chemical bonds must be** _____ **and/or new chemical bonds are** _____.

- This happens in a process called a **chemical reaction**, which we will study in chapter 6.

A *major principle* of chemistry is that the observed (macroscopic) properties of a substance are related to its "microscopic" structure.

- The *microscopic* structure entails details such as the kind of atoms/ions and the pattern in which they are **bonded** to each other.

Pure Substances

Compounds
Consist of **two or more** elements
Examples:
- water (H_2O)
- carbon dioxide (CO_2)
- sodium chloride (NaCl)

Elements
Consist of only **one** element
Examples:
- gold
- oxygen (O_2)
- helium

Ionic Compounds

Covalent Compounds
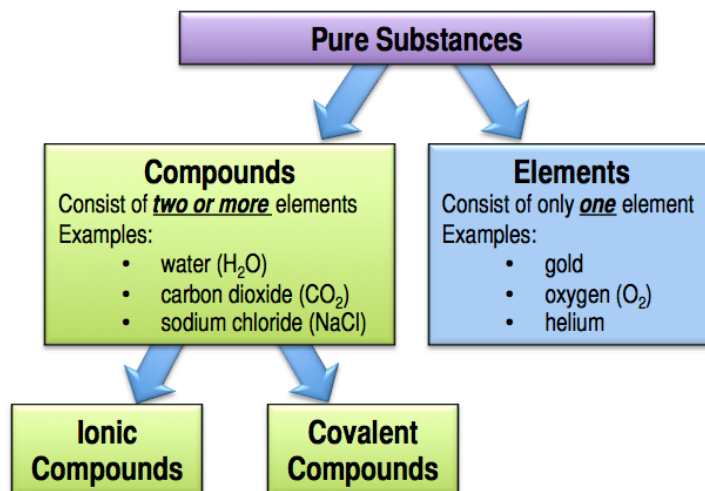
Covalent Chemical Bonding

Covalent bonding is defined as the chemical bonding *force* that results from the

_____ between two atoms.

The resulting collection of atoms results in the formation of either _____ or *polyatomic ions*.

A **molecule** is an electrically _____ group of atoms *held together by covalent bonds*.

Covalent bonding occurs between _____atoms.

Covalent bonding occurs because the bound atoms are at a _____ energy than the unbound atoms.

Why does sharing of electron pairs result in an attractive electrostatic force capable of holding atoms together?

Consider the two *hydrogen atoms* coming together to form a covalent bond.
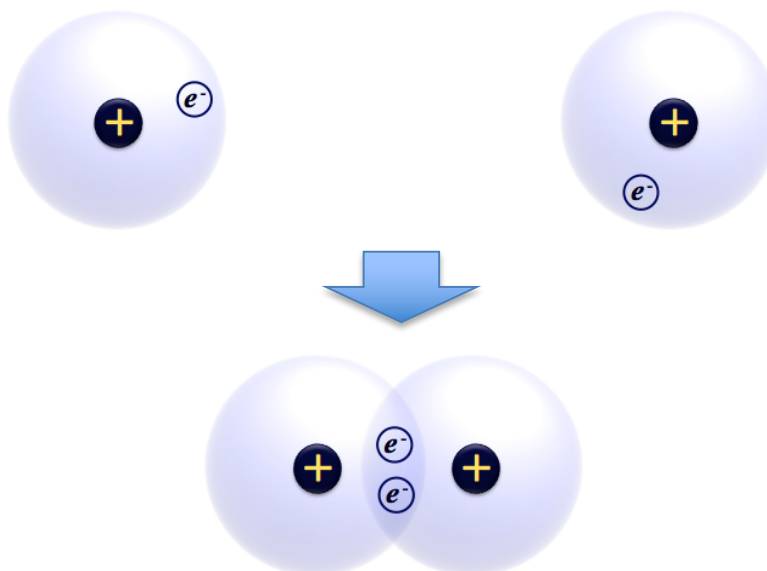
In covalent bonding, the atoms _____ *electron pairs*.

The shared electron pair spends significantly *more* _____ in the area between the positive nuclei of the hydrogen atoms than in other regions.

The electron pair between the nuclei create a **positive-negative-positive** electrostatic attractive "sandwich" and this _____ holds the atoms together.

The Octet Rule in the Formation of Molecules

The positive-negative-positive model **cannot** explain why a covalent bond *does not* form between two *helium* atoms.

The octet rule in the formation of molecules is: *molecules tend to form such that the atoms are surrounded by an octet (eight) of valence electrons (except for hydrogen and helium that have two electrons).*

Example: H₂
(recall that H and He are stable with two valence electrons)

When a covalent bond forms, each hydrogen atom "feels" **two** electrons in its outermost shell.
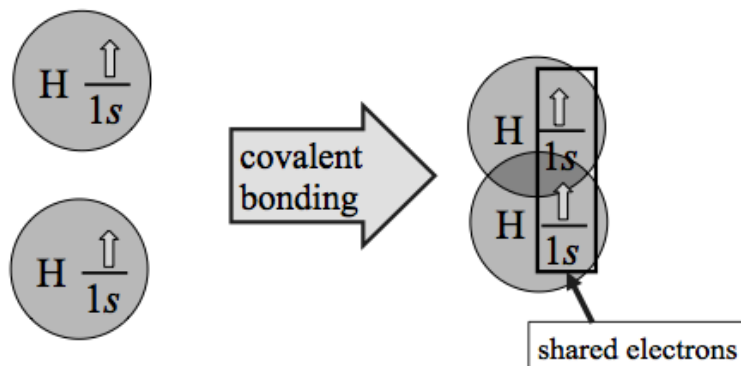
The H₂ covalent bond can also be illustrated with electron dot structures.

H· ——— ·H

H:H
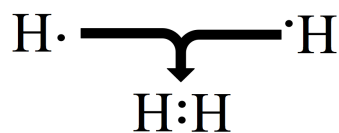
The two electrons _____ the atoms are shared in a covalent bond.
Chemist use a line to represent ____ electrons in a covalent bond.

H−H
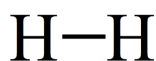
These drawings are called _____.

Let's do another example: **Hydrogen Chloride (HCl)**

When a covalent bond forms, the hydrogen atom "feels" **two** electrons in its outermost shell, and the chlorine atom "feels" **eight** electrons in its outermost shell.
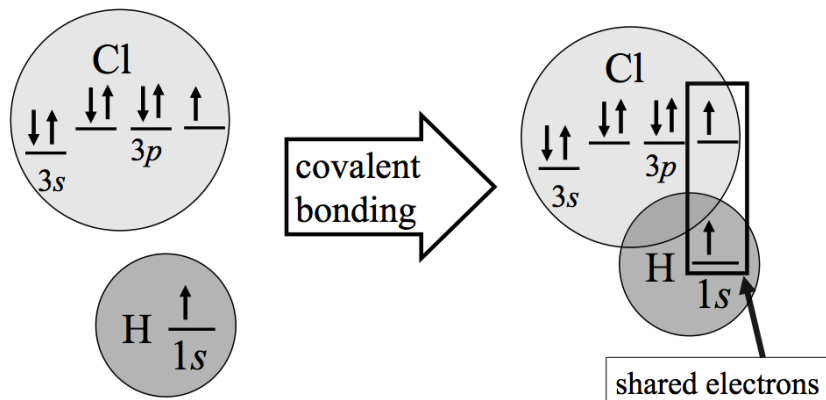
The HCl covalent bond can also be illustrated using electron dot structures.

H· ·C̈l:

H:C̈l:

H−C̈l:

line bond structure

Cl
↓↑ ↓↑ ↓↑ ↑
3s   3p

Cl
↓↑ ↓↑ ↓↑ ↑
3s   3p

covalent bonding

Cl
↓↑ ↓↑ ↓↑ ↑
3s   3p

↓↑ ↓↑ ↓↑ ↑
3s   3p
Cl

shared electrons
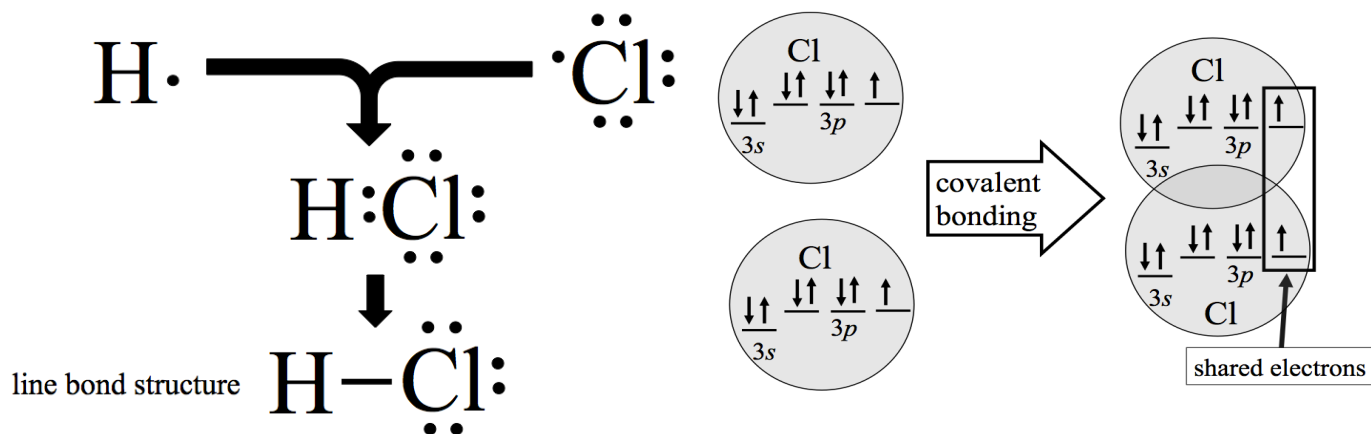
Let's do another example: **Cl₂ (chlorine gas)**.

When a covalent bond forms, each chlorine atom "feels" **eight** electrons in its outermost shell.

O
↓↑ ↓↑ ↑ ↑
2s   2p

O
↓↑ ↓↑ ↑ ↑
2s   2p

covalent bonding

O
↓↑ ↓↑ ↑ ↑
2s   2p

↓↑ ↓↑ ↑ ↑
2s   2p
O
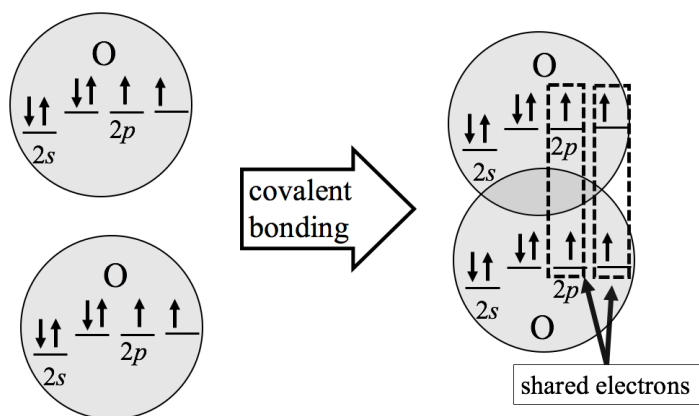
shared electrons

You try it:
Draw the *line bond structure* for Cl₂.
- Start with the electron dot structure for two Cl atoms.

Let's do **oxygen gas (O₂)**.

In O₂, **two pairs** of electrons are shared.

When a covalent bond forms, each oxygen atom "feels" **eight** electrons in its outermost shell.

Let's draw the line bond structure for **oxygen gas (O₂)**.
- Oxygen atoms have 6 valence electrons.
- We will rotate the electrons so they can form bonding pairs.

:Ö: ───── :Ö:

:Ö⣿Ö:

21
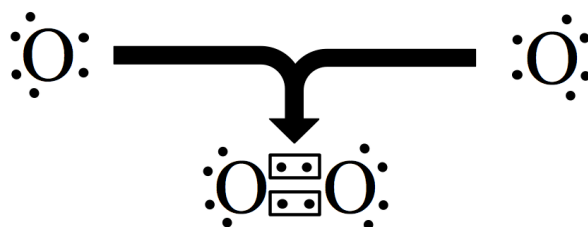
We use lines to represent _____ electron pairs.

When atoms are bonded with 2 pairs of electrons it is called a _____ _____.

Double Bond

$$\ddot{\text{O}} = \ddot{\text{O}}$$
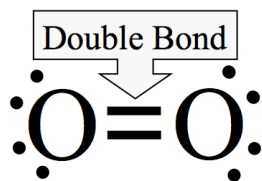
Let's draw the line bond structure for nitrogen gas (N_2)

- Nitrogen atoms have 5 valence electrons.
- We will rotate the electrons so they can form bonding pairs.

:N̈: ⎯⎯⎯⌐ ⌐⎯⎯⎯ :N̈:

↓

:N⊞N:
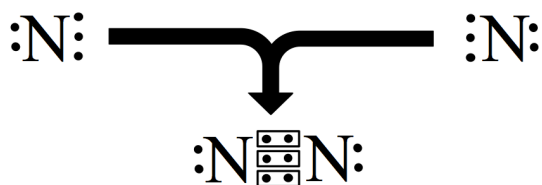
We use lines to represent electron pairs.

When atoms are bonded with **3 pairs** of electrons it is called a _____ _____.

Triple Bond
↓

:N≡N:
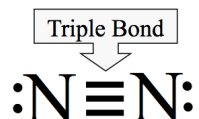
Naming Covalent Compounds

The covalent bonding that we will see in this course will *always* involve _____ **elements only**.

The nonmetal atoms can share electrons to form **molecules** (*molecular compounds*) or **polyatomic ions**.

A chemical substance whose simplest units are **molecules** is called a _____ *compound*.

When discussing molecules we use a _____ _____ that shows the *types (elements)* and *numbers of atoms* that make up a single molecule.

The number of atoms of each element contained in the molecule is written as a *subscript* after the element's symbol.

- **Examples:**

line bond structure	molecular formula
H−H	H_2
H−Ö−H	H_2O

When there is only **one atom** of a particular element present in a molecule the subscripted "**1**" is *omitted* for that element.

Some molecules *only* contain *one* element, for example H_2, Cl_2, and O_2.

- These molecules often take the name of the elements they contain.
- **Examples:**

molecular formula	name
H_2	hydrogen
O_2	oxygen

Naming Binary Covalent (Molecular) Compounds

_____ **covalent compounds** contain only *two* _____ (the "**bi-**" prefix indicates "*two*").

- Examples of binary covalent compounds are **HCl**, **H₂O**, and **CO₂**.

Educational Goals:
Given the **name** of a *binary covalent molecule*, be able to write the **molecular formula**.
Given the **molecular formula** of a *binary covalent molecule*, be able to write the **name** of the molecule.

Method for *Naming* Binary Covalent (Molecular) Compounds

1. List the name of the first element in the formula.

2. List the second element and add the –**ide** _____.

3. Use Greek _____ to indicate the number of each atom in the formula.

    - **Exception:** If there is just one atom of the _____ element in the formula, do not use **mono-** for the *first element in the name*.

        - **Example: CO₂**
          ~~mono~~carbon dioxide ➜ carbon dioxide

    - The "**o**" or "**a**" at the *end of the Greek prefix* is omitted when the element's name begins with a vowel.

        - **Example: CO**
          carbon mon~~o~~oxide ➜ carbon monoxide

Greek Prefix	Number
mono	1
di	2
tri	3
tetra	4
penta	5
hexa	6
hepta	7
octa	8
nona	9
deca	10

Example Problem:

Name the following compound: **CCl₄**

  Answer: carbon tetrachloride

Understanding Check
Write the **names** of the following molecules:
CF₄ _____
N₂O _____
SF₆ _____

Method for Writing the *Molecular Formula* of a Binary Covalent Compound

1. Write the symbol of the *first element* in the compound's name, then the symbol of the *second element* in the compound's name.

2. Indicate *how many atoms* of each element the molecule contains using *subscripts* after the atomic symbol.

    - The *numbers of atoms* are given in the Greek prefixes in the molecule's name.

    - NOTE: If there is no Greek prefix in front of the first element in the name, that means the number is **1**.

Example:
Write the *molecular formula* for **dinitrogen tetrafluoride**.
N_2F_4

For covalent compounds with ***more than two types of atoms***, we use *common names* or *IUPAC* system names. You are not responsible for knowing *common names*. You will learn some IUPAC system names in later chapters.

Examples of *common names*:
- Glucose ($C_6H_{12}O_6$)
- Acetone (C_3H_6O)

Ionic Compounds

Definition of **ionic bonding**: Chemical bonding that results from the electrostatic attraction between _____ **numbers** of *cations* and *anions*.

- Compounds composed of ions are called **ionic compounds**.

Example of an ionic compound: sodium chloride (NaCl)

Many sodium ions combine with **many** chloride ions in a *three-dimensional pattern* that minimizes the distance between the oppositely charged cations and anions and maximizes the distance between the like-charged particles.
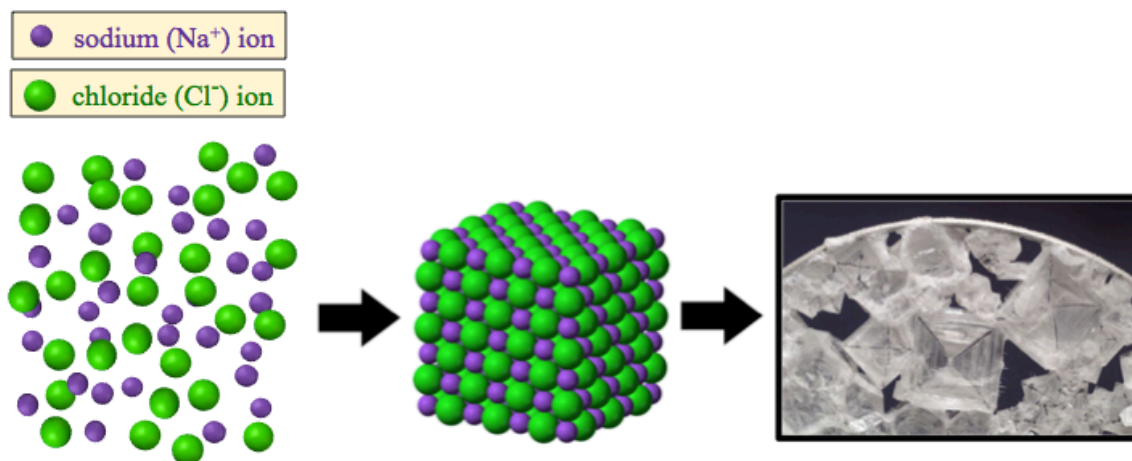
We call this structure a _____ or *crystal* _____.

It is this regular, repeating structure on the scale of the individual ions that give crystals the interesting geometrical shapes that we see on the macro-scale when we look at them with our eyes or with a microscope.

Ionic bonding (ionic compounds) results from:
- Combining **metal ions** with **nonmetal** ions.
- Combining **polyatomic ions** with *other* ions.

The cations and anions will combine in a ratio such that the **total** of the *positive* (+) and *negative* (−) *charges* equals _____!

- **Example:** Sodium Chloride (NaCl)

sodium (Na^+) ion

chloride (Cl^-) ion
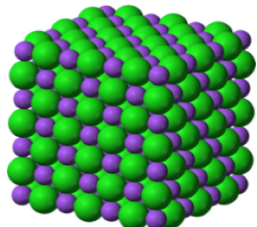
Sodium ions have a charge of 1+

Chloride ions have a charge of 1-

They combine in a 1-to-1 _____ in the crystal

For every sodium ion, there is one chloride ion!

The charges _____ up to ZERO!

Formula Units

The use of *molecular formulas* would not make sense for ionic compounds; they do not form molecules, instead they form crystals.

We write _____ _____ (as opposed to *molecular formulas*) for **ionic compounds**.

The *formula unit* looks like the molecular formula used for covalent compounds, however it means something *entirely* different.

The *formula unit* uses **subscripted numbers** after the ion's symbol that indicate the **ratio** that the cations and anions combine in the ionic crystal.

- As in the case of molecular formula, when a subscript would have a value of "1," the subscript is omitted.

- We write the cation symbol first followed by a numerical subscript (if needed), then we write the anion symbol followed by a numerical subscript (if needed).

Example: For sodium chloride, since sodium ions and chloride ions combine in a **one-to-one ratio**, we write the formula unit of sodium chloride as:

$$NaCl$$

Example: *Calcium* ions combine with *fluoride* ions to form an **ionic compound**.

Calcium ions have a charge of 2+

Fluoride ions have a charge of 1-

They combine in a _____ ratio in the crystal

For *every* calcium ion, there are _____fluoride ions.

We write the **formula unit** for calcium fluoride as:

$$CaF_2$$

Understanding Check:
Write the *formula unit* for the compound formed by combining magnesium and chloride ions.

$$Mg_{\square}Cl_{\square}$$
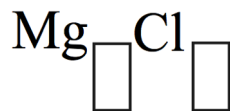
Understanding Check:
Write the *formula unit* for the compound formed by combining potassium and oxide ions.
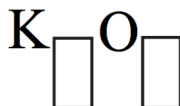
$$K_{\square}O_{\square}$$

Understanding Check:
Write the *formula unit* for the compound formed by combining magnesium and nitride ions.

$$Mg_{\square}N_{\square}$$

Dr. Zoval's Caveman Style, Works Every Time Method:

$$\overset{2+}{Mg}\underset{3}{}\overset{3-}{N}\underset{2}{}$$
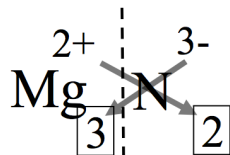
The Criss-Cross Method

Formula Units

Write the formula for the ionic compound formed between each of the following pairs of ions:

Cu^+ and O^{2-}

Fe^{3+} and S^{2-}

Cu^{2+} and Cl^-

Mg^{2+} and O^{2-}

Sn^{4+} and S^{2-}

V^{3+} and Cl^-
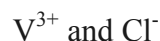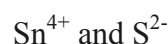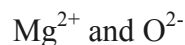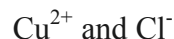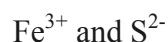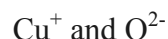
Formula Unit vs. Molecular Formula

Formula Unit =
Lowest **RATIO** of ions

Example: NaCl
Ratio of Na^+ to $Cl^- = 1$ to 1

| sodium (Na^+) ion |
| chloride (Cl^-) ion |
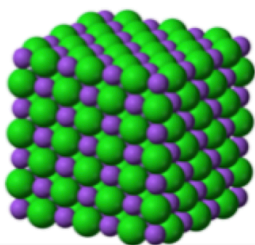
Molecular Formula =
Actual **number** of atoms

Example: H_2O
two hydrogen atoms and
one oxygen atom
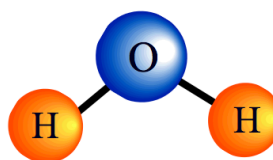
Naming Ionic Compounds

Method for Writing Formula Units for Ionic Compounds

1) Write the symbol of the first ion (the cation) in the compound's name, then the symbol of the second ion (the anion) in the compound's name.

2) Indicate the **ratio** of the ions in the compound using *subscripts* after each ion.

The ratio of the ions is deduced by *balancing the charges* of the ions so that the total charge in the crystal is equal to **zero**.

- We find the ion's charge from its position on the periodic table or, for polyatomic ions, we look it up in a table.

- You will know the charge for the metals t*hat occur with various charges* because the charge will be written in the compound's name in Roman numerals.

For _____ *ions*:
When the *subscript* for a **polyatomic ion** is *greater than 1*, the polyatomic ion formula is written in parenthesis and the subscript is written after/outside of the parenthesis.

Example: Write the *formula unit* for **iron(III) bromide**.

- You will know the **charge** for the metals t*hat occur with various charges* because the charge will be written in the compound's name in **Roman numerals**.

iron(III) bromide

$$Fe^{3+} \quad Br^{1-} \quad \Longrightarrow \quad FeBr_3$$

$$\text{Fe}_1 \quad \text{Br}_3$$
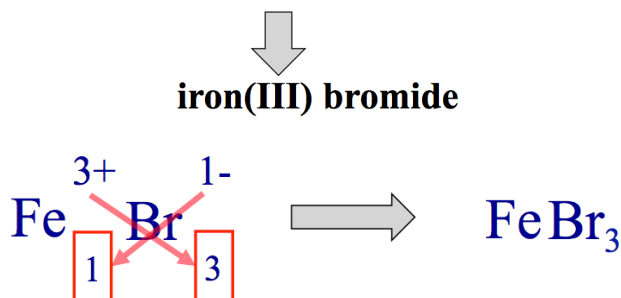
Example: Write the *formula unit* for **magnesium nitrate**.

$$Mg^{2+} \quad NO_3^{1-} \quad \Longrightarrow \quad Mg(NO_3)_2$$

$$\text{Mg}_1 \quad \text{NO}_3{}_2$$
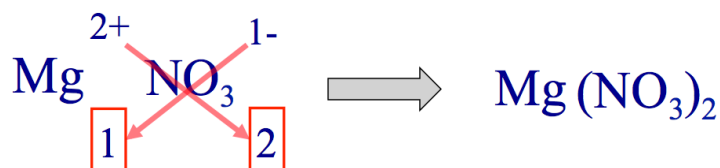
- **For polyatomic ions**:
When the *subscript* for a **polyatomic ion** is *greater than 1*, the polyatomic ion formula is written in parenthesis and the subscript is written after/outside of the parenthesis.

Method for Writing the Names of Ionic Compounds

1. Write the _____ name first, then the _____ name.

   • Monoatomic **anions** (anions composed of one element) use the "ide" suffix.

   • We get the names of *polyatomic ions* from the polyatomic ion table.

2. If the cation is one of the *metals with various charges*, write the charge using parenthesis and Roman numerals after the metal's name.

Example: Name the following compound: **$MgCl_2$**

Name: **magnesium chloride**

Example: Name the following compound: **$CuBr_2$**

   • What *must* the charge of the copper ion be? **2+**

Name: **copper(II) bromide**

Complete the names of the following ionic compounds with variable charge metal ions:

$FeBr_2$ iron(__) bromide

$CuCl$ copper(__) chloride

SnO_2 _____(__) _____

Fe_2O_3 _____

Name the following ionic compounds:

$NaCl$ _____

ZnI_2 _____

Al_2O_3 _____

Naming Compound Summary

Determine if the Compound is **Binary Covalent** (Molecular) or **Ionic**: Does the compound contain **only** *two types of nonmetal elements?*

Yes → Binary Covalent (Molecular) Compound

No → Ionic Compound
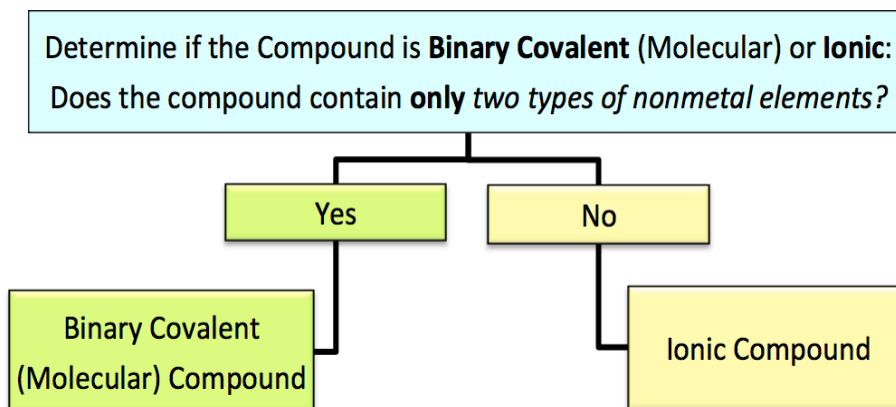
Given the Molecular Formula, Write the Name

Determine if the Compound is **Binary Covalent (Molecular)** or **Ionic**:

Does the compound contain **only** *two types of nonmetal elements?*

Yes ↓

No ↓

Binary Covalent (Molecular) Compound:

1) List the name of the first element in the formula.
2) List the second element and add the "ide" suffix.
3) Use Greek prefixes to indicate the number of each atom in the formula.
   - Exception: **Do not use** mono- for the first element in the name.
   - The *o* or *a* at the end of the Greek prefix is dropped when the element name begins with a vowel.

Ionic Compound:

1) Write the cation name first, then name the anion.

   - Monoatomic anions use the "ide" suffix

2) If the cation is one of the metals with various charges, write the charge using parenthesis and Roman numerals after the metal name.

Given the Name, Write the Molecular Formula

Determine if the Compound is **Binary Covalent (Molecular)** or **Ionic:**

Does the compound contain **only *two*** types of *nonmetal* elements?

Yes   No

Binary Covalent (Molecular) Compound:

1) Write the symbol of the first element in the compound's name, then the symbol of the second element in the compound's name.
2) Indicate how many atoms of each element the molecule contains using subscripts after the atomic symbol.
   - The numbers of atoms are given in the molecule's name in Greek prefixes
     - NOTE: If there is no Greek prefix in front of the first element in the name that implies the number is 1.
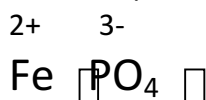
Ionic Compound:

1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.
2) Indicate the ratio of the ions in the compound using subscripts after each ion.
   - The ratio of the ions is deduced by balancing the charges of the ions.
   - *IMPORTANT: When there is more than one of a polyatomic ion in the formula unit we use parenthesis. Example Mg(NO₃)₂*

Molar Mass of Compounds

In this video, you will learn how to calculate the **molar mass** of a compound and how to use the molar mass of a compound to do *mole-mass conversions*.

1) Molar Mass of **Covalent Compounds** (**Molecules**)

2) Molar Mass of **Ionic Compounds**

Molar Mass of Covalent Compounds (Molecules)

The **molar mass** of a _____ tells us the mass (grams) of **1 mole** of the *molecules*.

- The *molar mass* of a molecule is also called the **molecular mass**.

To calculate the *molar mass* of a **molecule** we **add up** the *atomic molar masses* of **all** _____ in the molecule.

Example: Let's calculate the molar mass of H_2O.
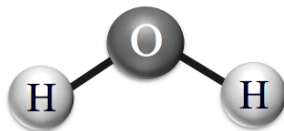
Atom	# of Atoms	Atomic Molar Mass	Total
oxygen	1	X 16.00 g/mole	16.00 g/mole
hydrogen	2	X 1.01 g/mole	2.02 g/mole
		Molar Mass of H_2O =	18.02 g/mole

One mole of H_2O
(6.022×10^{23} molecules) $\Big\}$ — has a mass of 18.02 grams

---

Understanding Check: Calculate the molar mass of CH_4 (methane).

Mass-Mole-Molecules Conversions

Note that, as in the case of atoms, the molar mass of a compound is the ***relationship*** between *moles* and *mass (grams)*, therefore we can **convert** between moles and grams of compounds.

Molecules   Mass (grams)

Use Avogadro's Number

1 mole = 6.022×10^{23} molecules

Use Molar Mass

\# grams/mole
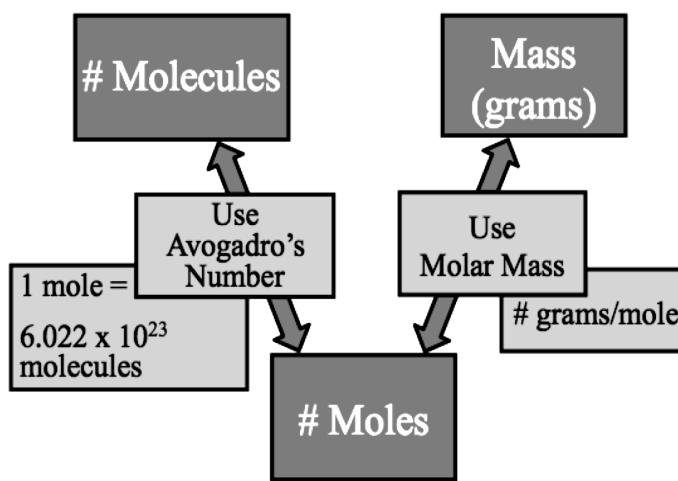
Moles

Example: How many *grams* of CH_4 is contained in 3.65 *moles*?

Use the molar mass to write an *equivalence statement*:

- **1 mole CH_4 = 16.05 grams**

The equivalence statements can be written as conversion factors:

$$\left(\frac{1 \text{ mole } CH_4}{16.05 \text{ grams}} \right) \xleftrightarrow[\text{Factors}]{\text{Conversion}} \left(\frac{16.05 \text{ grams}}{1 \text{ mole } CH_4} \right)$$

$$\frac{3.65 \text{ moles } CH_4}{} \left| \frac{16.05 \text{ grams } CH_4}{1 \text{ mole } CH_4} \right. = 58.6 \text{ grams } CH_4$$

You have just learned how to convert between moles and mass of a compound and vice versa.

We do a **two-step calculation** to convert between **mass** and number of **molecules**.

We can *convert between molecules and moles* since **Avogadro's Number applies to molecules**; one mole of a molecular compound contains 6.022×10^{23} molecules.

# Molecules		Mass (grams)

Use Avogadro's Number
1 mole = 6.022×10^{23} molecules

Use Molar Mass
grams/mole

Moles
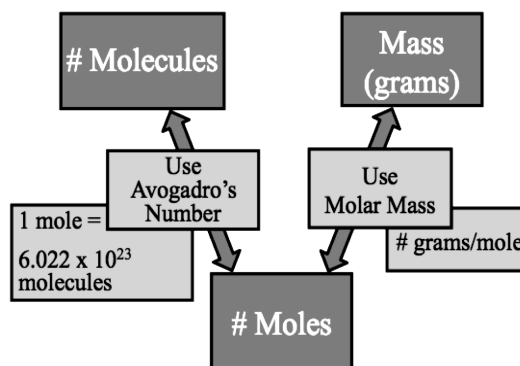
You try one: How many H_2O *molecules* are contained in 237 grams?

Molar Mass of Ionic Compounds

When using the **molar mass** of *ionic compounds*, we calculate the mass of a compound based on the number of each ion as it appears in the formula unit.

- For this reason, the *molar mass of an ionic compound* is also called _____ **mass**.

Example: The molar mass of sodium chloride (NaCl)

The **formula unit** for *sodium chloride* is **NaCl** because there is a 1:1 ratio of sodium ions to chloride ions in the crystal.

One **mole** of sodium chloride contains *one* **mole** of *sodium ions* and *one* **mole** of *chloride ions*.

Although **ions** have *extra* or *missing* elections, their molar masses are calculated by adding the *atomic molar masses* of the elements they contain.

- The reason we can do this is because the mass of electrons is negligible compared to the mass of protons and neutrons.

Ion	# of ions in the Formula Unit	Molar Mass of ion	Total
Sodium	1	X 22.99 g/mole	= 22.99 g/mole
Chloride	1	X 35.45 g/mole	= 35.45 g/mole
Molar Mass (Formula Mass) of NaCl			**= 58.44 g/mole**

Example: What is the molar mass of iron(II) phosphate, $Fe_3(PO_4)_2$?

One mole of iron(II) phosphate contains *three* moles of *iron(II) ions* and *two* moles of *phosphate ions*.

three moles of *iron(II) ions*   *two* moles of *phosphate ions*

$$Fe_3 \qquad\qquad (PO_4)_2$$
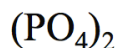
The molar mass of **each** *iron(II)* ion is: 55.85 g/mole.

each phosphate ion contains:
- one mole of phosphorus
- four moles of oxygen

The molar mass of **each** *phosphate ion* is: **94.97 g/mole**.

The molar mass (or formula mass) is calculated by adding the molar masses of the ions:

Ion	# of Ions in the Formula Unit	Molar Mass of ion	Total
Iron(II)	3	X 55.85 g/mole	= 167.55 g/mole
Phosphate	2	X 94.97 g/mole based on: one phosphorus **and** four oxygens *per ion*	= 189.94 g/mole
Molar Mass (Formula Mass) of Fe₃(PO₄)₂			**= 357.49 g/mole**

An Alternative Method:

$$Fe_3 \qquad\qquad (PO_4)_2$$

three **moles** of *iron(II) ions*   *two* **moles** of *phosphate ions* contain:
- *two* moles of phosphorous
- *eight* (2 x 4) moles of oxygen

Three moles of **Fe**: 3 x 55.85 g/mole =   **167.55** g/mole
Two moles of **P**: 2 x 30.97 g/mole =   **061.94** g/mole
Eight moles of **O**: 8 x 16.00 g/mole =   **128.00** g/mole
The molar mass of $Fe_3(PO_4)_2$ is   **357.49** g/mole

Understanding Check: What is the molar mass of magnesium nitrate, $Mg(NO_3)_2$?

Mole-Mass Conversions for Ionic Compounds

Mole-Mass conversions for ionic compounds are done *exactly* as we did for covalent compounds; use the molar mass as a conversion factor.

Mass
(grams)

Use
Molar Mass

grams/mole
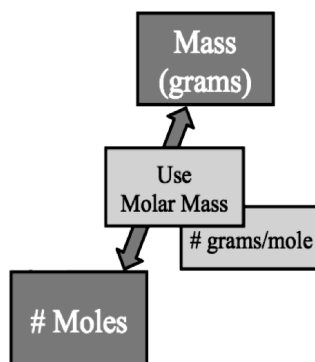
Moles

You Try One: What is the **mass** (grams) of 4.95 **moles** of $Mg(NO_3)_2$?

Naming Compounds Tutorial and Worksheet

Since we use different methods in naming binary covalent (molecular) compounds and ionic compounds, the **first step** in naming or writing the formula of a compound is to **determine which of the 2 compound classes it belongs**. This can be done as follows:

Determine if the Compound is **Binary Covalent** (Molecular) or **Ionic**: Does the compound contain **only** *two types of nonmetal elements?*

Yes

No

Binary Covalent (Molecular) Compound

Ionic Compound
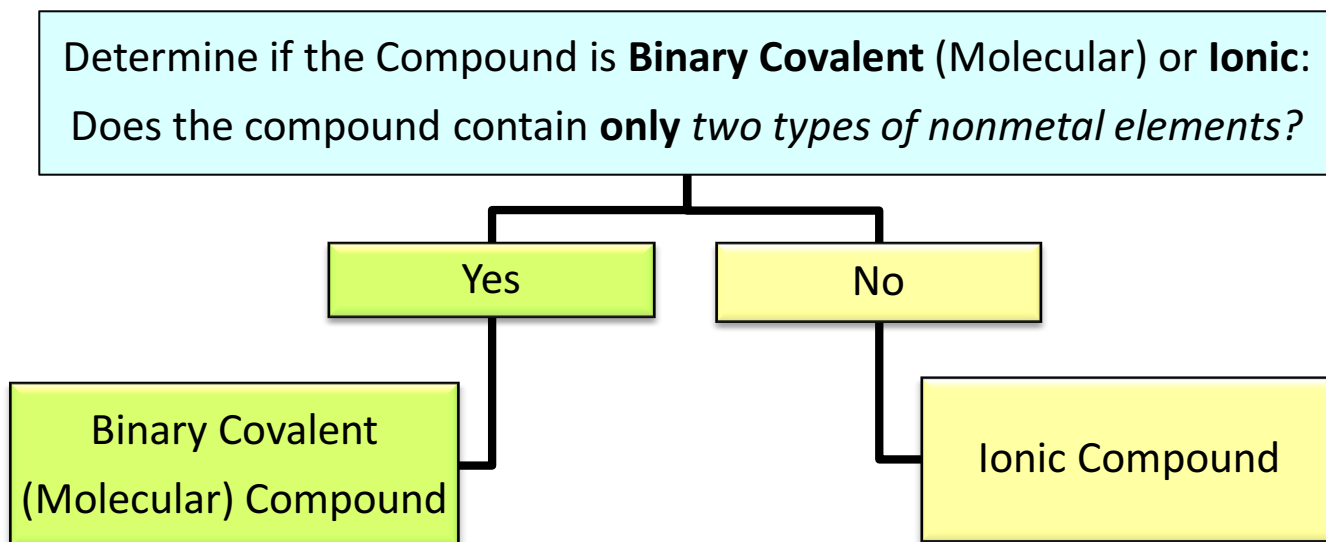
Binary covalent compounds will contain **only** *two types of non-metal elements*. There may be more than one of each element. For example CO_2 contains just two types of elements, carbon and oxygen. We will discuss naming covalent compounds that contain more than two types of elements, like glucose $C_6H_{12}O_6$, in later chapters.

Once it is determined that the compound is **ionic** or **covalent**, the student can be asked to do either of the following:

1) Given the **name** of the compound, write the **formula**.

Or

2) Given the **formula** of the compound, write the **name**.

In this tutorial we will review the process for achieving these 2 objectives and practice with some worksheet problems. First, we will review and practice how to write formulas for compounds when given the compound's name. Second, we will review and practice how to write the name of a compound when given the compound's formula.

Given the Name of the Compound, Writing Formulas for Compounds

Determine if the Compound is Binary Covalent (Molecular) or Ionic:

Does the compound contain only _two_ types of _nonmetal_ elements?

Yes

No

Binary Covalent (Molecular) Compound:

1) Write the symbol of the first element in the compound's name, then the symbol of the second element in the compound's name.
2) Indicate how many atoms of each element the molecule contains using subscripts after the atomic symbol.
   - The numbers of atoms are given in the molecule's name in Greek prefixes
     - NOTE: If there is no Greek prefix in front of the first element in the name that implies the number is 1.

Ionic Compound:

1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.
2) Indicate the ratio of the ions in the compound using subscripts after each ion.
   - The ratio of the ions is deduced by balancing the charges of the ions.
   - _IMPORTANT: When there is more than one of a polyatomic ion in the formula unit we use parenthesis. Example $Mg(NO_3)_2$_

Writing the Formulas of Ionic Compounds

Example: Write the formula for **calcium bromide**.

1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.

   Ca Br

2) Indicate the ratio of the ions in the compound using subscripts after each ion.
   - This step involves filling in the subscripts boxes as we did in the lecture:

   Ca☐ Br☐

   - The ratio of the ions is deduced by **balancing the charges** of the ions.
     - This is done so that the **total charge** in the crystal, when large numbers of cations and anions combine, is **equal to zero**.
     - We find the ion's charge from its position on the periodic table <u>or</u> we look it up in a table in the case of polyatomic ions.
     - Transition metal with varying charges will be written in the compound name in Roman numerals.

   - First, temporarily write the charge of each ion above the ion's symbol.

   $$^{2+} \quad ^{1-}$$
   Ca☐ Br☐

   - Next, place numbers in the subscripts such that the total charge of the compound is zero. Note that in this example, we need **two** bromide ions, each has a charge of (1-) to cancel the (2+) charge of the calcium ion:
     - $2(-1) + (+2) = 0$ zero total charge.
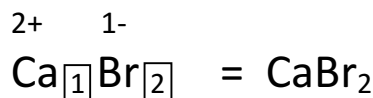
   $$^{2+} \quad ^{1-}$$
   $$Ca_{\boxed{1}} Br_{\boxed{2}} \quad = CaBr_2$$

     - We saw a shortcut way to do this called the Criss-Cross Method (see your chapter 3 notes)

   $$^{2+} \quad ^{1-}$$
   $$Ca_{\boxed{1}} Br_{\boxed{2}} \quad = CaBr_2$$
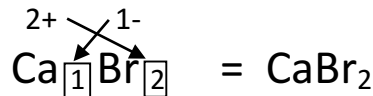
     - Note, we do not leave the charges written above the symbols in the completed formula.

IMPORTANT: When there is more than one of a polyatomic ion in the formula, we use parenthesis.
     - Not applicable in this example since there are no polyatomic ions in calcium bromide.

Examples: Writing the Formulas of Ionic Compounds

Write the formula for **magnesium nitrate**.
1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.
   - When you see a polyatomic ion (nitrate), look up the formula and charge in the table of polyatomic ions.

   $Mg \quad NO_3$

2) Indicate the ratio of the ions in the compound using subscripts after each ion.
   a. This step involves filling in the subscripts boxes as we did in the lecture:

   $Mg_\square NO_3{}_\square$
   - The ratio of the ions is deduced by **balancing the charges** of the ions.
     - This is done so that the **total charge** in the crystal, when large numbers of cations and anions combine, is **equal to zero**.
     - We find the ion's charge from its position on the periodic table **or** we look it up in a table in the case of polyatomic ions.
     - Transition metal with varying charges will be written in the compound name in Roman numerals.

   - First, temporarily write the charge of each ion above the ion's symbol.

   $\overset{2+}{Mg}_\square \overset{1-}{NO_3}{}_\square$

   - Next, place numbers in the subscripts such that the total charge of the compound is zero. Note that in this example, we need **two** nitrate ions, each has a charge of (1-) to cancel the (2+) charge of the magnesium ion:
     - 2(-1) + (+2) = 0 zero total charge.
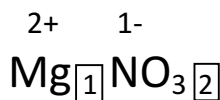
   $\overset{2+}{Mg}_{\boxed{1}} \overset{1-}{NO_3}{}_{\boxed{2}}$

   - We saw a shortcut way to do this called the Criss-Cross Method (see your chapter 3 notes)

   $\overset{2+}{Mg}_{\boxed{1}} \overset{1-}{NO_3}{}_{\boxed{2}}$
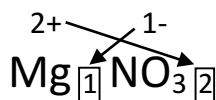
*IMPORTANT: When there is more than one of a polyatomic ion in the formula unit we use parenthesis. There are **2 ions** of nitrate in magnesium nitrate*

$$Mg_{\boxed{1}} NO_3{}_{\boxed{2}} = Mg(NO_3)_2$$
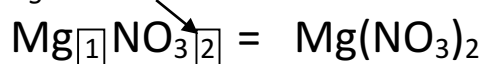
In compound where there is just **one formula unit** of a polyatomic ion, no parenthesis are needed. An example of this is **sodium nitrate: NaNO₃**

Examples: Writing the Formulas of Ionic Compounds

Write the formula for **iron(II) phosphate**.

1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.
   - When you see a polyatomic ion (phosphate in this case), look up the formula and charge in the table of polyatomic ions.

   Fe PO_4

2) Indicate the ratio of the ions in the compound using subscripts after each ion.
   b. This step involves filling in the subscripts boxes as we did in the lecture:

   Fe □PO_4 □

   c. The ratio of the ions is deduced by **balancing the charges** of the ions.
   - This is done so that the **total charge** in the crystal, when large numbers of cations and anions combine, is **equal to zero**.
   - We find the ion's charge from its position on the periodic table **or** we look it up in a table in the case of polyatomic ions.
   - **Transition metal with varying charges will be written in the compound name in Roman numerals.**
     - In this example, now we know the charge on **the Fe ion is 2+**

   d. First, temporarily write the charge of each ion above the ion's symbol.

   2+   3-
   Fe □PO_4 □

   e. Next, place numbers in the subscripts such that the total charge of the compound is zero. Note that in this example, we need **two** phosphate ions, each has a charge of (3-) and three Fe^{2+} ions to balance the charge:
   - 2(-3) + 3(+2) = 0 zero total charge.
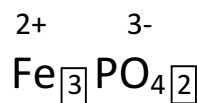
   2+   3-
   Fe□$_3$ PO_4□$_2$

   - We saw a shortcut way to do this called the Criss-Cross Method (see your chapter 3 notes)
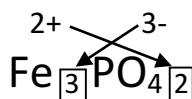
   2+ ⤢ 3-
   Fe□$_3$$PO_4$□$_2$

*IMPORTANT: When there is more than one of a polyatomic ion in the formula unit we use parenthesis. There are **2 ions** of phosphate in iron(II)phosphate.*

Fe□$_3$$PO_4$□$_2$ = $Fe_3(PO_4)_2$
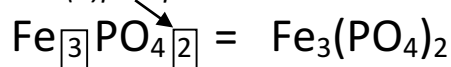
Examples: Writing the Formulas of Ionic Compounds

Write the formula for **barium sulfide**.

1) Write the symbol/formula of the first ion in the compound's name, then the symbol/formula of the second ion in the compound's name.

$$Ba \quad S$$

2) Indicate the ratio of the ions in the compound using subscripts after each ion.

- This step involves filling in the subscripts boxes as we did in the lecture:

$$Ba_\square S_\square$$

- The ratio of the ions is deduced by **balancing the charges** of the ions.
  - This is done so that the **total charge** in the crystal, when large numbers of cations and anions combine, is **equal to zero**.
  - We find the ion's charge from its position on the periodic table **or** we look it up in a table in the case of polyatomic ions.
  - Transition metal with varying charges will be written in the compound name in Roman numerals.

- First, temporarily write the charge of each ion above the ion's symbol.

$$\overset{2+}{Ba_\square} \ \overset{2-}{S_\square}$$

- Next, place numbers in the subscripts such that the total charge of the compound is zero. Note that in this example, we need **one** sulfide ion, with a charge of (2-) to cancel the (2+) charge of the barium ion:
  - (-2) + (+2) = 0 zero total charge.
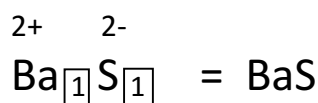
$$\overset{2+}{Ba_{\boxed{1}}} \overset{2-}{S_{\boxed{1}}} \ = BaS$$

- We saw a shortcut way to do this called the Criss-Cross Method (see your chapter 3 notes)

$$\overset{2+}{Ba_{\boxed{2}}} \overset{2-}{S_{\boxed{2}}} \ = BaS$$
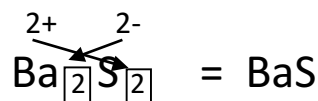
- Note, the subscripts in ionic compound represent the ratio in which large numbers of anions and cations combine to form the ionic compounds. Since we want the **lowest ratio**: we use 1:1, since 2:2 = 1:1

$$\cancel{Ba_2S_2} \ = \ BaS$$
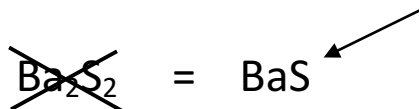
Write the formula for the following ionic compounds: (see next page for key)

sodium bicarbonate _____

sodium fluoride _____

iron (III) chloride _____

sodium carbonate _____

copper (II) sulfate _____

magnesium hydroxide _____

barium nitrate _____

lithium sulfate _____

magnesium chloride _____

silver nitrate _____

aluminum sulfate _____

calcium hydroxide _____

calcium sulfate _____

mercury (II) nitrate _____

lead (IV) nitrate _____

magnesium iodide _____

sodium nitride _____

Practice Problems KEY

sodium bicarbonate $NaHCO_3$

sodium fluoride   NaF

iron (III) chloride $FeCl_3$

sodium carbonate Na_2CO_3

copper (II) sulfate $CuSO_4$

magnesium hydroxide $Mg(OH)_2$

barium nitrate $Ba(NO_3)_2$

lithium sulfate Li_2SO_4

magnesium chloride $MgCl_2$

silver nitrate $AgNO_3$

aluminum sulfate $Al_2(SO_4)_3$

 calcium hydroxide $Ca(OH)_2$

calcium sulfate $CaSO_4$

mercury (II) nitrate $Hg(NO_3)_2$

lead (IV) nitrate $Pb(NO_3)_4$

magnesium iodide MgI_2

sodium nitride Na_3N

Writing the Formulas of Covalent Compounds

1) Write the symbol/formula of the first element in the compound's name, then the symbol/formula of the second element in the compound's name.
2) Indicate how many atoms of each element the molecule contains using subscripts after the atomic symbol.
   - The numbers of atoms are given in the molecule's name in Greek prefixes
   - NOTE: If there is no Greek prefix in front of the first element in the name, that means the number is 1.

Example: Write the formula of **dinitrogen tetrafluoride**.

1) Write the symbol/formula of the first element in the compound's name, then the symbol/formula of the second element in the compound's name.

$$N \quad F$$

2) Indicate how many atoms of each element the molecule contains using subscripts after the atomic symbol.

$$N_\square F_\square$$

   - The numbers of atoms are given in the molecule's name in Greek prefixes.
      - **di**nitrogen **tetra**fluoride
      - see your chapter 3 notes for a list of the Greek prefixes

   $$N_2F_4$$

   - **NOTE**: If there is no Greek prefix in front of the first element in the name, then the number is 1.
      - Example carbon tetrachloride = CCl_4

Example: Write the formula of **carbon disulfide**.

1) Write the symbol/formula of the first element in the compound's name, then the symbol/formula of the second element in the compound's name.

$$C \quad S$$

2) Indicate how many atoms of each element the molecule contains using subscripts after the atomic symbol.

$$C_\square S_\square$$

   - The numbers of atoms are given in the molecule's name in Greek prefixes.
      - carbon **di**sulfide
      - see your chapter 3 notes for a list of the Greek prefixes

   $$C_1S_2 \quad = CS_2$$

   - **NOTE**: If there is no Greek prefix in front of the first element in the name, then the number is 1.

Write the formulas for the following covalent compounds:

See next page for KEY

a. disulfur tetrafluoride   _____

b. carbon trioxide _____

c. nitrogen pentoxide _____

d. nitrogen tribromide _____

e. dinitrogen heptachloride _____

f. carbon tetrachloride_____

g. hydrogen monochloride_____

h. trihydrogen monophosphide _____

i. dihydrogen monoxide _____

a. disulfur tetrafluoride S_2F_4

b. carbon trioxide CO_3

c. nitrogen pentoxide NO_5

d. nitrogen tribromide NBr_3

e. dinitrogen heptachloride N_2Cl_7

f. carbon tetrachloride CCl_4

g. hydrogen monochloride HCl

h. trihydrogen monophosphide H_3P

i. dihydrogen monoxide H_2O

Given the Formulas for Compounds, Write the Name

Determine if the Compound is **Binary Covalent (Molecular)** or **Ionic**:

Does the compound contain **only** *two types of nonmetal elements*?

Yes

No

Binary Covalent (Molecular) Compound:

1) List the name of the first element in the formula.
2) List the second element and add the "ide" suffix.
3) Use Greek prefixes to indicate the number of each atom in the formula.
   - Exception: **Do not use** mono- for the first element in the name.
   - The *o* or *a* at the end of the Greek prefix is dropped when the element name begins with a vowel.

Ionic Compound:

1) Write the cation name first, then name the anion.
   - Monoatomic anions use the "ide" suffix

2) If the cation is one of the metals with various charges, write the charge using parenthesis and Roman numerals after the metal name.

Writing the Names of Ionic Compounds

Example: Write the name for **CaBr$_2$**

1) Write the cation name first, then name the anion.
    - monoatomic anions use the "ide" suffix

calcium bromide

2) If the cation is one of the transition metals with various charges, write the charge using parenthesis and Roman numerals after the metal name.
    - Not necessary here, there is not a transition metal present

Example: Write the name for **Mg(NO$_3$)$_2$**

1) Write the cation name first, then name the anion.
    - monoatomic anions use the "ide" suffix
        - Here we notice that the anion is a **polyatomic ion**. Get the name from the polyatomic ion table (in your notes or textbook). *You will be given a copy of the polyatomic ion table on your exams*.
        - **Do not** change the suffix to "ide" with polyatomic ions:

magnesium nitrate

2) If the cation is one of the transition metals with various charges, write the charge using parenthesis and Roman numerals after the metal name.
    - Not necessary here, there is not a transition metal present

Writing the Names of Ionic Compounds

Example: Write the name for **CuF_2**

1)   Write the cation name first, then name the anion.
   - monoatomic anions use the "ide" suffix

   copper fluoride

2)   If the cation is one of the ***transition metals*** with various charges, write the **charge using parenthesis and Roman numerals** after the metal name.

   copper(?) fluoride

   - We must figure out what the charge is on the copper, we can deduce the charge on the transition metal cations from the charge on the anions
     - Recall that the total charge for any compound must equal zero.
     - Since there are two fluorides, each with a charge of (1-) and there is only one copper, we can conclude that the charge on the copper must be (2+).
       - You can think of this as the reverse criss-cross! See chapter 3 notes for more details.

   copper(II) fluoride

   write the **charge in parenthesis in Roman numerals after the cation name**

Write the names of the following compounds:

See next page for key

NaCl _____

$Fe_2(CO_3)_3$ _____

$Cu(OH)_2$ _____

$(NH_4)_2SO_4$ _____

$LiNO_3$ _____

$BaSO_4$ _____

$Mg(NO_3)_2$ _____

AgCl _____

$Al(OH)_3$ _____

$CaSO_4$ _____

FeS _____

$FeCl_3$ _____

NaI _____

$MgCO_3$ _____

KEY

NaCl   sodium chloride

$Fe_2(CO_3)_3$ iron(III) carbonate

$Cu(OH)_2$ copper(II) hydroxide

$(NH_4)_2SO_4$ ammonium sulfate

$LiNO_3$ lithium nitrate

$BaSO_4$ barium sulfate

$Mg(NO_3)_2$ magnesium nitrate

AgCl   silver chloride

- (note: silver is one of the transition metals that only occurs as a (1+) ion)

$Al(OH)_3$ aluminum hydroxide

$CaSO_4$ calcium sulfate

FeS Iron(II) sulfide

$FeCl_3$ iron(III) chloride

NaI sodium iodide

$MgCO_3$ magnesium carbonate

Writing the Names of Covalent Compounds

1) List the name of the first element in the formula.

2) List the second element and add the –ide suffix.

3) Use Greek prefixes to indicate the number of each atom in the formula.
- Exception: do not use mono- for the first element in the name.
- The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel

Example: Write the name for **N_2S_4**

1) List the name of the first element in the formula.

    nitrogen

2) List the second element and add the –ide suffix.

    nitrogen   sulfide

3) Use Greek prefixes to indicate the number of each atom in the formula.
- See your textbook or lecture notes for a table of the Greek prefixes.

    _____nitrogen   _____sulfide

    dinitrogen   tetrasulfide
- Exception: do not use mono- for the first element in the name.
  - Not applicable in this example
- The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel
  - Not applicable in this example

Example: Write the name for **SO_3**

1) List the name of the first element in the formula.

    sulfur

2) List the second element and add the –ide suffix.

    sulfur   oxide

3) Use Greek prefixes to indicate the number of each atom in the formula.

    _____ sulfur   _____ oxide

    sulfur   trioxide
- Exception: do not use **mono-** for the ***first*** element in the name.
  - NOTE, we did not write **mono**sulfur because of this rule!
- The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel
  - Not applicable in this example

Example: Write the name for **SO$_2$**

1) List the name of the first element in the formula.

      sulfur

2) List the second element and add the –ide suffix.

      sulfur   oxide

3) Use Greek prefixes to indicate the number of each atom in the formula.

      _____ sulfur _____ oxide

      sulfur   dioxide

- Exception: do not use **mono-** for the ***first*** element in the name.
  - NOTE, we did not write **mono**sulfur because of this rule!
- The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel
  - Not applicable in this example

Example: Write the name for **CO**

1) List the name of the first element in the formula.

      carbon

2) List the second element and add the –ide suffix.

      carbon   oxide

3) Use Greek prefixes to indicate the number of each atom in the formula.

      _____ carbon _____ oxide

      carbon   monoxide

- Exception: do not use **mono-** for the ***first*** element in the name.
  - NOTE, we did not write **monocarbon** because of this rule!
- The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel
  - NOTE, we did not write **mono<u>o</u>xide** because of this rule!

Write the names of the following compounds:
See next page for key

    a. Br$_2$I$_4$ _____

    b. P$_5$F$_8$ _____

    c. NO$_5$ _____

- Remember: The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel

    d. NBr$_3$ _____

    e. N$_2$O$_5$ _____

    f. BrCl$_3$ _____

    g. H$_2$S   _____

    h. N$_2$O _____

KEY

a. Br_2I_4 dibromine tetriodide

b. P_5F_8 pentaphosphorus octafluoride

c. NO_5 nitrogen pentoxide
   - The *o* or *a* at the end of the Greek pre-fix is usually dropped when the element name begins with a vowel
     - NOTE, we did not write **pent<u>a</u>oxygen** because of this rule!

d. NBr_3 nitrogen tribromide

e. N_2O_5 dinitrogen pentoxide

f. $BrCl_3$ bromine trichloride

g. H_2S dihydrogen monosulfide

h. N_2O dinitrogen monoxide

Molar Mass Worksheet and Key

For the following compounds, write the chemical formula and determine the molar mass. Write the units!

water

sodium carbonate

carbon dioxide

barium nitrate

sodium chloride

hydrogen monochloride

calcium hydroxide

sulfuric acid (H$_2$SO$_4$)

potassium permanganate (KMnO$_4$)

acetic acid (C$_2$H$_4$O$_2$)

Molar Mass Worksheet Key

Water (H₂O)

Element	Number	MM
H	2	1.01 g/mole
O	1	16.00 g/mole

Total MM = 18.02 g/mole

carbon dioxide, CO₂

Element	Number	MM
O	2	16.00 g/mole
C	1	12.01 g/mole

Total MM = 44.01 g/mole

sodium chloride, NaCl

Element	Number	MM
Cl	1	35.45 g/mole
Na	1	22.99 g/mole

Total MM = 58.44 g/mole

calcium hydroxide, Ca(OH)₂

Element	Number	MM
H	2	1.01 g/mole
O	2	16.00 g/mole
Ca	1	40.08 g/mole

Total MM = 74.10 g/mole

potassium permanganate (KMnO₄)

Element	Number	MM
O	4	16.00 g/mole
Mn	1	54.94 g/mole
K	1	39.10 g/mole

Total MM = 158.04 g/mole

sodium carbonate, Na₂CO₃

Element	Number	MM
O	3	16.00 g/mole
Na	2	22.99 g/mole
C	1	12.01 g/mole

Total MW = 105.99 g/mole

barium nitrate, Ba(NO₃)₂

Element	Number	MM
O	6	16.00 g/mole
Ba	1	137.33 g/mole
N	2	14.01 g/mole

Total MM = 261.35 g/mole

hydrogen monochloride, HCl

Element	Number	MM
Cl	1	35.45 g/mole
H	1	1.01 g/mole

Total MM = 36.46 g/mole

sulfuric acid (H₂SO₄)

Element	Number	MM
S	1	32.07 g/mole
H	2	1.01 g/mole
O	4	16.00 g/mole

Total MM = 98.09 g/mole

acetic acid (C₂H₄O₂)

Element	Number	MM
H	4	1.01 g/mole
O	2	16.00 g/mole
C	2	12.01 g/mole

Total MM = 60.06 g/mole

Moles, Molecules, and Grams Worksheet and Key

Atoms
Or
Molecules

Mass (grams)

Use Avogadro's Number

Use Molar Mass

$1 \text{ mole} = 6.022 \times 10^{23}$

Moles

$\left(\dfrac{\text{grams}}{\text{mole}}\right)$
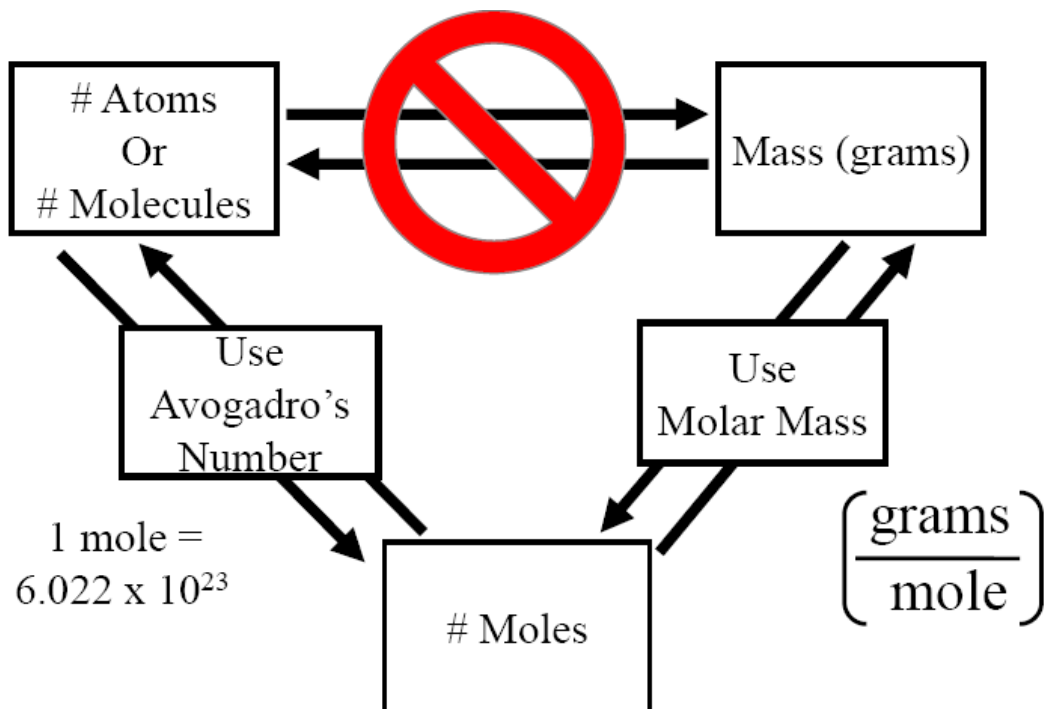
1) How many moles are there in 24.0 grams of FeF_3?

2) How many moles are there in 458 grams of Na_2SO_4?

3) How many grams are there in 2.30×10^{24} atoms of silver?

4) How many grams are there in 7.40 moles of $AgNO_3$?

SEE LAST PAGE FOR KEY

5) How many grams are there in 7.50×10^{23} molecules of H_2SO_4?

6) How many molecules are there in 122 grams of NO_2?

7) How many grams are there in 9.40×10^{25} molecules of H_2?

8) How many molecules are there in 237 grams of CCl_4?

9) How many molecules are there in 2.30 grams of NH_3?

10) How many grams are there in 3.30×10^{23} molecules of N_2I_6?

11) How many moles are there in 2.00×10^{19} molecules of CCl_4?

12) How many grams are there in 1.00×10^{24} molecules of BCl_3?

13) How many grams are there in 4.50 moles of $Ba(NO_2)_2$?

14) How many molecules are there in 9.34 grams of water?

Moles, Molecules, and Grams Worksheet – Answer Key

1) How many moles are there in 24.0 grams of FeF_3? **.213 moles**
2) How many moles are there in 458 grams of Na_2SO_4? **3.22 moles**
3) How many grams are there in 2.30×10^{24} atoms of silver? **412 grams**
4) How many grams are there in 7.40 moles of $AgNO_3$? **1260 grams (note:3 significant figures)**
5) How many grams are there in 7.50×10^{23} molecules of H_2SO_4? **122 grams**
6) How many molecules are there in 122 grams of NO_2? **1.60×10^{24} molecules**
7) How many grams are there in 9.40×10^{25} molecules of H_2? **315 grams**
8) How many molecules are there in 237 grams of CCl_4? **9.28×10^{23} molecules**
9) How many molecules are there in 2.30 grams of NH_3? **8.13×10^{22} molecules**
10) How many grams are there in 3.30×10^{23} molecules of N_2I_6? **433 grams**
11) How many moles are there in 2.00×10^{19} molecules of CCl_4? **3.32×10^{-5} moles**
12) How many grams are there in 1.00×10^{24} molecules of BCl_3? **195 grams**
13) How many grams are there in 4.50 moles of $Ba(NO_2)_2$? **1030 grams (3 significant figures)**
14) How many molecules are there in 9.34 grams of water? **3.12×10^{23} molecules**

Educational Goals

1. Given the formula of a diatomic or small molecule, draw the **line bond structure.**
2. Understand and construct **condensed** and **skeletal structural formulas** given the line bond structures and vice versa.
3. Given the structural formula, determine the **formal charge** of **O** *and* **N** *atoms*.
4. Given the line bond structure of a *small molecule*, predict the **molecular shape** and **bond angle(s)**.
5. Given the structure of a *large molecule*, predict the **bond angle(s)** around any atom.
6. Define **electronegativity** and explain its relationship to *polar covalent bonds*.
7. Give a simple rule that can be used to predict whether or not a *covalent bond* is **polar**.
8. Classify diatomic, small, and large *molecules* as **polar** or **nonpolar**.
9. Describe, compare, and contrast the five **noncovalent interactions**.
10. Describe, compare, and contrast the four classes of **hydrocarbons**.
11. Given the structural formula of an alkane, alkene, or alkyne, be able to give the name and vice versa.
12. Explain the difference between **constitutional isomers**, **conformations**, and the **stereoisomers** known as **geometric isomers**. Give examples of two different classes of hydrocarbons that can exist as geometric isomers.
13. Define the term **functional group** and describe the structural features that distinguish hydrocarbons, alcohols, carboxylic acids, and esters from one another.

Organic chemistry is the chemistry of carbon-containing molecules.

Review: The Octet Rule in the Formation of Molecules

Octet Rule: *Chemical compounds tend to form so that each atom, by gaining, losing, or sharing electrons, has an _____ of electrons in its outermost shell (n).*

Exception to the octet rule _____ and _____.

- *Hydrogen* and *helium* have filled outer shells with just _____ electrons.

Covalent bonding results from the *sharing* of electron pairs between two atoms.

Method for Drawing Line Bond Structures

Step 1: Count the total number of _____ _____ from all the atoms in the molecule.

Example: H_2O

    2 H atoms 2 x $1e^- = 2e^-$

         1 O atom 1 x $6e^- = \underline{6e^-}$

      Total number of valence *e-* = 8e-
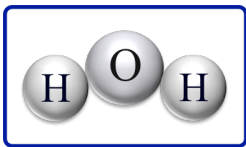
       The line bond structure of H_2O will have 8 electrons

Step 2: Draw the "Skeleton Structure"
   - Attach the atoms together with _____ _____in the most symmetric way possible.

$$H - O - H$$

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

$$\begin{array}{ll} \text{Total number of valence } e^- & 8e^- \\ \textit{Minus} \text{ electrons used in skeleton} & \underline{- 4e^-} \\ \text{Electrons remaining } \textbf{to be added} = & 4e\text{-} \end{array}$$

Step 4: Add the remaining electrons as _____ _____ as evenly as possible on all atoms except hydrogen.

$$\text{H} - \overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{O}}} - \text{H}$$
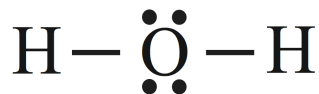
Step 5: Check for _____.

– Are there 8 electrons around all atoms (except hydrogen)?
   If YES, you are finished!

$$\text{H} \overset{\boxed{8}}{\underset{\boxed{6}}{\overset{\boxed{2}}{-}}}\text{O} \overset{\boxed{4}}{-} \text{H}$$
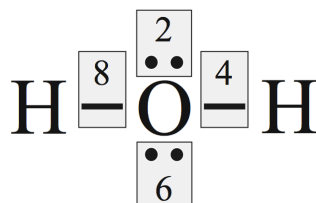
Step 6 (if needed): Use lone pairs to make _____ or _____ bonds until the octet rule is satisfied for *all atoms* in the molecule.

- Let's do a couple of examples to see how that works!
- We will do O_2, and N_2.

Example O_2

Step 1: Count the total number of valence electrons from all the atoms in the molecule.
   - How many **valence electrons** in O_2?
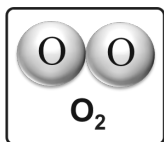
$$\begin{array}{ll} 2 \text{ O atoms} \quad 2 \text{ x } 6e^- = 12e^- \\ \textbf{Total number of valence } e^- = 12e^- \end{array}$$

O O
O_2

Step 2: Draw the "Skeleton Structure"
   -Attach the atoms together with single bonds in the most symmetric way possible.

$$\text{O} - \text{O}$$

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

$$\begin{array}{ll} \text{Total number of valence } e^- & 12e^- \\ \textit{Minus} \text{ electrons used in skeleton} & \underline{- 2e^-} \\ \text{Electrons remaining } \textit{to be added} = & 10e\text{-} \end{array}$$

Step 4: Add the remaining electrons as lone pairs as evenly as possible on all atoms except hydrogen.

$$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{O}}} - \overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{O}}}$$

Step 5: Check for Octets

      − Are there 8 electrons around all atoms (except hydrogen)?

$$:\!\overset{\displaystyle\cdot\cdot}{\underset{\displaystyle\cdot\cdot}{O}} - \overset{\displaystyle\cdot\cdot}{\underset{\displaystyle\cdot\cdot}{O}}\!:$$

      − If NO, use lone pairs to make double or triple bonds.

Step 6 (if needed): Use lone pairs to make **double** or **triple bond**s until the octet rule is satisfied for *all atoms* in the molecule.

double bond

$$:\!\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}} - \overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!: \quad\longrightarrow\quad \overset{\cdot\cdot}{\underset{\cdot\cdot}{O}} = \overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}$$
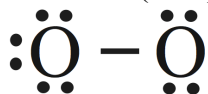
Example N$_2$

Step 1: Count the total number of valence electrons from all the atoms in the molecule.
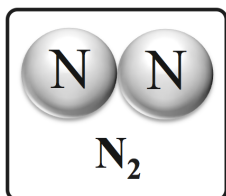
    - How many **valence electrons** in N$_2$?

        2 N atoms   2 x $5e^- = 10e^-$

        Total number of valence e^- = $10e^-$

[N][N] N$_2$

Step 2: Draw the "Skeleton Structure"

    -Attach the atoms together with single bonds in the most symmetric way possible.

$$N - N$$

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

        Total number of valence e^- $10e^-$
      Minus electrons used in skeleton $- 2e^-$
      Electrons remaining *to be added* = $8e-$

Step 4: Add the remaining electrons as lone pairs as evenly as possible on all atoms except hydrogen.

$$\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}} - \overset{\cdot\cdot}{\underset{\cdot\cdot}{N}}$$
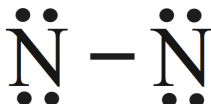
Step 5: Check for Octets

      − Are there 8 electrons around all atoms (except hydrogen)?

      − If NO, use lone pairs to make double or triple bonds.

Step 6 (if needed): Use lone pairs to make **double** or **triple bond**s until the octet rule is satisfied for *all atoms* in the molecule.

triple bond

$$\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}} - \overset{\cdot\cdot}{\underset{\cdot\cdot}{N}} \;\Rightarrow\; \overset{\cdot\cdot}{\underset{\cdot\cdot}{N}} = \overset{\cdot\cdot}{\underset{\cdot\cdot}{N}} \;\Rightarrow\; :\!\underset{\cdot\cdot}{N} \equiv \underset{\cdot\cdot}{N}\!:$$

Draw the line bond structure for ammonia: **NH₃**

Step 1: **Count the total number of valence electrons from all the atoms in the molecule.**	Step 2: **Draw the "Skeleton Structure"**
Molecular formula of molecule _____ <table><tr><td>Atom</td><td>Number of atoms</td><td></td><td>Number of valence electrons per atom</td><td>Totals</td></tr><tr><td>N</td><td>1</td><td>x</td><td></td><td>=</td></tr><tr><td>H</td><td>3</td><td>x</td><td></td><td>=</td></tr></table> Total # of electrons in line bond structure =_____	-Attach the atoms together with single bonds in the most symmetric way possible. Central atom is:_____ Draw skeleton: # of electrons used in skeleton = _____ (multiply # of bonds in skeleton by 2)
Step 3: **Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons**. Total # of electrons in structure _____ (from step 1 above) # of electrons used in skeleton - _____ (from step 2 above) Remaining # electrons to be added= _____	Step 4: **First:** Re-draw skeleton here: **Next, Add the remaining electrons as <u>lone pairs</u> as evenly as possible on all atoms except hydrogen.**
Step 5: **Check for Octets** Check the structure in step 4 for octets of electrons around each atom (except for hydrogen). If the octet rule is satisfied, **you are done**. If the octet rule is **<u>not</u>** satisfied, go the **Step 6**.	Step 6 (if needed): Use lone pairs to make **double** or **triple** bonds until the octet rule is satisfied for all atoms in the molecule.

Understanding Check: Draw the line bond structure for sulfur trioxide: **SO₃**

Step 1: Count the total number of valence electrons from all the atoms in the molecule.	**Step 2: Draw the "Skeleton Structure"** -Attach the atoms together with single bonds in the most symmetric way possible.
Molecular formula of molecule _____	Central atom is:_____

<table>
<tr><td>Atom</td><td>Number of atoms</td><td></td><td>Number of valence electrons per atom</td><td>Totals</td></tr>
<tr><td></td><td></td><td></td><td></td><td>=</td></tr>
<tr><td></td><td></td><td></td><td></td><td>=</td></tr>
</table>

Draw skeleton:

Total # of electrons in line bond structure =_____

# of electrons used in skeleton = _____
(multiply # of bonds in skeleton by 2)

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.	**Step 4: First:** Re-draw skeleton here:
Total # of electrons in structure _____ (from step 1 above)	
# of electrons used in skeleton - _____ (from step 2 above)	**Next, Add the remaining electrons as lone pairs as evenly as possible on all atoms except hydrogen.**
Remaining # electrons to be added= _____	

Step 5: Check for Octets Check the structure in step 4 for octets of electrons around each atom (except for hydrogen).	**Step 6 (if needed):** Use lone pairs to make **double** or **triple** bonds until the octet rule is satisfied for all atoms in the molecule.
If the octet rule is satisfied, **you are done**. If the octet rule is **not** satisfied, go the **Step 6**.	

Structural Formulas

A **molecular formula** shows us the number and types of atoms contained in a molecule.

- **Example** of a *molecular formula*: H_2O

Drawings, such as *line bond structures*, that show the _____ of atoms within molecules are called _____ **formulas.**

- **Example** of a *structural formula*: $H-\overset{\displaystyle ..}{\underset{\displaystyle ..}{O}}-H$

Structural Formulas vs. Molecular Formulas

The **molecular formula** of *isopropyl alcohol* (often called rubbing alcohol) is C_3H_8O.

The **structural formula** of *isopropyl alcohol* is:
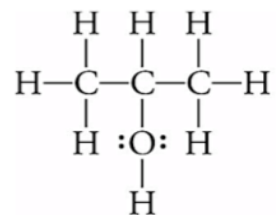
Which of these two types of formulas, the **molecular formula** or the **structural formula**, do you think is more informative?

There are actually **three** *completely different molecules* that have this same molecular formula of C_3H_8O:

isopropyl alcohol   1-propanol   ethyl methyl ether
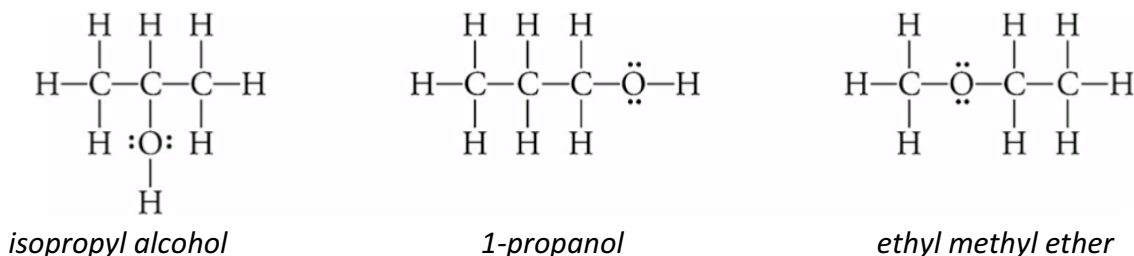
Line bond structural formulas **explicitly** show all the information about how the atoms are connected and the presence of all single bonds, double bonds, triple bonds and lone pairs.

In practice, chemists often use one of two **short-cut** forms of structural formulas:

- _____ *structural formulas*

or

- _____ *structural formulas*

Condensed Structural Formulas (Condensed Structures)

When drawing **condensed structures**:
- Single bonds between carbon and hydrogen *are omitted*.
  - **Example:** a carbon bonded to three hydrogen atoms is drawn as "**CH₃**"
- Single bonds between carbons (C-C) *can be* omitted.
- Single bonds between oxygen or nitrogen *and* hydrogen *can be* omitted.
  - **Example:** an oxygen bonded to one hydrogen atom can be drawn as "**OH**."
- Bonds between *all other* pairs of atoms **must** be drawn.
- Lone pairs *can be* omitted.
- Double and triple bonds *are always drawn*.

Example: Propane (C_3H_8)

The **connectivity** of the carbon and hydrogen atoms can be seen _____ in propane's *line bond structure*:

$$
\begin{array}{ccccc}
 & H & H & H & \\
 & | & | & | & \\
H- & C & -C & -C & -H \\
 & | & | & | & \\
 & H & H & H &
\end{array}
$$
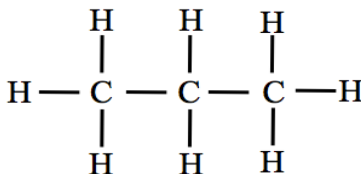
In *condensed structures*, _____ bonds between carbon and hydrogen atoms *are omitted*. We can draw the condensed structure of propane as:

$$CH_3-CH_2-CH_3 \quad \underline{or} \quad CH_3\diagdown_{CH_2}\diagup CH_3$$
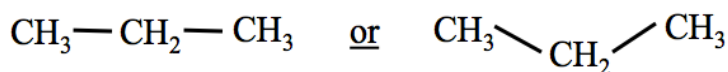
When drawing condensed structures, carbon-carbon single bonds can be omitted when the carbon atoms are in a _____ _____ such as the three carbons in propane:

$$CH_3CH_2CH_3$$
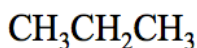
Even though not all of the bonds are drawn in condensed structures, they are _____ and can be *unequivocally* known.

Example: Isopentane (C_5H_{12})
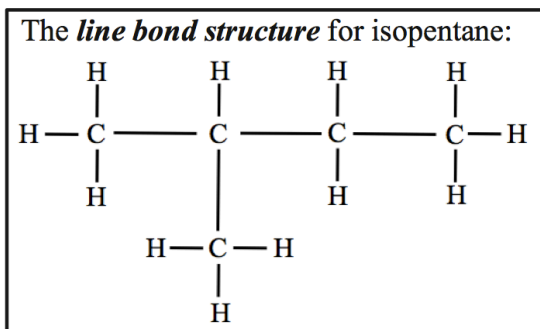
The *line bond structure* for isopentane:

$$
\begin{array}{ccccccc}
 & H & & H & & H & & H \\
 & | & & | & & | & & | \\
H- & C & - & C & - & C & - & C-H \\
 & | & & | & & | & & | \\
 & H & & | & & H & & H \\
 & & H- & C & -H & & & \\
 & & & | & & & & \\
 & & & H & & & &
\end{array}
$$

In isopentane, there are four carbons bonded in a *linear sequence*.

There is one carbon that "_____" from the *linear sequence*.

In *condensed structures*, **single bonds** between carbon and hydrogen atoms *are omitted*. We can draw the condensed structure of isopentane as:
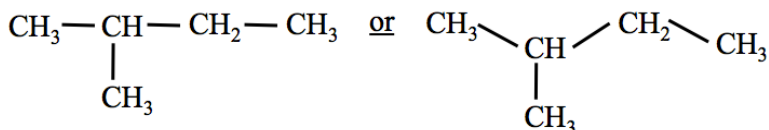
$$CH_3-CH-CH_2-CH_3 \quad \underline{or} \quad CH_3\diagdown_{CH}\diagup CH_2\diagdown CH_3$$
$$\quad\quad\quad | \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad |$$
$$\quad\quad\quad CH_3 \quad\quad\quad\quad\quad\quad\quad\quad\quad CH_3$$

Further condensation is possible.
- *Single bonds* between **carbon** atoms *in a linear sequence* can be omitted as in the case of the four carbons in a **linear sequence** in isopentane (as shown below).

$$CH_3-CH-CH_2-CH_3 \quad \Longrightarrow \quad CH_3CHCH_2CH_3$$
$$\quad\quad\quad | \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad |$$
$$\quad\quad\quad CH_3 \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad CH_3$$
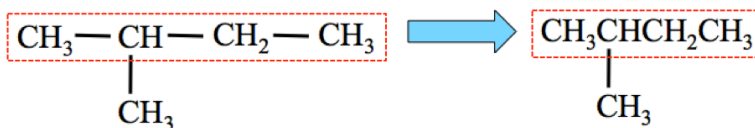
If you **are not** a Saddleback College student, check with your instructor as to which form of condensed structures she/he wishes you to use.

Example: Isopropyl bromide (C₃H₇Br)

The *line bond structure* of isopropyl bromide is:
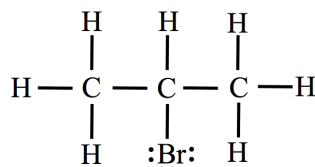
In *condensed structures*, single bonds between atom pairs *other than* **C-C**, **C-H**, **O-H**, and **N-H** are *always drawn*.

-   Therefore the **C-Br** bond is drawn in the condensed structures:
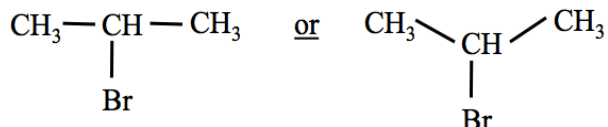
-   Lone pairs *can be omitted* in condensed structures.

Further condensation is possible.

-   *Single bonds* between **carbon** atoms *in a linear sequence* can be omitted as in the case of the three carbons in a **linear sequence** in isopropyl bromide.
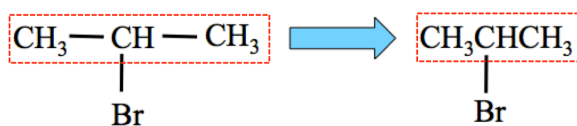
Skeletal Structural Formulas (Skeletal Structures)

Another *structural formula* that chemists use in order to more easily and quickly draw molecules is called the _____ **structure**.

When drawing **skeletal structures**:

-   Carbons are not drawn; they are *implied* to exist where lines (bonds) _____ or at the _____ of a line (bond).
-   Hydrogens are *omitted* **if** they are bonded to carbon.
-   Bonds between oxygen or nitrogen *and* hydrogen may be omitted.
-   Atoms other than carbon and hydrogen are *always* drawn.
-   Lone pairs *can be* omitted.

Example: Propane (C₃H₈)
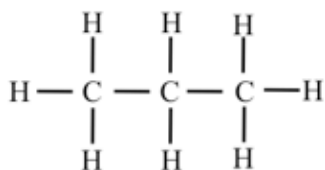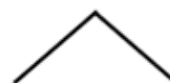
If the hydrogens bonded to carbon are omitted from skeletal structures, how do we determine how many hydrogens are bonded to each carbon? The answer to this is quite simple and is related to the octet rule:

-   We *never* find *lone pairs* on carbon in any molecule that contains more than one carbon atom.

-   The octet rule requires that carbons will **always** have *four pairs of shared electrons around them*, therefore we can deduce the number of *hydrogens* that are bonded to each carbon in a skeletal structure.

Example: 2-Fluorobutane
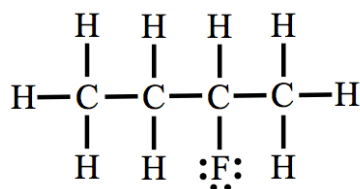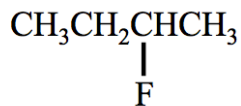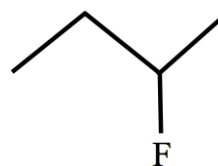
Line Bond Structure   Condensed Structure   Skeletal Structure

Example: Ethanol
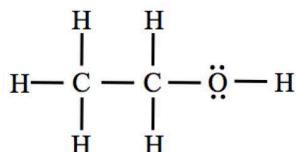
Line Bond Structure   Condensed Structure   Skeletal Structure
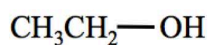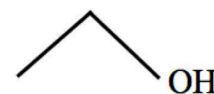
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Understanding Check: Draw **condensed** *and* **skeletal structur** of diethyl ether.

diethyl ether
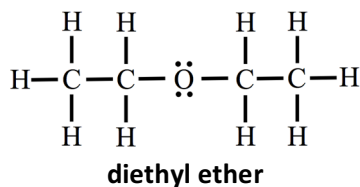
Understanding Check: Draw **condensed** *and* **skeletal structure** of ethylamine.

ethylamine

9
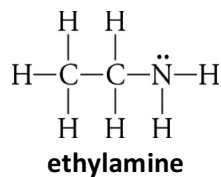
Understanding Check: The line bond structure of a large hydrocarbon molecule is shown below. Draw the **condensed structure** **and** the **skeletal structure** of this molecule.
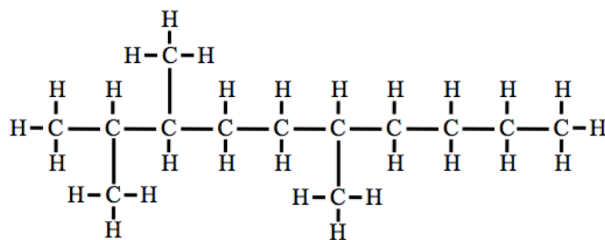
Structural Formulas of Cyclic Compounds

Many compounds contain atoms bonded, not in a *linear sequence*, but in a "**ring**" pattern.

Molecules that contain rings of atoms are called _____ compounds.

- An example of a *cyclic compound* is a molecule called cyclohexane. The three structural formulas for cyclohexane are:
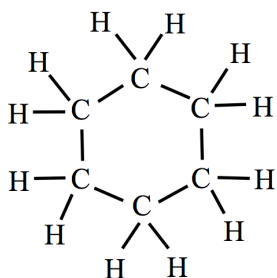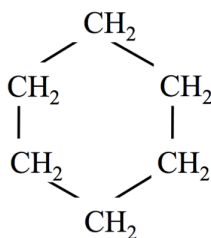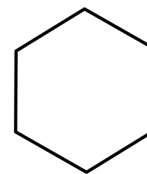
| Line Bond Structure | Condensed Structure | Skeletal Structure |

Molecular Geometry

Let's define **molecular geometry** as the _____ *arrangement* of a molecule's atoms.

Molecules very rarely take the shapes that are drawn in their structural formulas.

Structural formulas, whether line bond, condensed, or skeletal, are either **one-** or **two-dimensional**.

Most molecules are _____ *dimensional*.

- Line bond structures are commonly drawn with the lines/bonds at 90° angles, but the **bond angles** in molecules (the angle between covalent bonds), with rare exceptions, are not at 90°.

- Skeletal and condensed structures often use bond angles of 90° or approximately 120° only for convenience in depicting the bonding pattern connectivity, not necessarily to represent the actual bond angles/geometry of the molecule.

Example: Fentanyl

The *skeletal structure* of fentanyl is:
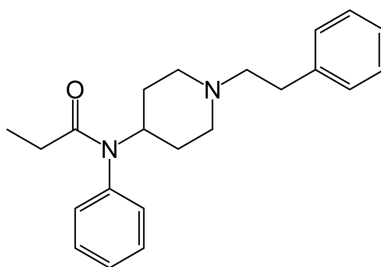
The "*geometry*" of the molecule can be depicted in two types of views:

ball-and-stick model

space-filling model
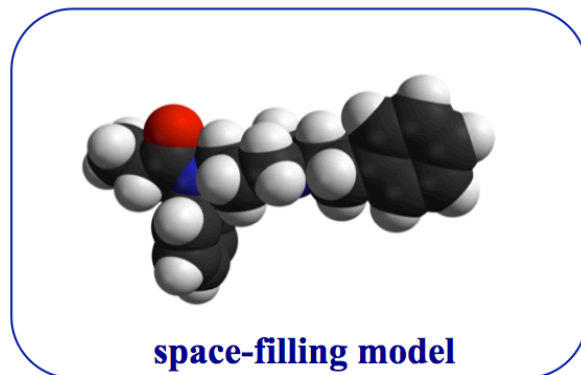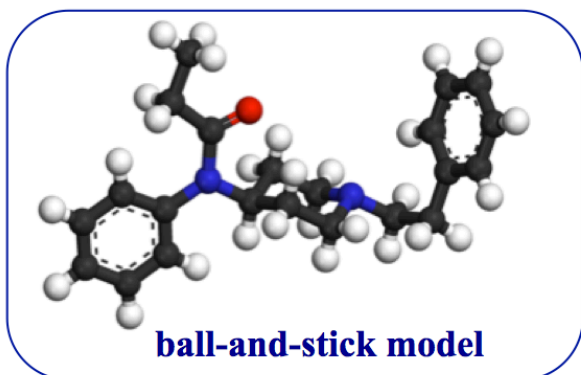
Definition: a _____ _____ is the angle between two covalent bonds.

Structural formulas, whether line bond, condensed, or skeletal, *do not **explicitly** show the* _____ *bond angles within molecules.* However, **the actual bond angles can be** _____ **from a molecule's structural formula**.
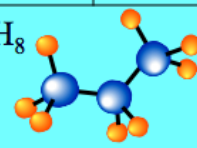
To know the *exact* molecular geometry, we must know all of the **bond angles** *and* **bond lengths** (distance between bonded atoms) within a molecule.

ball-and-stick model of fentanyl
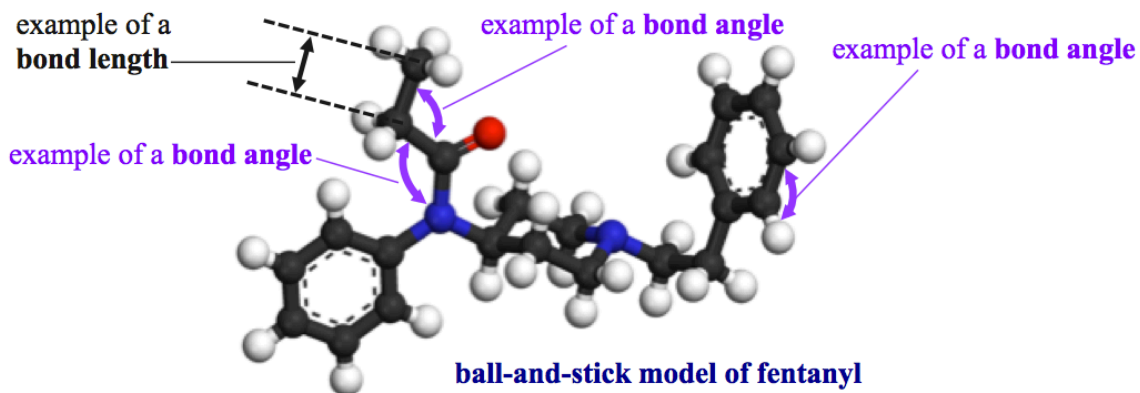
We will **ignore** variations in bond lengths since these relatively minor deviations in length *do not significantly affect the concepts to be discuss*ed.

Therefore, for our purposes, *predicting molecular geometry will be equivalent to predicting the **bond angles** within a molecule*.

When discussion molecular geometry and other concepts in this course, we will often use the following molecular size categories:

Molecular Size Category	Description	Example(s)	
Diatomic Molecule	Molecule contains **only two atoms**	H_2	HCl
Small Molecule	Molecule has **one central atom** with **all other** atoms bonded to the central atom	CH_4	H_2O
Large Molecule	Larger than *Small Molecule*; there **is not just one single, central atom** with **all** the other atoms bonded to it	C_3H_8	

For **diatomic molecules**, the geometry of the molecule is always _____; the two atoms that make up the molecule exist on the same **line**.

- Examples: H_2 and HCl

For small and large molecules: **bond angles** can be predicted from the _____ *formula* using a model called **Valence Shell Electron Pair Repulsion (VSEPR) Theory.**

Valence Shell Electron Pair Repulsion (VSEPR) Theory: Predicting Bond Angles

The bond angles around *any particular atom of interest* in a molecule can be predicted because the **groups of electrons** surrounding this atom **will** _____ *each other*.

- These _____ _____ (abbreviated as **EG**) consist of, as the name implies, groups of electrons that are localized to a certain area.
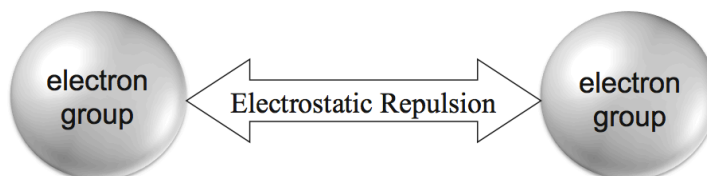
You can easily recognize an **EG** by looking for one of the following:

(1) **A** _____ _____ (an atom **bonded to** the *atom of interest*).
- Each *bonded atom* counts as **one** electron group.
- Whether the bonded atom is connected to the atom of interest with a **single**, **double**, or **triple bond**, *all of these shared electrons are localized within a particular region and therefore count as **one EG**.*

(2) **A** _____ _____ (**on** the *atom of interest*).
- Each lone pair counts as *one electron group* (EG
- Even though lone pairs are not attached to other atoms, they do occupy a localized area around the atom of interest and therefore repel other electron groups.

Example: 2 Electron Groups

What do you think will happen to these two balloons if they both have a negative charge?
Draw the balloons inside the right-most sphere.
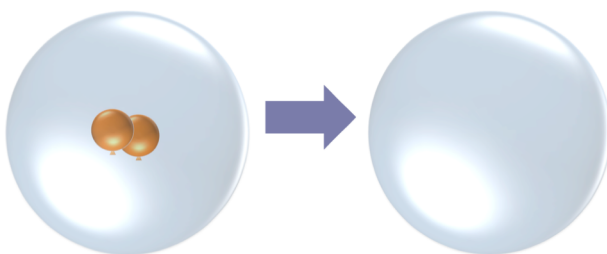
Electrostatic _____ will cause the balloons to move as far apart from each other as possible.

The same thing happens with _____ _____.

Draw the line bond structure for **CO_2**.

The central atom (C) goes in the _____ of the sphere.
- There are _____ electron groups around the central atom!
- Each bonded atom counts as _____ electron group.

The electron groups are placed as _____ apart from each other as possible!

Both electron groups are on the same _____ and are at a _____ angle.

180°
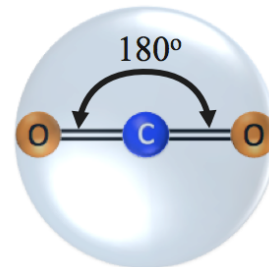
Example: 3 Electron Groups
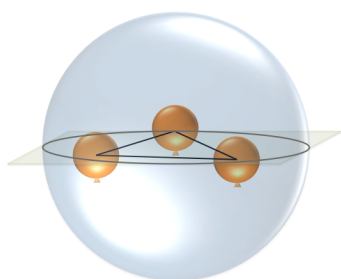
If 3 negatively charged balloons are placed into a hollow, clear plastic sphere, electrostatic repulsion will cause the balloons to move as far apart from each other as possible.

The same thing happens with *electron groups*.

Draw the line bond structure for **SO_3**.

The central atom (S) goes in the middle of the sphere.

There are _____ electron groups around the central atom!

All electron groups are on the same _____ and are at _____ angles.

120°

13
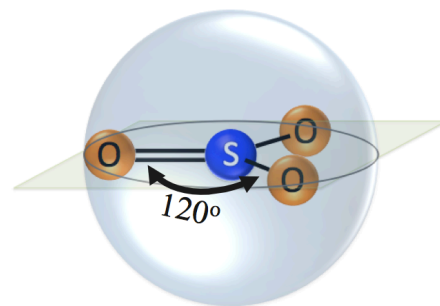
Example: 4 Electron Groups
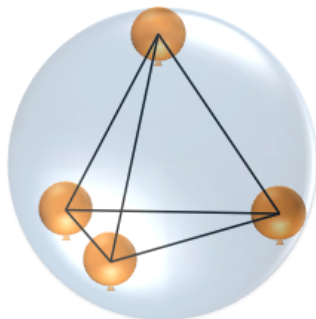
If 4 negatively charged balloons are placed into a hollow, clear plastic sphere, electrostatic repulsion will cause the balloons to move as far apart from each other as possible.

The same thing happens with *electron groups*.

Draw the line bond structure for a methane molecule (CH_4).

The central atom (C) goes in the middle of the sphere.
How many electron groups are around the central atom?
There are **4** electron groups around the central atom!
The electron groups are placed as far apart from each other as possible!
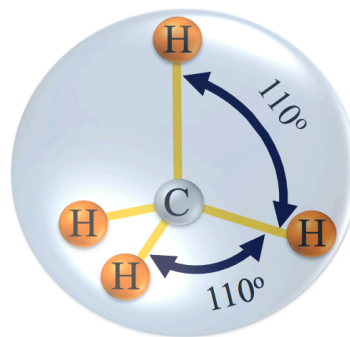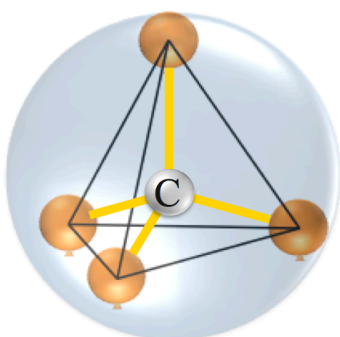
This arrangement is a 4-sided, 3-dimensional structure with electron groups at about _____ angles.

Electron Arrangement Review

180°
EG   EG

2 Electron Groups

EG
EG   EG
120°

3 Electron Groups

EG
110°
EG   EG
110°
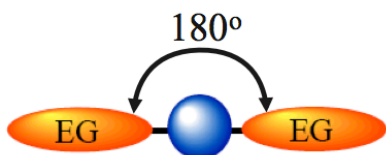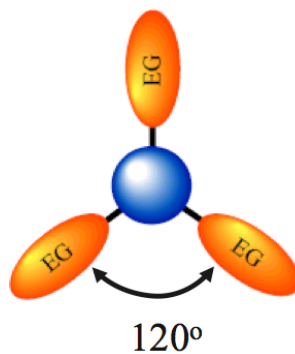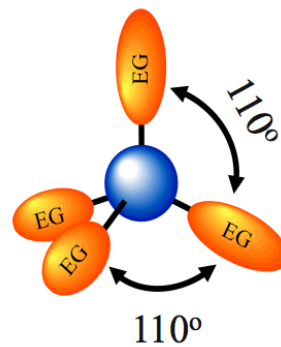
4 Electron Groups

For three or four electron groups, the angles will deviate slightly from **120°** and **110°** when one (or more) of the electron groups is a **lone pair**.

- In this course, these slight deviations in bond angles can be *ignored* because their effects are **not significant** in the chemistry that will be discussed.
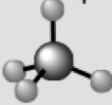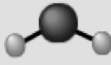
The Geometry of Diatomic Molecules

Molecular Size Category	Description	Example(s)	
Diatomic Molecule	Molecule contains **only two atoms**	H_2	HCl

For *diatomic molecules*, the geometry of the molecule is always **linear**; the two atoms that make up the molecule exist on the same line.
- Since there is only one bond (whether single, double, or triple), it does not make sense to talk about a bond angle.
- To discuss a bond angle, there must be two bonds originating from the same atom.

The Molecular Shape of Small Molecules

Molecular Size Category	Description	Example(s)	
Small Molecule	Molecule has <u>**one**</u> **central atom** with *all other* atoms bonded to the central atom	CH_4	H_2O

For *small molecules*, there exists one **central atom** with all other atoms bonded to the central atom, therefore the *only* bond angles that exist are between bonds _____ from the **central atom**.

This simplified geometry allows us to categorize (name) particular ***molecular*** _____ seen in **small molecules**.

Given the line bond structure, small molecules can be categorized by their **molecular shape** as follows:

Step 1. Get the Electron Group Arrangement

Find the *angle* between the electron groups and their arrangement around the **central atom**.
- **Two electron groups:** 180° angle, both electron groups are on the same line as the central atom.
- **Three electron groups:** 120° angles, all electron groups are on the same plane as the central atom.
  - Angles will deviate **slightly** from 120° if *one of the electron groups* is a ***lone pair***
- **Four electron groups:** 110° angles, occupies three dimensions in space.
  - Angles will deviate **slightly** from 110° if *one or more of the electron groups* is a ***lone pair***

**Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.**
Small molecules are categorized according to the arrangement of the atoms **only**.

Although **lone pairs** are also electron groups and are therefore important in determining the electron group arrangement in Step 1, they are treated as being "_____" when assigning molecular shape category names.

Draw the line bond structure of CO_2

Example: The Molecular Shape of CO_2

Step 1. Get the Electron Group Arrangement

How many electron groups are around the central atom? ___

What is the bond angle in a 2-electron group arrangement?
     Choices: a) $180°$ b) $120°$ c) $110°$

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

$180°$
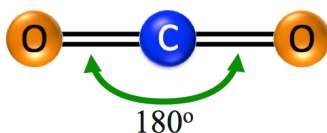
This molecular shape is called _____.

A very helpful tool for determining **molecular shape** is called the "**ABE Method**."
    "**A**" represents the central atom (**carbon** in our CO_2 example).
    "**B**" represents atom(s) bonded to the *central atom*.
         (each **oxygen** in our CO_2 example)
    "**E**" represents lone pair(s) *on the central atom*.
         (none seen in CO_2 since there are no lone pairs *on the central atom*)
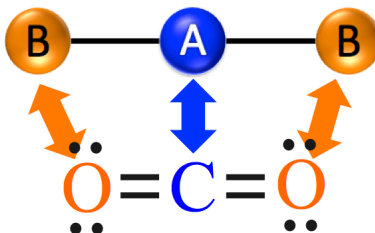
The **ABE** Method uses a "general notation" that indicates the type and number of
_____   _____ (**B** or **E**) that surround the central atom (**A**).

We write the **ABE** Method notation for CO_2 and *all* other small molecules that have *two* **bonded atoms** and *no* lone pairs *on the central atom* as "_____."

• There are two oxygens bonded to the central atom therefore we write "**B₂**."

All AB₂ molecules have _____ **bond angles** and are in the _____ **molecular shape** category.
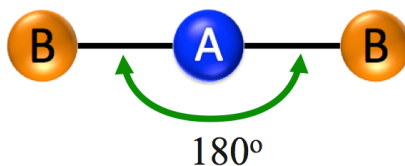
$180°$

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Molecular Shape Table

Number of Lone Pairs

	0 Lone Pairs	1 Lone Pair	2 Lone Pairs
2 EG			
3 EG			
4 EG			

Number of Electron Groups (EG)

Three Electron Groups

Example: Draw the line bond structure of **SO_3**

Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

EG

EG   EG

120º

3 Electron Groups
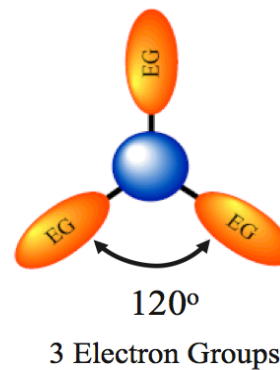
Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.
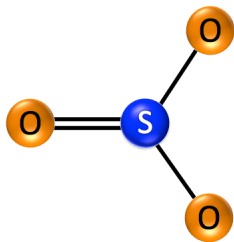
This molecular shape is called _____ _____.

We write the **ABE** Method notation for SO_3 and *all* other small molecules that have *three* **bonded atoms** and *no* lone pair *on the central atom* as "_____."

- There are three oxygens bonded to the central atom therefore we write "**B₃**."

All AB₃ molecules have _____ bond angles and are in the ***trigonal planar*** molecular shape category.
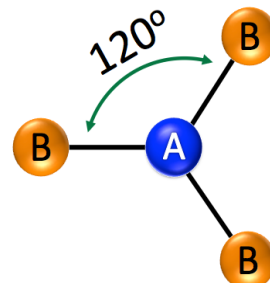
> **Example:** Draw the line bond structure of **ozone gas (O_3).**

Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

  - **Three electron groups:** $120°$ angles, all electron groups are on the same plane as the central atom. Angles will deviate **slightly** from $120°$ if *one of the electron groups* is a ***lone pair***.
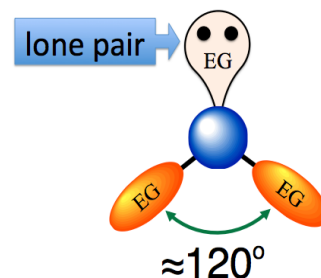
Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.
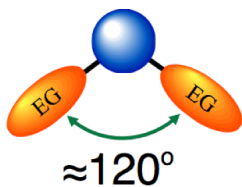
- When determining **molecular shape**, we treat lone pair(s) as if they were **invisible**!

This molecular shape is called _____.

We write the **ABE** Method notation for O_3 and *all* other small molecules that have *two* **bonded atoms** and *one* lone pair *on the central atom* as "_____."

- There are two oxygens bonded to the central atom therefore we write "**B₂**."
- There is **one lone pair** on the *central atom* therefore we write "**E**."

All AB₂E molecules have _____ bond angles and are in the ***bent*** molecular shape category.
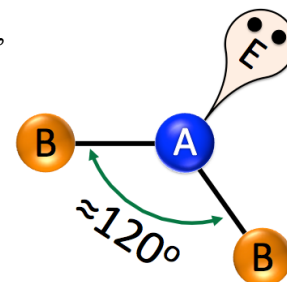
Four Electron Groups

> **Example:** Draw the line bond structure of **methane gas (CH_4).**

Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

  - **Four electron groups:** 110° angles, occupies three dimensions in space

$110°$
$110°$

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

This molecular shape is called _____ .

We often use a _____ _____ _____ representation in order to illustrate a three-dimensional molecule on a two-dimensional surface such as a page or computer screen.
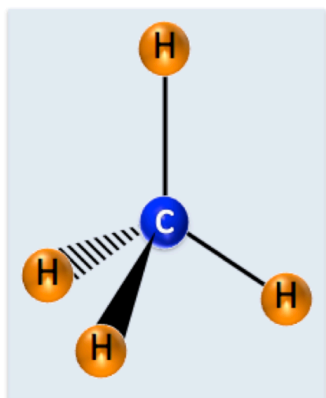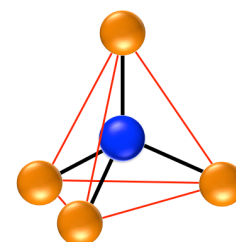
a wedge and dash representation
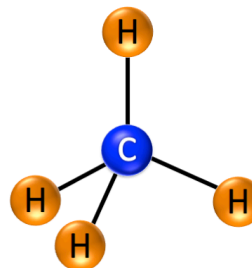
a perspective representation
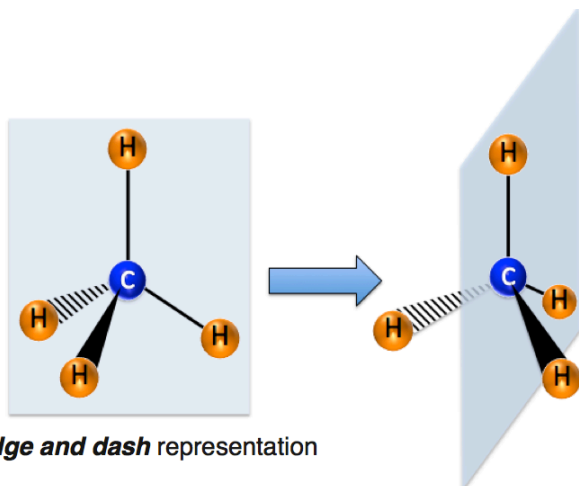
a wedge and dash representation

The implication of a wedge and dash representation

Solid wedges indicate bonds that would be coming *out and above* the page (toward the viewer) in the three-dimensional object.

Dashed shapes indicate bonds that would be coming *out and behind* the page (away from the viewer) in the three-dimensional object.

Regular lines (neither wedge nor dash) indicate bonds that exist on the plane of the page in the three-dimensional object.

19
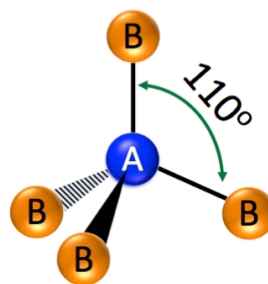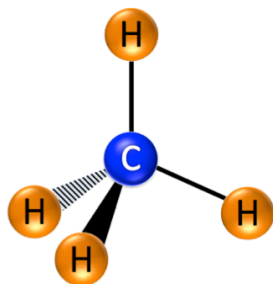
We write the **ABE** Method notation for CH_4 and **all** other small molecules that have **four** bonded atoms and **no** lone pair *on the central atom* as "_____."

- There are four hydrogens bonded to the central atom therefore we write "**B₄**."

All **AB₄** molecules have _____ **bond angles** and are in the **tetrahedral** molecular shape category.

Four Electron Group Example: Consider the line bond structure of **ammonia (NH₃).**
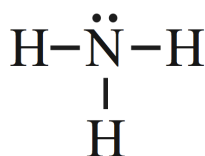
$$H-\ddot{N}-H$$
$$|$$
$$H$$

Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

  - **Four electron groups:** $110°$ angles, occupies three dimensions in space. Angles will deviate **slightly** from $110°$ if *one or more of the electron groups* is a **lone pair**.
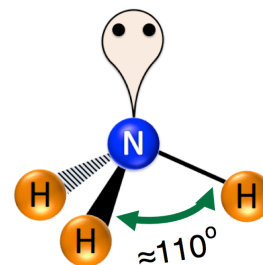
Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.
- When determining **molecular shape**, we treat lone pair(s) as if they were **invisible**!
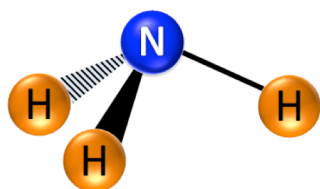
This molecular shape is called _____.
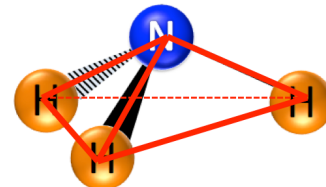
We write the **ABE** Method notation for NH_3 and **all** other small molecules that have **three** bonded atoms and **one** lone pair *on the central atom* as "_____."
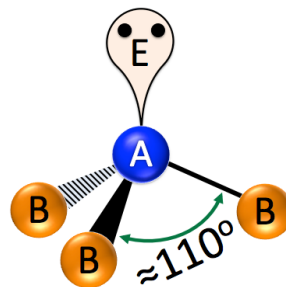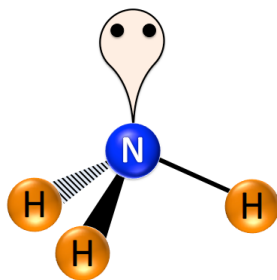
- There are three hydrogens bonded to the central atom therefore we write "**B₃**."
- There is **one lone pair** on the *central atom* therefore we write "**E**."

All **AB₃E** molecules have _____ **bond angles** and are in the **pyramidal** molecular shape category.

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Four Electron Group Example: Consider the line bond structure of a **water molecule (H_2O):**

$$H - \overset{\cdot\cdot}{\underset{\cdot\cdot}{O}} - H$$

Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

  - **Four electron groups:** 110° angles, occupies three dimensions in space. Angles will deviate **slightly** from 110° if *one or more of the electron groups* is a **lone pair**.

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

- When determining **molecular shape**, we treat lone pair(s) as if they were **invisible**!

  This molecular shape is called _____.

We write the **ABE** Method notation for H_2O and *all* other small molecules that have *two* bonded atoms and *two* lone pairs *on the central atom* as "_____."
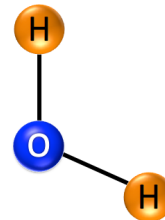
- There are two hydrogens bonded to the central atom therefore we write "**B₂**."
- There are **two lone pairs** on the *central atom* therefore we write "**E₂**."

All AB₂E₂ molecules have _____ bond angles and are in the **bent** molecular shape category.

Molecular Shape Table
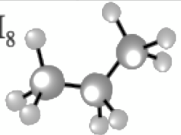
Number of Lone Pairs

	0 Lone Pairs	1 Lone Pair	2 Lone Pairs
2 EG	AB_2 Linear — $180°$		
3 EG	AB_3 Trigonal Planar — $120°$	AB_2E Bent — $\approx 120°$	
4 EG	AB_4 Tetrahedral — $110°$	AB_3E Pyramidal — $\approx 110°$	AB_2E_2 Bent — $\approx 110°$

Number of Electron Groups (EG)

Understanding Check: Molecular Shapes for Small Molecules

Determine the **bond angles** (or approximate bond angles) and the **molecular shape** category for each of the following *small molecules*:

a) NF_3

b) H_2S

c) SO_2

d) CS_2

e) carbon tetrachloride

The Molecular Geometry of Large Molecules

	Larger than *Small Molecule*; there is **not** just one single, central atom with **all** the other atoms bonded to it	C_3H_8
Large Molecule		

The **bond angles** around any _____ *of interest* in a **large molecule** can be predicted in the same manner that we used for small molecules.

- Simply use the **ABE** method, but in this case let "**A**" represent the *atom of interest* in the large molecule instead of the central atom of a small molecule.

Example: Consider the line bond structure of an ethane molecule:

$$H-\underset{\underset{H}{|}}{\overset{\overset{H}{|}}{C}}-\underset{\underset{H}{|}}{\overset{\overset{H}{|}}{C}}-H$$
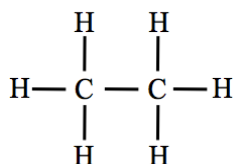
What are the **bond angles** around **each** of the **carbon atoms** in an ethane molecule?

The Geometry of Large Molecules: ABE Method

ABE Class	Bond Angles
AB_2	180°
AB_3	120°
AB_2E	≈ 120°
AB_4	110°
AB_3E	≈ 110°
AB_2E_2	≈ 110°

The Geometry of Large Molecules: ABE Method
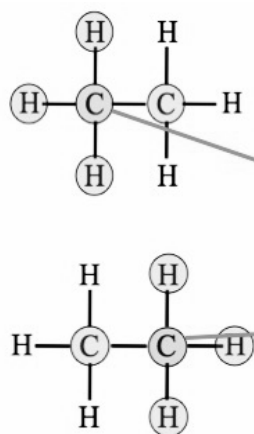
ABE Class	Bond Angles
AB_2	180°
AB_3	120°
AB_2E	≈ 120°
AB_4	110°
AB_3E	≈ 110°
AB_2E_2	≈ 110°
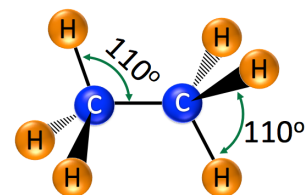
The illustration on the right shows the significance of lines, wedges, and dashes implied in the wedge and dash representation of the ethane molecule.
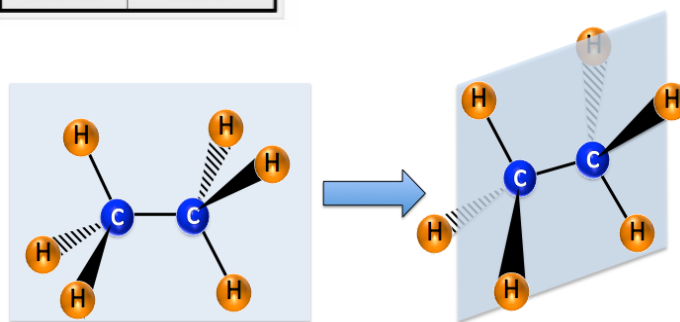
You may have noticed that we only discussed **molecular geometry (*bond angles)*** for *large molecules*; we do not categorize large molecules by "*molecular shape*" as we did for small molecules.

The reason for this is that _____ bonds can "_____" and therefore large molecules are **always *changing their shape***.

It is important to understand that although single bonds are capable of rotation, ***the bond angles around any particular atom do not change upon rotation***.

Only single bonds freely rotate; because of the nature of ***double* and *triple bonds***, they *do not* rotate.
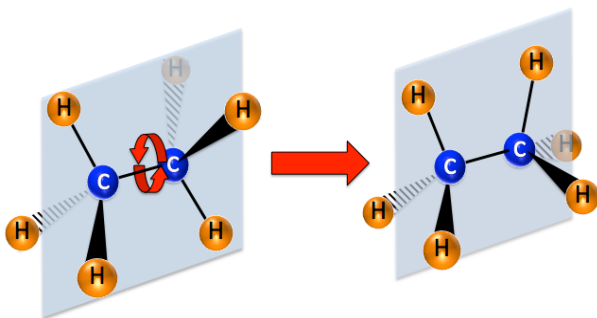
Another example for the geometry of large molecules: Consider the line bond structure of an *ethanol* molecule (shown on the right).

What is the bond angle for the bonds coming from ***the oxygen atom*** in an ethanol molecule?

$$H - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - \overset{..}{\underset{..}{O}} - H$$

The Geometry of Large Molecules: ABE Method	
ABE Class	**Bond Angles**
AB$_2$	180°
AB$_3$	120°
AB$_2$E	≈ 120°
AB$_4$	110°
AB$_3$E	≈ 110°
AB$_2$E$_2$	≈ 110°
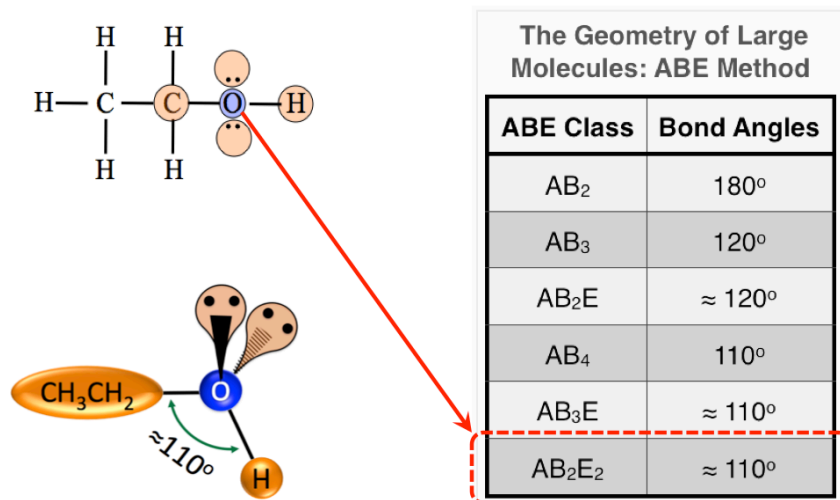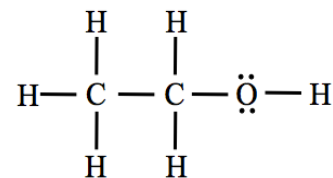
Understanding Check: Predicting Bond Angles in Large Molecules

Consider the line bond structure of an acetone molecule:

$$H - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - \overset{\displaystyle :O:}{\overset{||}{C}} - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - H$$
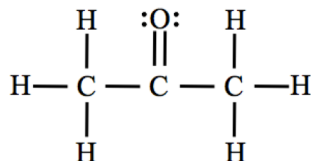
a) What are the bond angles around the left-most carbon atom?
b) What are the bond angles around the carbon atom in the middle of the molecule?
c) What are the bond angles around the right-most carbon atom?

Reflection and Looking Forward

You have seen how the connectivity of atoms shown in structural formulas, such as line bond structures, can be used to determine molecular geometries (bond angles).
For example:

$$H - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - \overset{\displaystyle H}{\underset{\displaystyle H}{\overset{|}{\underset{|}{C}}}} - H$$
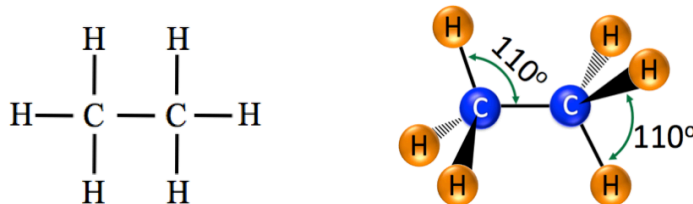
The molecular geometries are quite important because the observed (macroscopic) properties of a molecular compound are related to its **nanoscopic** structure. The *nanoscopic* structure of molecules includes details such as the kind of atoms, the pattern in which they are **bonded** to each other, the molecular geometry, and **how the electrons are distributed within the molecule**.

Throughout the remainder of this course, you will see how the nanoscopic details of a molecule will affect observed, macroscopic properties such as biological effects, melting and boiling temperatures, rates of evaporation, and the ability of one substance to dissolve another substance.

23

The Distribution of Electrons in Molecules

Molecular geometry plays a major role in *how the electrons are distributed in molecules*.

The **electron distribution** is a major factor that determines the chemical and physical _____ of molecular compounds.

- For example, consider two molecules that are quite similar in size - CO_2 and H_2O. Both molecules contain three atoms, however at room temperature they are in different phases; CO_2 exists as a gas, whereas H_2O exists as a liquid (water).

Representations of Methane (CH$_4$)
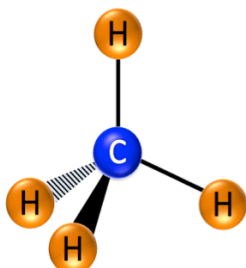
Space-filling models are images that show *molecular geometry* and also indicate the approximate *area that electrons occupy.*

line bond structure   ball-and-stick model   space-filling model

Here is a new concept: ***the electrons are*** _____ ***within molecules.***

- Sometimes electrons spend _____ time in one particular region of the molecule giving that region *additional* _____ *charge*.

- Sometimes a particular region of a molecule is *electron* _____ , giving that region of the molecule *additional* _____ *charge*.

The existence of this ***uneven charge*** within a molecule is a major factor that makes the **properties** of molecules such as CH_4, CO_2, and H_2O, quite different.

Let's first consider the H_2 molecule: $$H-H$$

The two electrons in this ***covalent bond*** are "*shared evenly*" by the hydrogens.

The electrons do not spend more time, *on average*, closer to any one of the two hydrogen atoms.

This is because the bond is between _____ *atoms*; the electrons are equally attracted to **each** of the positively-charged hydrogen nuclei.

When electrons are shared between *like atoms*, such as in H_2, they are, on average, **evenly** distributed between the atoms.

Next, let's consider the HCl molecule: $$H-\ddot{\underset{\cdot\cdot}{Cl}}:$$

The two electrons in the **H-Cl** *bond* are *not* shared *equally* by the chlorine and hydrogen atoms.

The shared electrons spend, on average, a bit more time nearer the chlorine than the hydrogen.

This is because the bond is between _____ atoms (chlorine vs. hydrogen).

- The shared electrons happen to be more strongly attracted to the chlorine than they are to the hydrogen.

H − H
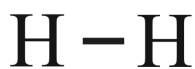
When electrons in bonds are **evenly** shared, as is the case for *like atoms* (such as H_2), we call the bond a _____ _____.

H−C̈l:

When electrons in bonds are not equally shared, as is the case for *un-like atoms*, we call the bond a _____ _____.

Scientists and engineers use the term _____ _____ to describe this physical state that results when there is a separation of charge over a short distance such as the length of a chemical bond.

H−C̈l:

Hydrogen acquires a *partial positive charge*

Chlorine acquires a *partial negative charge*
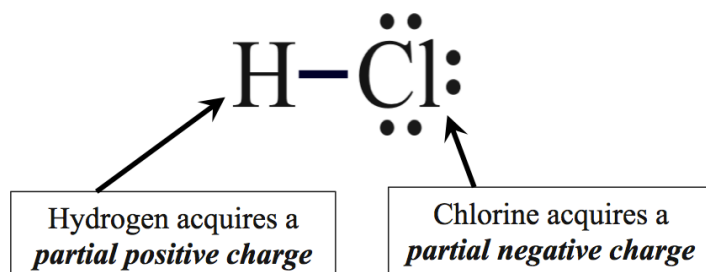
Representations of Bond Polarity in HCl

δ^+ δ^-

H—C̈l:

H—C̈l:

H   Cl
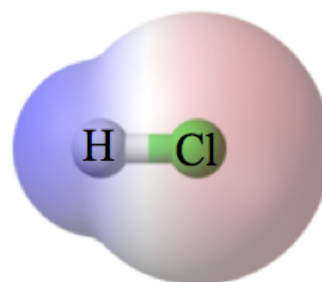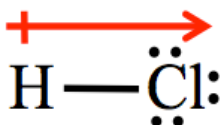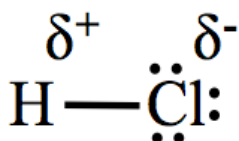
The line bond structure (above, left) uses the Greek lowercase letter delta (δ) to indicate a *partial positive charge* (δ^+) or a *partial negative charge* (δ^-) near the appropriate atoms.

Another way to show bond polarity and partial charge is to use the **dipole arrow** (above, middle).

- When using *dipole arrows*, the arrow points to the partial negative charged region and a crossed line (looks like + on the end of the arrow) is used to indicate the partial positive charged region.

The space-filling model (above, right) not only shows the region that the molecule's electrons occupy, but is also shaded to indicate the *electron distribution*.

- The area where electrons spend more time and therefore has a partial negative charge is shaded red.
- The area that is electron deficient has a partial positive charge and is shaded blue.

Electronegativity

The relative ability of an atom in a bond to attract electrons is called its _____.

- The *more* electronegative atom in the bonded pair will have a stronger attraction to the shared electrons, the electrons will spend a bit more time in the vicinity of that atom, therefore the atom will have a **partial negative charge**.
- The *less* electronegative atom in the bond will have a **partial positive charge**.

Electronegativity Values

H 2.20																		He
Li 0.98	Be 1.57												B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
Na 0.93	Mg 1.31												Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.60
Cs 0.79	Ba 0.89	*	Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn 2.2
Fr 0.7	Ra 0.9	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo

* Lanthanoids	La 1.1	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.2	Gd 1.2	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.1	Lu 1.27
** Actinoids	Ac 1.1	Th 1.3	Pa 1.5	U 1.38	Np 1.36	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr 1.3

Note that there is a **periodic trend** in electronegativity values of the **s-** and **p-**block elements; electronegativity increases going from left to right (in a row) and bottom to top (in a column).

You can determine which atom in a polar bond is ***partially positive*** and which is ***partially negative*** by comparing the **electronegativity values** of the two atoms.

Example: Consider the line bond structure of hydrogen monobromide (HBr).

$$\delta^+ \quad \quad \delta^-$$
$$H-\overset{..}{\underset{..}{Br}}:$$

Hydrogen has an electronegativity of **2.20**	Bromine has an electronegativity of **2.96**
partially positive	**partially** negative
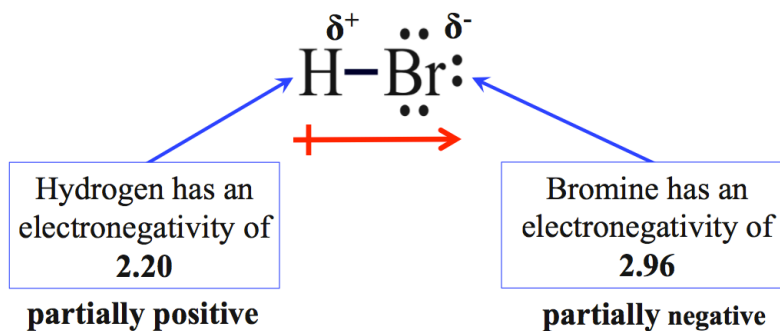
Understanding Check: Bromine monofluoride (BrF) exists as a brown gas and is used as an algaecide, fungicide, and disinfectant in some industrial applications. Draw the line bond structure of bromine monofluoride.

a) Predict which atom is **partially positive** and which atom is **partially negative**.

b) Add the δ^+ or δ^- symbols to the appropriate atom.

c) Add a dipole arrow below the line bond structure to indicate the polarity.

The **degree of bond polarization** depends on the _____ in electronegativities between the two bonded atoms.

- Greater differences in the abilities of the bonded atoms to attract the shared electrons results in *more polarized bonds*.

Example: The electronegativity of hydrogen, fluorine, and bromine are 2.20, 3.98, 2.96, respectively. Which bond is *more polarized*, the **H-F** or **H-Br** bond?

> **H-F**:   The *difference* in electronegativity between F and H: 3.98 - 2.20 = **1.78**
>
> **H-Br**: The *difference* in electronegativity between Br and H: 2.96 - 2.20 = **0.76**

Since there is a greater difference in electronegativity between F and H vs. Br and H, **the H-F bond is _____ polarized than the H-Br bond.**

Summary of Bond Polarity

We can classify covalent bonds as being *either* _____ or _____.

- **Polar bonds** occur because of *unequal sharing* of electrons in covalent bonds when two *un-like* atoms (such as H-Br or H-Cl) are bonded together.

- **Nonpolar bonds** occur when the electrons are shared evenly between two *like* atoms (such as H-H or F-F).

The Polarity of Molecules
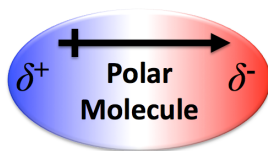
Similar to the concept of *bond polarity*, when electrons are not symmetrically distributed **in a molecule**, it results in a **polar** _____; a molecule with one end that has a partial negative charge and one end that has a partial positive charge.

The existence and degree of polarity (strength of the dipole) in molecules has implications in many of the chemistry concepts that you will learn throughout this course.

For example, one type of force responsible for attracting molecules *to other molecules* that is, in part, responsible for whether the molecules exist close to each other in the liquid or solid phase instead of the gas phase is called the **dipole-dipole force**.

- The partially positive (δ^+) end of one molecule's dipole is attracted to the partially negative (δ^-) end of another molecule's dipole (and vice versa) by an electrostatic attraction as illustrated below.

In this video, you will learn how to determine if a **molecule** is *polar* or *nonpolar* based on *both* the existence (or not) of _____ _____ **and** its molecular _____.

I will show you a method for determining the polarity of a molecules for each of our *molecular size categories* (diatomic, small, and large molecules).

The Polarity of *Diatomic* Molecules

Molecular Size Category	Description	Example(s)	
Diatomic Molecule	Molecule contains only two atoms	H_2	HCl

Since diatomic molecules contain **only one bond**, the polarity of the molecule depends only on the polarity of that bond.

- A _____ *diatomic molecule*, such as H_2, contains **like-atoms** and a *nonpolar* bond, therefore the molecule is _____.

- A _____ *diatomic molecule*, such as HCl, contains two **un-like** atoms and a *polar* bond, therefore the molecule is _____.

Diatomic Molecule Polarity

Are the Two Atoms Identical?

Yes — No

| Homo-nuclear Molecule | Hetero-nuclear Molecule |

| Nonpolar Molecule | Polar Molecule |
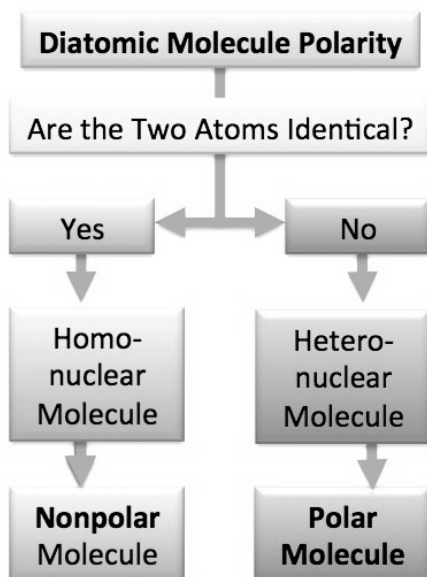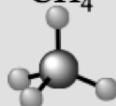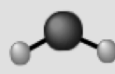
Understanding Check:
Determining the Polarity of Diatomic Molecules

Categorize each of the diatomic molecules listed below as **polar** or **nonpolar**.

a) O_2

b) carbon monoxide (CO)

c) N_2

d) nitrogen monoxide (NO)

The Polarity of *Small* Molecules

Molecular Size Category	Description	Example(s)	
Small Molecule	Molecule has **one central** atom with **all other** atoms bonded to the central atom	CH_4	H_2O

Small molecules contain more than one bond.

The *individual bonds within a molecule* can be polar and/or nonpolar.

Just because a small molecule contains polar bonds does not necessarily mean that it is a polar molecule.

In order to determine if a small molecule is polar, we must look at what happens when we **_add up_** all of the dipoles.

Dipoles are physical quantities that not only have a magnitude (amount of charge), but also have a direction.

An analogous physical quantity that you are familiar with is *velocity*. When you drive your car, to completely describe your path you would use both the *speed* (miles per hour) and the *direction* you are traveling.

Another physical quantity with both magnitude and direction is a **force**. When you pull on an object, how fast and where the object moves depends on how hard you pull **and** in what *direction* you pull.
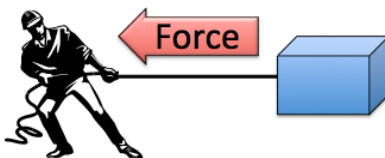
Quantities with both magnitude and direction are called **vector quantities**.

Covalent bond electric dipoles are vector quantities; they have both *magnitude* (based on differences in electronegativity of the bonded atoms) and *direction* (based on bond angles).

Before we discuss "*adding up*" dipole vectors, let's *add up* some vector quantities of which you have prior knowledge. We will consider adding a couple of force vectors:
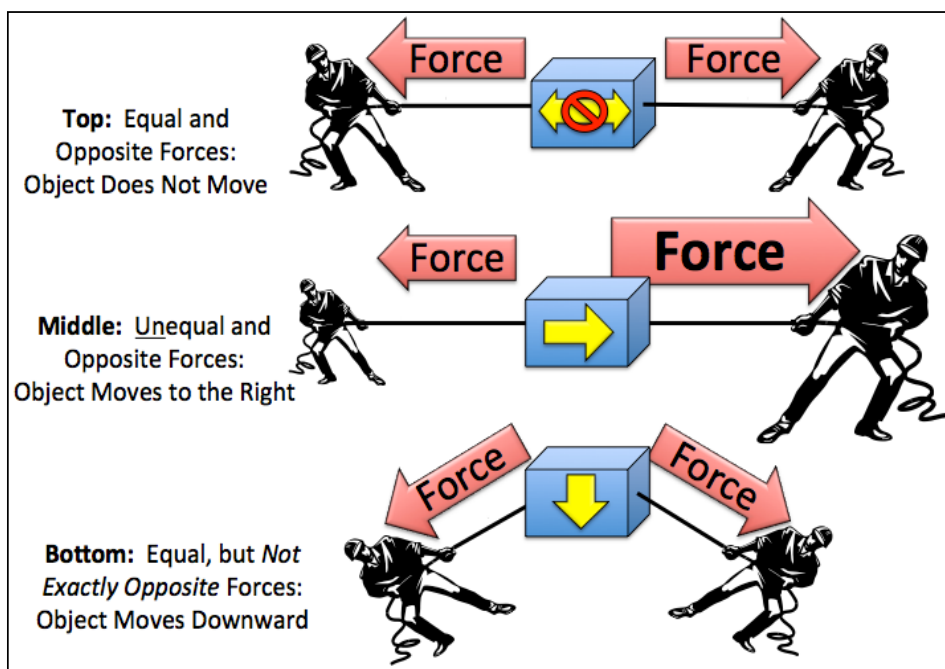
Top: Two equal tensions (represented by the red vector arrows of the same length) are exerted in opposite directions. The blue box does not move because the forces are "balanced" or "cancel"; they *add up to zero*.

Middle: The two tension forces are in opposite directions, however the force pulling to the right is larger (represented by a larger vector arrow). The blue box moves to the right because the forces are not "balanced" and do not "cancel" - they **do not** add up to zero.

Bottom: The two tension forces are equal but they are <u>not</u> oriented in exactly *opposite directions*. The blue box moves downward because the forces are not "balanced" and do not "cancel" - they **do not** add up to zero.

To determine if a *small* molecule is polar:

We must look at what happens when we _____ up all the dipoles.

Example: CO_2

There are 2 polar bonds in a CO_2 molecule.

This results in two_____.

- The oxygens have a _____ negative charge.
- The carbon has a partial positive charge.
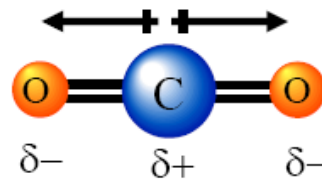
Since the molecule is _____, the dipoles cancel each other and the molecule is _____.

- All *symmetric* small molecules are ***nonpolar***.

Let's look at what happens when we add up all the dipoles in another molecule:

Example: H_2O

There are 2 polar bonds in an H_2O molecule.

This results in two dipoles.

- The oxygen has a partially negative charge.
- The hydrogens have a partially positive charge.
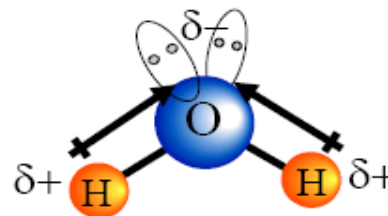
Since the molecule is <u>not</u> symmetric, the dipoles *do not cancel* each other and the molecule is

_____.

Since dipoles in ***nonsymmetric*** molecules do not cancel each other out, they ***add up*** to yield a **molecule with a dipole**.

Nonsymmetric small molecules with polar bonds are **polar** molecules.
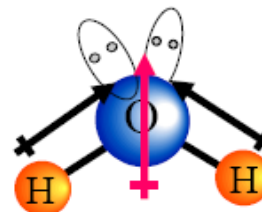
General Rule to Know if a molecule is Symmetric or Nonsymmetric:

Symmetric molecules have the *central atom* surrounded by _____electron groups.

Examples of symmetric and *non*symmetric molecules:

CO_2	CH_4	CH_3F	NH_3
Symmetric (Nonpolar)	Symmetric (Nonpolar)	**Non**symmetric (Polar)	**Non**symmetric (Polar)
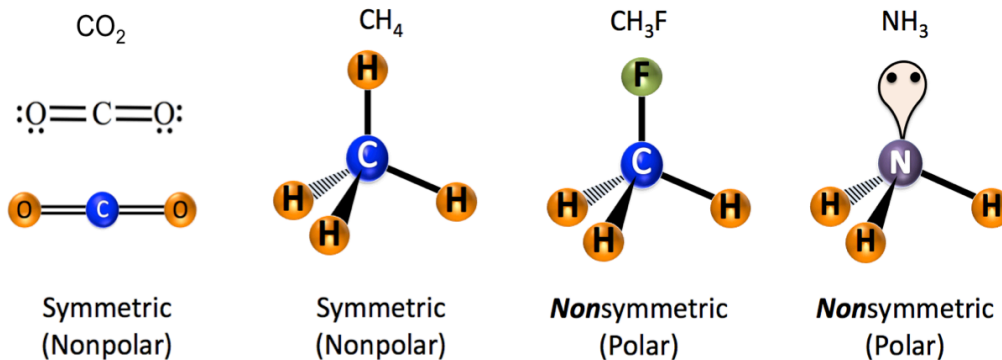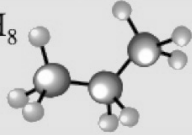
Polarity of Small Molecules Summary
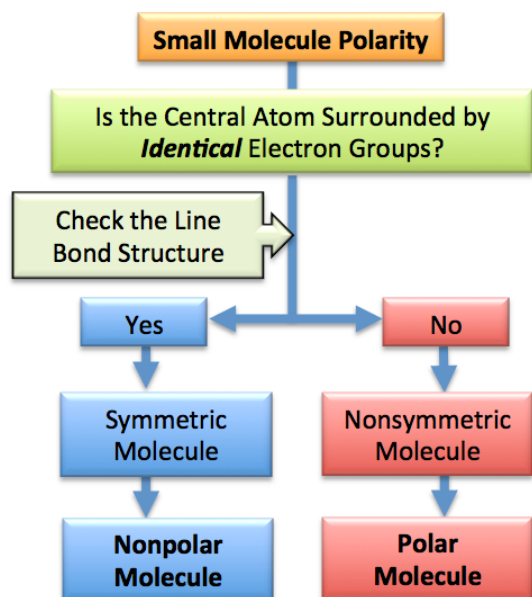
Understanding Check:
Determining the Polarity of Small Molecules
Categorize each of the small molecules listed below as **polar or nonpolar**. Note that you will need to begin with the line bond structure of a molecule in order to determine its polarity.

a) NF_3

b) H_2S

c) O_3

d) CS_2

e) CCl_4

The Polarity of *Large* Molecules

Molecular Size Category	Description	Example(s)
Large Molecule	Larger than *Small Molecule*; there **is not just one single, central atom** with **all** the other atoms bonded to it	C_3H_8

In this course, we will be working with large molecules (organic and biochemistry).

Large molecules will be considered polar (or have polar regions) if they have _____ _____ bonds.

- o The ***important highly polar covalent bonds***, especially in organic and biochemistry, are those in which either **hydrogen** or **carbon** atoms are covalently attached to **nitrogen**, **oxygen**, **fluorine**, or **chlorine** atoms.
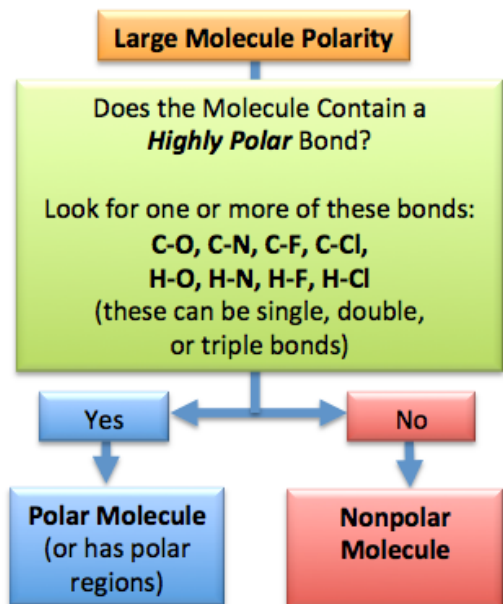
Example:

Cyclohexane　　vs.　　**Cyclohexanol**
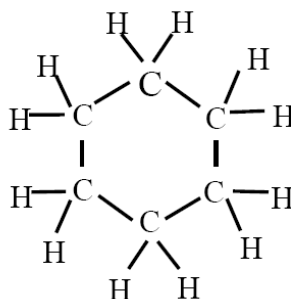
No *highly polar* bonds
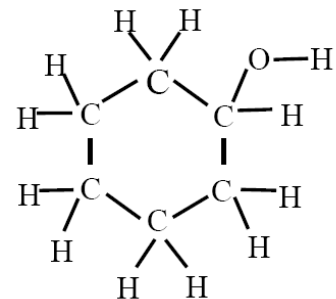
Two *highly polar* bonds
(C-O and O-H)

Nonpolar　　　　　　**Polar**

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Formal Charge

There is **one more** phenomenon that results in the *uneven distribution of charge.*

We will use the concept of "_____ _____" to account for electrically-charged regions within molecules (and polyatomic ions).

The **formal charge** concept involves identifying _____ in molecules (or in polyatomic ions) that have an **excess** or **deficiency of electrons**.

- An excess of electrons on a particular atom means that there are more electrons in the vicinity of an atom than there are protons in the atom. If there is one extra electron in the vicinity of a particular atom, the *formal charge* of the atom would be 1-.

- Conversely, when we say that an atom is electron deficient, this means that there are fewer electrons in the vicinity of a particular atom than there are protons in the atom. If an atom has a deficiency of one electron (one more proton than electrons), the formal charge of the atom would be 1+.

What Do You Need to Know About Formal Charge?

We will soon be focusing on organic biomolecules. Biomolecules consist primarily of C, H, O, and N.

- In the compounds that you will come across in this course, *carbon* and *hydrogen* atoms *will never* have a formal charge.

- *Oxygen* and *nitrogen* **may or may not** have a formal charge.

I will only need you to be able to determine the formal charge on two elements -

_____ and _____.

1) **The Formal Charge on Oxygen:**

- Oxygen has a formal charge of **1-** when it has *just* _____ *single bond* (three lone pairs).

$$ -\ddot{\underset{\displaystyle ..}{O}}\text{:}^{-} $$
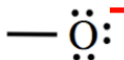
- In **all other cases that we discuss in this course**, oxygen will **not** have a formal charge (formal charge = zero).

      • Examples:

$$ \begin{array}{cc} :\overset{\displaystyle ..}{O}: & \\ \| & \qquad -\ddot{\underset{\displaystyle ..}{O}}- \end{array} $$
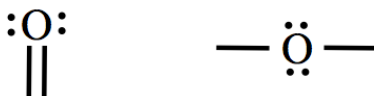
2) The Formal Charge on Nitrogen:

- Nitrogen will have *no formal charge* when it has *one or more lone pairs on it*.

$$\overset{\displaystyle ..}{-\,\ddot{N}\,-} \qquad -\,\ddot{N}= \qquad :N\equiv$$
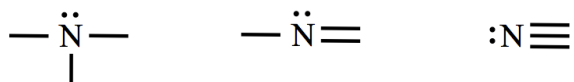
- In _____ *other cases*, nitrogen has a **1+** formal charge.

$$-\,\overset{+}{N}\,- \qquad -\,\overset{+}{N}= \qquad -\,\overset{+}{N}\equiv$$
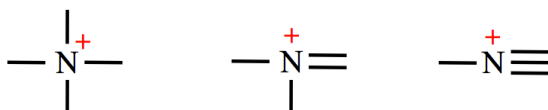
Determination of the formal charge of oxygen and nitrogen is summarized in the thought-map flowchart shown below.
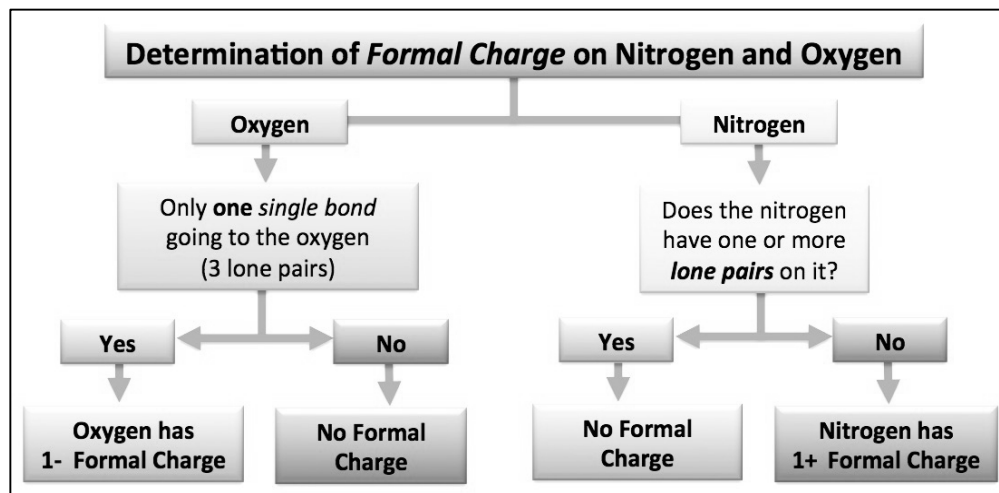
OPTIONAL: If you are interested in learning the details of how formal charges are assigned to oxygen, nitrogen, and other atoms based on their bonding patterns, you can find that information in Appendix 3 of your textbook.

Example: The line bond structure of the nitrate ion (NO_3^-) is shown below. Add the *formal charge* (as a superscript) to the line bond structure next to any **oxygen** or **nitrogen** atom that has a non zero formal charge.
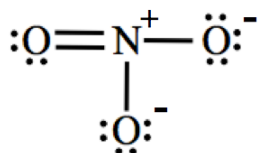
The nitrogen has *no lone pairs*, therefore it has a formal charge of **1+** (or **+**).

The oxygens below and to the right of the nitrogen have *just one single bond*, therefore they have a formal charge of **1-** (or **-**).

The oxygen to the left of the nitrogen *does not have just one single bond* (it has a *double bond*), therefore it has no formal charge (formal charge = zero).

Understanding Check: The line bond structure glycine, an amino acid present in many proteins, is shown below. Assign formal charges to the nitrogen and each oxygen atom in this compound.
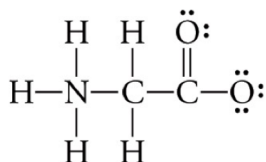
Understanding Check: Aspartic acid is one of the 20 common amino acids that make up the proteins in our bodies. The condensed structure of the aspartic acid is shown below. Add the formal charge (as a superscript) next to any *oxygen or nitrogen atom* in the condensed structure that has a non zero formal charge.
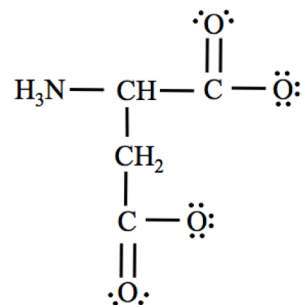
Summary

In the last two videos, you learned *two ways* to predict the ***distribution of charge***:

> **Molecular Polarity:** Because of the unequal sharing of electrons, regions of a molecule can have **partial charge**. These charged regions have a *partial positive charge* (δ^+) or *partial negative charge* (δ^-).

> **Formal Charge:** A region in the vicinity of a *particular atom* in a compound can have ***formal charge*** *because of an excess or deficiency* of electron(s) at that atom.

Both the polarity and presence of formal charges in molecules are important in understanding how ***compounds interact with each other***, and also in understanding the forces within large biomolecules such as DNA, RNA, proteins, and carbohydrates. These forces are crucial for the biological molecules maintaining their shape and biological function.

Noncovalent Interactions

Ionic compounds exist as crystalline solids at room temperature because the ions are held together by **ionic chemical bonds**.

Molecular compounds can also exist as crystalline solids.

- Example: H_2O (ice or snow flakes)

H_2O molecules are not ions, so **what forces are responsible for holding H_2O molecules, or other molecules, together in their solid states**?

The answer is that there are *electrostatic attractive forces* called _____ _____ that attract molecules to other molecules.

Noncovalent interactions are quite different from the ***covalent bonding forces*** that are present within molecules and polyatomic ions.

- _____ **bonding forces** result from **shared electrons**.

- ***Noncovalent interactions***, as the name implies, ***do not*** involve the sharing of electrons; they are strictly **electrostatic attractions**.

In this video, you will learn about **five** types of ***noncovalent interactions***.

1) Hydrogen Bonding

Hydrogen bonding is the result of the electrostatic attraction *between* the partial positive charged end of a ***particularly strong polar bond*** (O-H, N-H, or F-H) and the negative charge of a lone pair of electrons on a very electronegative atom (O, N, or F).
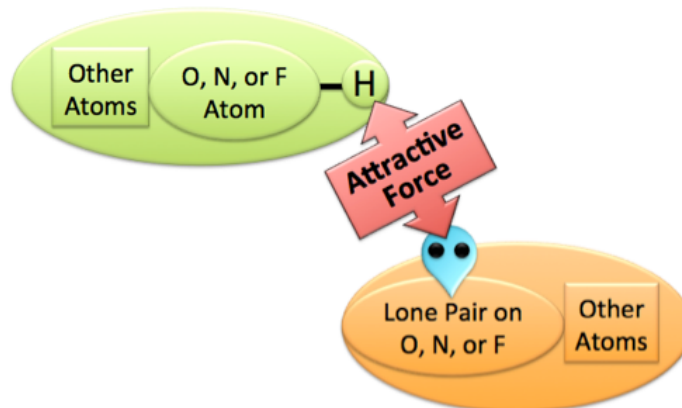
Example: *Hydrogen bonding* is the major force responsible for H_2O, a relatively small and light molecule, existing in the liquid phase instead of the gaseous phase at room temperature.
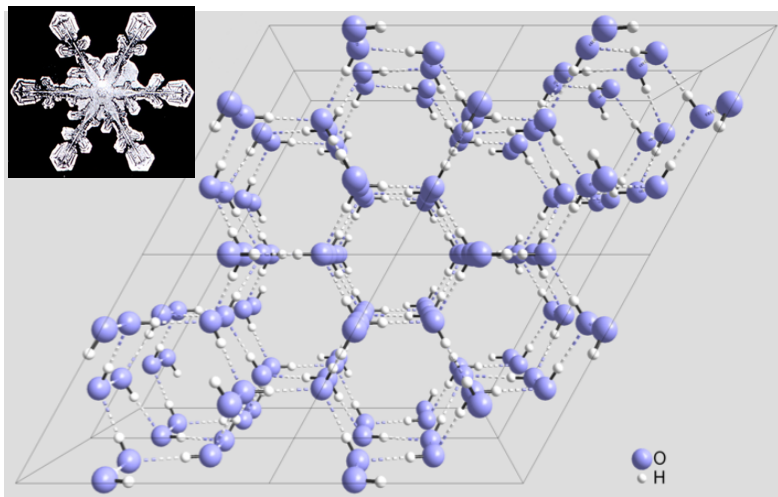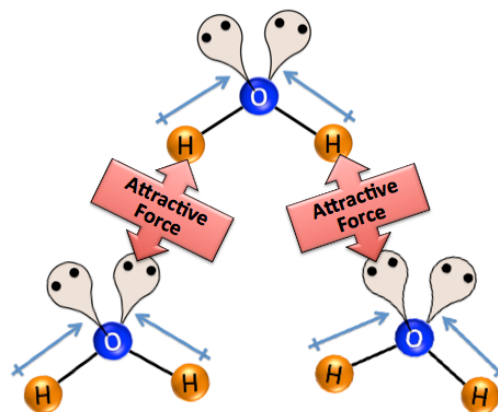
On the Left: Hydrogen bonds (as dashed lines) in a ball and stick model of an ice crystal.

Understanding Check:

The line bond structures of ammonia and acetone are shown below:
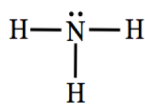
ammonia   acetone
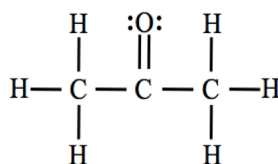
a. Can hydrogen bonding occur between two ammonia molecules?
b. Can hydrogen bonding occur between two acetone molecules?
c. Can hydrogen bonding occur between an ammonia molecule and an acetone molecule?

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2) Dipole-Dipole Forces
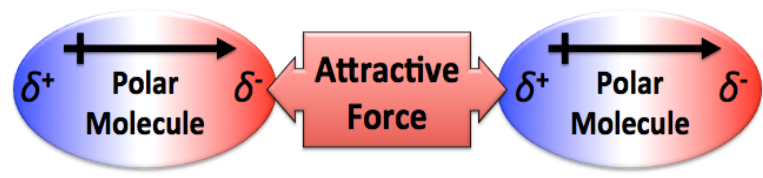
Polar molecules are attracted to other polar molecules by a type of noncovalent interaction called the _____ **force**.
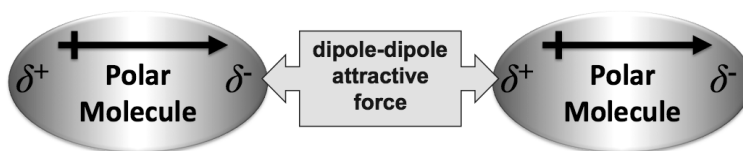
The partially positive (δ^+) end of one molecule's dipole is electrostatically attracted to the partially negative (δ^-) end of another molecule's dipole (and vice versa).

Example: Diethyl Ether

Understanding Check:
a. Can a dipole-dipole force occur between two H_2O molecules?
b. Can a dipole-dipole force occur between two methane (CH_4) molecules?
c. Can a dipole-dipole force occur between two acetone molecules?

acetone
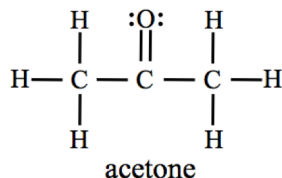
It is ***noncovalent interactions*** that hold molecules together such that they exist in the solid or liquid phases instead of the gaseous phase.
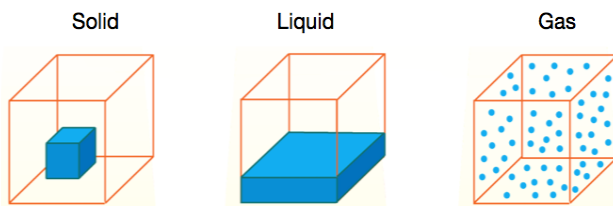
Whether a substance exists in the gas, liquid, or solid phase is determined by a _____ between noncovalent interactions (working to keep the particles close to one another) and temperature (kinetic energy working to distribute the particles randomly in their container).

- If the noncovalent interactions are dominant, then the substance will exist in the solid or liquid phase.
- If the temperature/kinetic energy can overcome the noncovalent interactions, then the substance will exist in the gaseous phase.

It was observed that nonpolar molecules such as CO_2, O_2, and N_2, which are ***not capable*** of interacting through dipole-dipole forces or hydrogen bonding, can be cooled to temperatures at which they exist in the liquid and solid phases.

In 1930, Fritz London, along with R. Eisenschitz, came up with a model to explain this observation.

3) London Dispersion Forces

The explanation is based on our third type of ***noncovalent interaction***, which came to be known as **London dispersion forces**, named in honor of Fritz London.

London dispersion forces are caused by an "instantaneous" dipole in one molecule _____ the formation of a "temporary" dipole in another molecule.
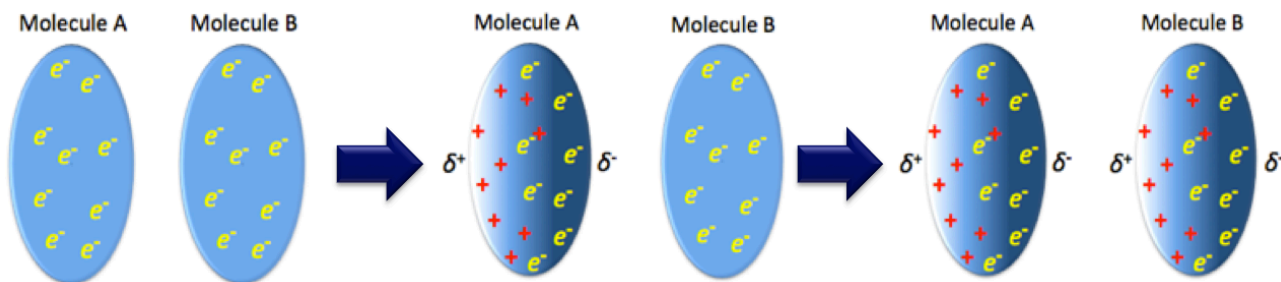
_____ *molecules*, polar and nonpolar, contain electrons and will therefore be attracted to each other through London dispersion forces.

The _____ a molecule is, the easier (lower in energy) it is to polarize its electrons, and therefore, **the stronger is its London dispersion force interactions**.

- This trend can be observed by noting the boiling points of the molecules in the table below:
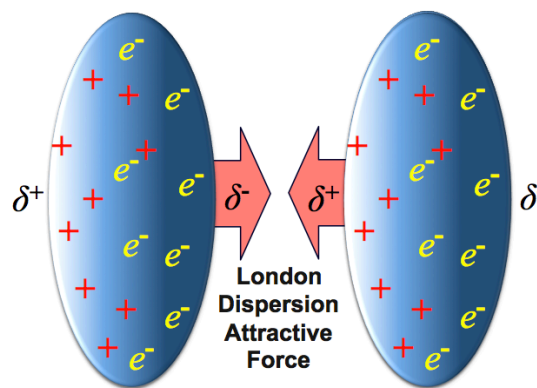
Effect of Molecular Size on London Dispersion Forces			
Molecule Name	Condensed Structure	Boiling Point (°C)	Phase at Room Temperature
methane	CH_4	-164	gas
ethane	CH_3CH_3	-89	gas
propane	$CH_3CH_2CH_3$	-42	gas
butane	$CH_3CH_2CH_2CH_3$	0	gas
pentane	$CH_3CH_2CH_2CH_2CH_3$	36	liquid

Understanding Check:
a. Can London dispersion forces occur between two CBr_4 molecules?
b. Can London dispersion forces occur between two H_2O molecules?
c. Which of the following substances is predicted to have the higher boiling point:

decane ($CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$)
or
nonane ($CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$)

4) Ion-Dipole Interactions

An **ion-dipole interaction**, as the name implies, is the electrostatic attractive interaction *between* an *ion* (or formal charge) *and* the _____ of a polar molecule.
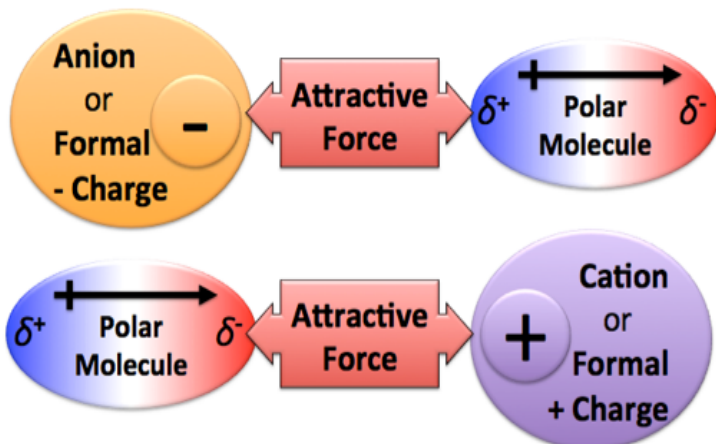
The attraction could be *between* an **anion** (or negative formal charge) *and* the partially positive end (δ^+) of a dipole, or vice versa, *between* a **cation** (or positive formal charge) *and* the partially negative end (δ^-) of a dipole.

The attraction could be *between* an **anion** (or negative formal charge) *and* the partially positive end (δ^+) of a dipole, or vice versa, *between* a **cation** (or positive formal charge) *and* the partially negative end (δ^-) of a dipole.

Examples: Sodium cations or chloride anions interacting with polar water molecules.

Understanding Check:

a. Can an ion-dipole interaction occur between ammonium (NH_4^+) and H_2O?

b. Can an ion-dipole interaction occur between bromide (Br^-) and I_2?

---

5) Salt Bridge Interactions

A **salt bridge** is the electrostatic attractive interaction **between** a negative formal charge **and** a positive formal charge in protein.

Salt bridges are one of the noncovalent interactions that are responsible for the way a protein **folds up onto itself** to give it the shape that is necessary for it to perform its biological function.

protein
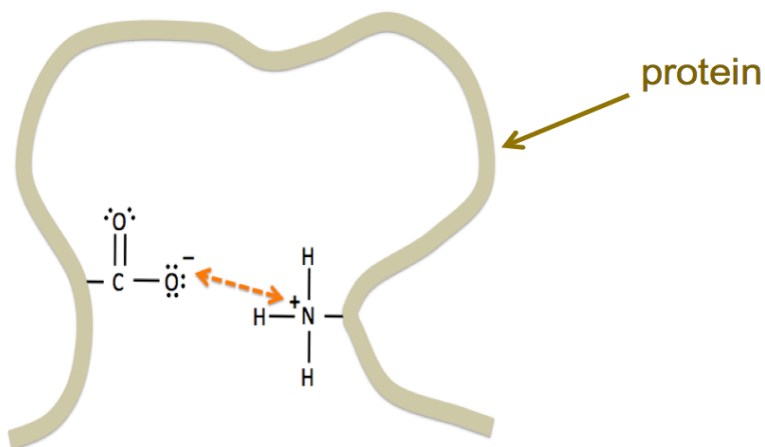
Summary of Noncovalent Interactions
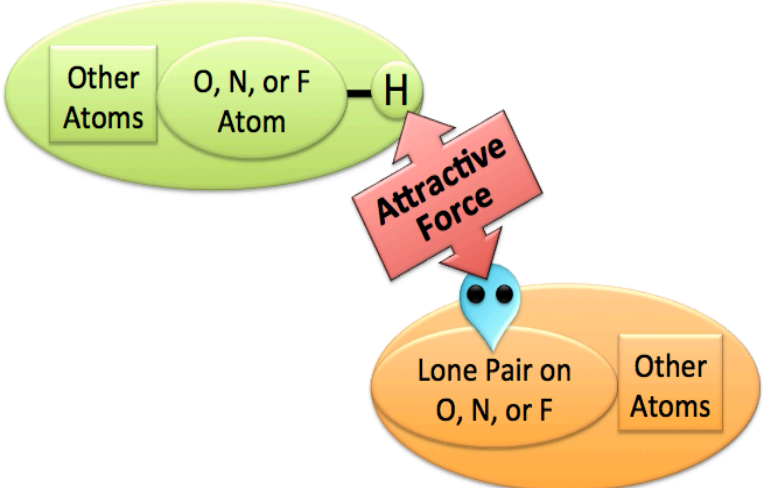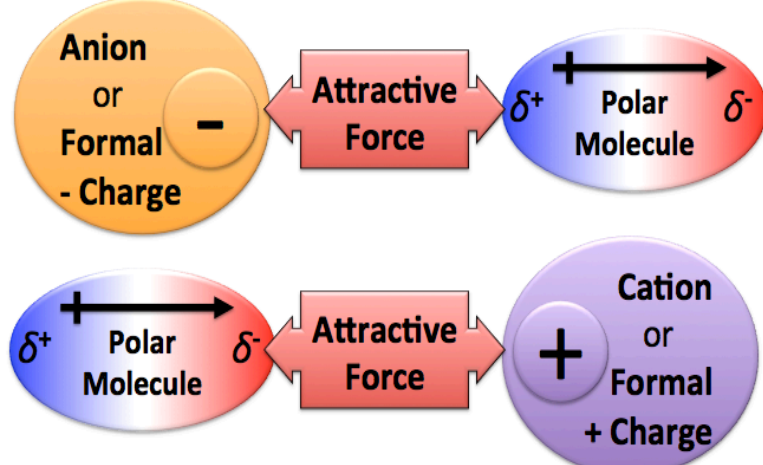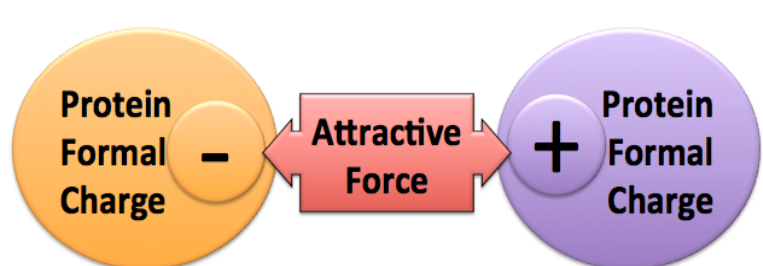
In this video, you learned about **five** types of **noncovalent interactions**.

When these interactions occur between molecules (as opposed to monatomic or polyatomic ions), they are sometimes referred to as **intermolecular forces**.

Noncovalent interactions cause molecules to be *attracted to each other* and can result in molecular compounds existing as liquids or solids.

In the case of large molecules or polyatomic ions that can *fold back upon themselves*, noncovalent interactions can occur between two regions **within an individual particle**.

Summary of Noncovalent Interactions

Noncovalent Interaction	Interaction Between:
Hydrogen Bonding Electrostatic attractive force between the partially positive charged hydrogen end of an O-H, N-H, or F-H bond and the negative charge of a lone pair on an O, F, or N.	
Dipole-Dipole Electrostatic attractive force between *two **polar** molecules*.	
London Dispersion Forces Electrostatic attractive force between ***any*** two molecules.	
Ion-Dipole Electrostatic attractive force between a *dipole* and *an ion or formal charge*. The partially positive charge of a dipole is attracted to a negatively charged ion *or* a negative formal charge. The partially negative charge of a dipole is attracted to a positively charged ion *or* positive formal charge.	
Salt Bridge Electrostatic attractive force between a negative formal charge and a positive formal charge in protein.	

Organic Chemistry

Organic chemistry is the chemistry of _____-*containing* compounds.

Hydrocarbons
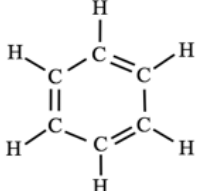
Hydrocarbons contain only _____ and _____ atoms.

Hydrocarbons are the main source of energy used by humans. Hydrocarbons are burned in a chemical process called combustion in order to do various types of work or to generate heat.

The majority of the hydrocarbons on earth exists as *crude oil (or petroleum)*, a mixture of various hydrocarbon molecules and small amounts of other substances. Crude oil is considered a "fossil fuel" because it is formed from huge amounts of dead organisms, primarily zooplankton and algae, that have been buried under sedimentary rock and exposed to high temperature and pressure. Under those conditions and in the absence of oxygen, the molecules from the dead organisms are converted to petroleum through a series of chemical reactions.

Fossil fuel is called a *non-renewable* energy source since its process of formation occurs over millions of years. The hydrocarbon molecules in crude oil are further separated (refined) into various materials such as gasoline, petroleum jelly, paraffin wax, diesel fuel, asphalt, and baby oil.

Hydrocarbons can be categorized into the four subcategories, shown in the table below, based on their chemical bonding patterns.

Category	Defining Feature	Saturation	Example
alkane	all single bonds	saturated	ethane $CH_3 - CH_3$
alkene	at least one carbon-carbon **double** bond	unsaturated	ethene $CH_2 = CH_2$
alkyne	at least one carbon-carbon **triple** bond	unsaturated	ethyne $CH \equiv CH$
aromatic	alternating double and single bonds in a **cyclic** hydrocarbon	unsaturated	benzene

Hydrocarbons are also classified as being either _____ (all single bonds) or _____ (contains one or more carbon-carbon double or triple bonds).

Another way that hydrocarbons are classified by their bonding pattern is either as **normal, branched**, or **cyclic**.

Example of a *branched* hydrocarbon:
The *line bond, condensed, and skeletal structures* for *isopentane* are shown below.
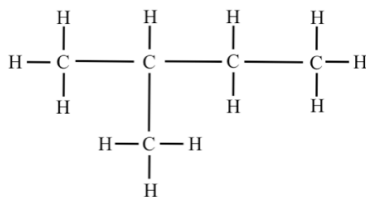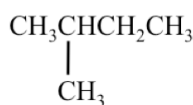
Line Bond Structure   Condensed Structure   Skeletal Structure

In *isopentane*, there are four carbons bonded in a **linear sequence**.

There is one carbon that "_____" from the linear sequence, therefore *isopentane* is classified as a **branched hydrocarbon**.

40

Example of a *normal* hydrocarbon:

The *line bond, condensed, and skeletal structures* for **propane** are shown below.

Line Bond Structure   Condensed Structure   Skeletal Structure
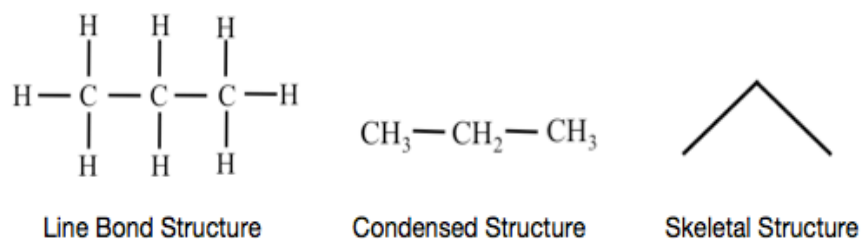
In *propane,* _____ **of the carbons** are bonded in a **linear sequence**, therefore *propane* is classified as a **normal hydrocarbon**.

For both *normal and branched alkanes,* if "*n*" is the number of carbon atoms in the molecule, then the alkane will have the molecular formula of $C_nH_{(2n+2)}$.
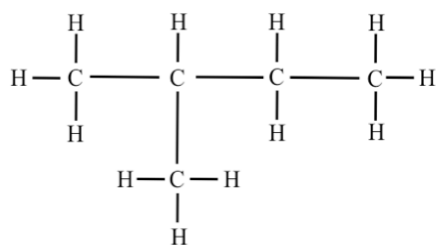
"*n*" (the number of carbon atoms) = 5

The molecular formula is $C_5H_{(2 \cdot 5 + 2)} = C_5H_{12}$

isopentane
(a **branched** hydrocarbon)
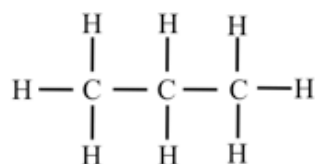
"*n*" = 3

The molecular formula is $C_3H_{(2 \cdot 3 + 2)} = C_3H_8$

propane
(a **normal** hydrocarbon)

Example of a *cyclic* hydrocarbon:

The *line bond, condensed, and skeletal structures* for **cyclohexane** are shown below.

Line Bond Structure   Condensed Structure   Skeletal Structure
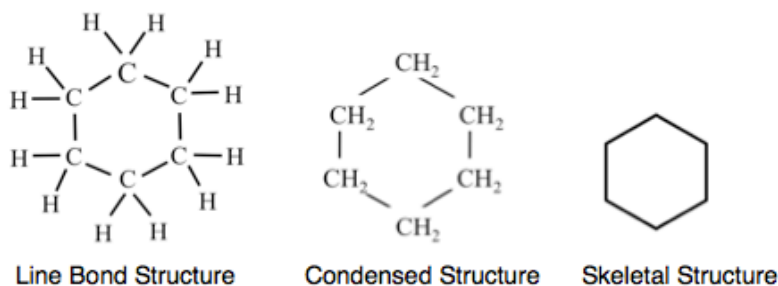
When the carbons in a hydrocarbon molecule are bonded together such that they form a _____, we call it a **cyclic** hydrocarbon.

41

Alkanes

Alkanes are molecules that consist *only of carbon and hydrogen* and contain *only single bonds*.

The primary source of alkanes is *crude oil* and *natural gas*. Natural gas is formed in the same way as crude oil, except that the original source of organics is from buried plants and animals. It is composed primarily of methane (CH_4) and ethane (C_2H_6), but also has significant amounts of propane (C_3H_8), butane (C_4H_{10}), pentane (C_5H_{12}), other hydrocarbons, and some non hydrocarbon gases. Alkanes with 4-12 carbons are the major component of gasoline. Gasoline that is high in branched alkanes is preferred because the branched molecules reduce engine "knocking." The "octane rating" of gasoline is related to the amounts and types of branched alkanes. Gasoline also contains small amounts of alkenes. Currently in the US, refineries are required to add alcohol (a renewable fuel source) to gasoline at a concentration of 10%. Diesel fuel is composed of alkane molecules with 9-16 carbons (75%) and aromatic hydrocarbons (25%). Alkane molecules with more than sixteen carbon atoms are used for fuel oil (kerosene) and lubricating oil. Paraffin wax is composed primarily of alkane molecules with 20-40 carbon atoms. Paraffin wax is used for candles, electrical insulation, and lubrication.

Naming Alkanes

IUPAC rules, devised by the **I**nternational **U**nion of **P**ure and **A**pplied **C**hemistry, are a widely used method of naming organic compounds.

Using the IUPAC rules involves identifying an alkane's _____ _____ (the longest continuous chain of carbon atoms in the molecule) and _____ (atoms or groups of atoms attached to the parent chain).

In alkanes, the substituents, called _____ _____, are constructed solely of carbon and hydrogen atoms.

Method for Naming Normal and Branched Alkanes

Step 1. Name the *parent chain*.

For normal and branched alkanes, the ***parent chain is the longest, continuous chain of carbons atoms***.

The parent chain is named by combining a **prefix**, that specifies the number of carbon atoms in the parent chain, with the "_____" suffix.

Example: If a linear or branched alkane has ***three carbon atoms*** in the parent chain, the parent chain name is ***propane***

In a **normal** (unbranched) **alkane**, there are ***no substituents***, and the molecule's name is identical to the **parent chain** name.

- **Example:** The name for the normal alkane with ***four carbons*** is **butane**.
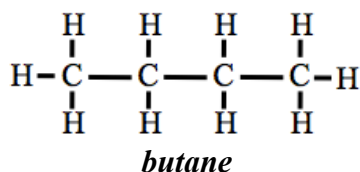
Prefixes for Naming Parent Chains	
Number of Carbons in Parent Chain	**Naming Prefix**
1	meth
2	eth
3	prop
4	but
5	pent
6	hex
7	hept
8	oct
9	non
10	dec

H-C—C—C—C-H
butane

Step 2. Name any alkyl group substituents.

Alkyl group substituents are comprised of the carbons and hydrogens that "branch" from the parent chain.

In the molecule drawn below (a branched alkane), the parent chain has four carbons and one **alkyl group substituent**.
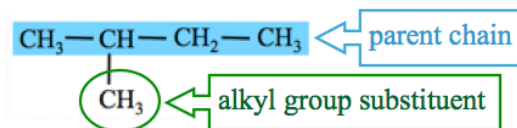
Alkyl group substituents are named based on the _____ of _____ in the substituent.

If there is *one carbon* in the substituent, we call it a _____ group.
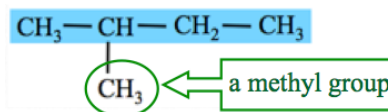
If there are *two carbons* in the substituent, we call it an _____ group.
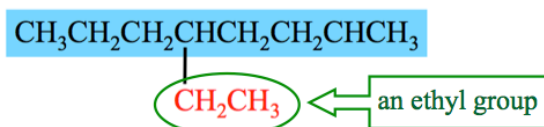
When *three carbons* are contained in a substituent, then there are *two* distinct bonding patterns that are possible.
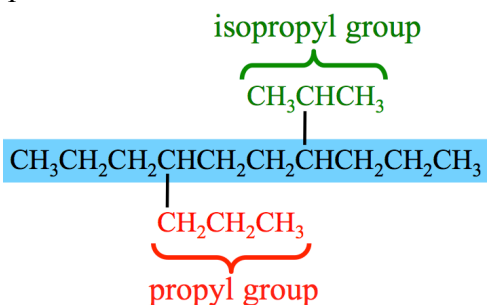
If a carbon on the *end of the substituent* is bonded to the parent chain, we call the substituent a _____ group.

If the carbon *in the center of the substituent* is bonded to the parent chain, we call the substituent an _____ group.

There are multiple, *correct* ways to draw **propyl groups** in structural formulas.

condensed formula   *skeletal formula*
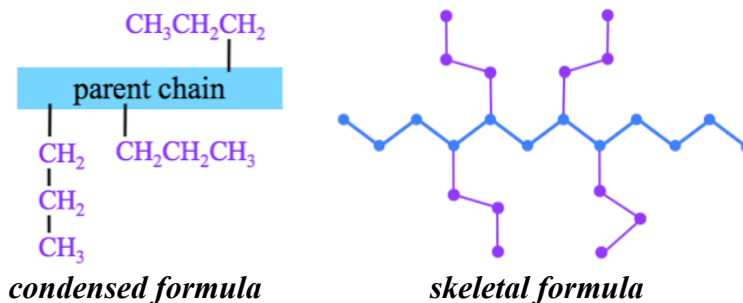
There are multiple, *correct* ways to draw **isopropyl groups** in structural formulas.

condensed formula   *skeletal formula*

43
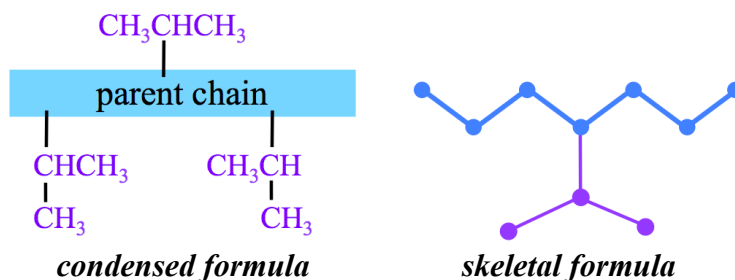
The condensed structures of alkyl group substituents with 1- 4 carbon atoms are shown on the right.

I ask my students to memorize the top four on the list (*methyl* through *butyl*).

- Check with your instructor to see which ones you need to memorize.

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

In order to uniquely name molecules, the name must indicate to which *parent chain-carbon* a substituent is attached.

- For example, there are *two different molecules* that both have a 5-carbon parent chain *and* one methyl group substituent.

$CH_3CHCH_2CH_2CH_3$
$|$
CH_3

$CH_3CH_2CHCH_2CH_3$
$|$
CH_3
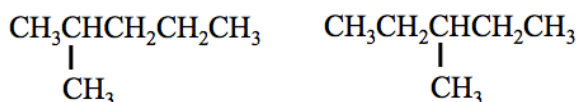
Alkyl Groups		
Number of Carbon Atoms	**Alkyl Group Name**	**Condensed Structure**
1	methyl	— CH_3
2	ethyl	— CH_2CH_3
3	propyl	— $CH_2CH_2CH_3$
3	isopropyl	— $CHCH_3$ $|$ CH_3
4	butyl	— $CH_2CH_2CH_2CH_3$
4	isobutyl	— CH_2CHCH_3 $|$ CH_3
4	*sec*-butyl	— $CHCH_2CH_3$ $|$ CH_3
4	*tert*-butyl (or *t*-butyl)	CH $|$ — $C-CH_3$ $|$ CH_3

Since there are two ends of the parent chain, we **begin numbering from the end of the parent chain that is _____ to a substituent**.

For example, the parent chain carbons are assigned position numbers for alkane shown below.

1   2   3   4   5
$CH_3—CH—CH_2—CH_2—CH_3$
$|$
CH_3
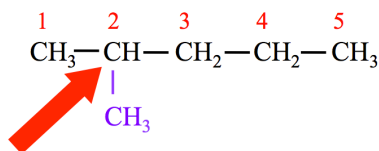
In the alkane shown above, note that the *point of attachment* of the **methyl group** substituent is to the carbon at position number "**2**" on the parent chain.

Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

Step 4A: List the alkyl groups along with their position numbers, ***in _____ order***.

- Write the position number(s) in front of the substituent(s).
  - In our example molecule, we write: **2-methyl**.
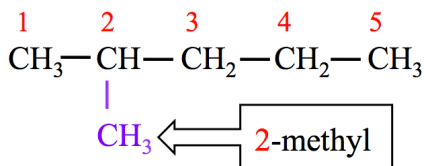
1   2   3   4   5
$CH_3—CH—CH_2—CH_2—CH_3$
$|$
CH_3 ⟵ 2-methyl

WHEN NEEDED: Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) identical substituents are present. *Not needed in this example.*

Step 4B: Write the parent chain name ***behind*** the list of alkyl groups.
- In our example, we have only one substituent: **2-methyl**.
- The parent chain (five carbons) is **pentane**.

We write the IUPAC name of this molecule as: **2-methylpentane**.

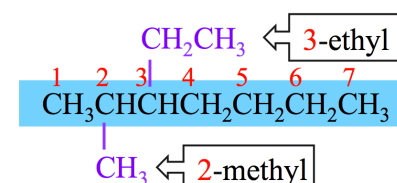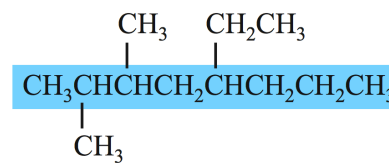**Example:** Give the IUPAC name for the alkane shown below.

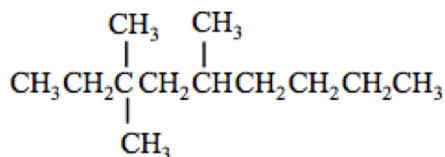$$\begin{array}{c} CH_2CH_3 \\ | \\ CH_3CHCHCH_2CH_2CH_2CH_3 \\ | \\ CH_3 \end{array}$$
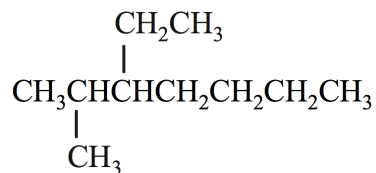
Step 1. Name the *parent chain*.
The parent chain (seven carbons) is **heptane**.
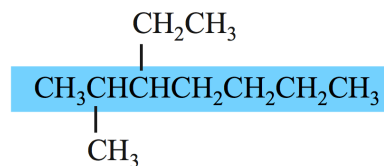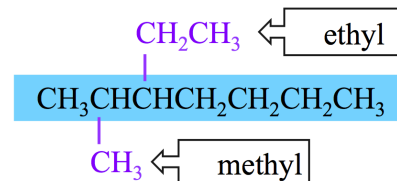
$$\begin{array}{c} CH_2CH_3 \\ | \\ CH_3CHCHCH_2CH_2CH_2CH_3 \\ | \\ CH_3 \end{array}$$

Step 2. Name any alkyl group substituents.

$$CH_2CH_3 \Leftarrow \boxed{ethyl}$$
$$CH_3CHCHCH_2CH_2CH_2CH_3$$
$$CH_3 \Leftarrow \boxed{methyl}$$

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

$$CH_2CH_3 \Leftarrow \boxed{3\text{-ethyl}}$$
$$\overset{1\ \ 2\ \ 3\ \ 4\ \ 5\ \ 6\ \ 7}{CH_3CHCHCH_2CH_2CH_2CH_3}$$
$$CH_3 \Leftarrow \boxed{2\text{-methyl}}$$

Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

<p align="center">3-ethyl-2-methylheptane</p>

Example: Give the IUPAC name for the alkane shown below.

$$\begin{array}{cc} CH_3 & CH_2CH_3 \\ | & | \\ CH_3CHCHCH_2CHCH_2CH_2CH_3 \\ | \\ CH_3 \end{array}$$
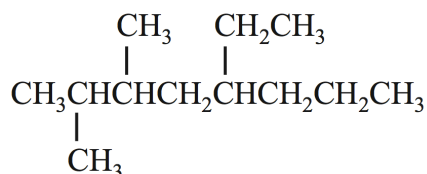
Step 1. Name the *parent chain*.
The parent chain (eight carbons) is **octane**.

$$\begin{array}{cc} CH_3 & CH_2CH_3 \\ | & | \\ CH_3CHCHCH_2CHCH_2CH_2CH_3 \\ | \\ CH_3 \end{array}$$

Step 2. Name any alkyl group substituents.

$$\boxed{methyl} \Rightarrow CH_3 \qquad CH_2CH_3 \Leftarrow \boxed{ethyl}$$
$$CH_3CHCHCH_2CHCH_2CH_2CH_3$$
$$CH_3 \Leftarrow \boxed{methyl}$$

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

$$\boxed{3\text{-methyl}} \Rightarrow CH_3 \qquad CH_2CH_3 \Leftarrow \boxed{5\text{-ethyl}}$$
$$\overset{1\ \ 2\ \ 3\ \ 4\ \ 5\ \ 6\ \ 7\ \ 8}{CH_3CHCHCH_2CHCH_2CH_2CH_3}$$
$$CH_3 \Leftarrow \boxed{2\text{-methyl}}$$

Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

WHEN NEEDED: Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) identical substituents are present.

We will use the "**di" prefix** for the *methyl groups* (**dimethyl**)

Since one of the methyl groups is on carbon number **2** and the other is on carbon number **3**, we write **2,3-dimethyl**.

Place a **comma** *between position numbers*; note that we used "2,3-"

Place a **dash** between position *numbers* and *letters*.

NOTE:

Alphabetize using the alkyl group name *only*; **disregard** the Greek prefixes (di, tri, tetra).

⬇   ⬇

5-ethyl   **2,3-dimethyl**

5-ethyl-2,3-dimethyloctane

Common Errors

Do not assume that the parent chain position numbers always start with carbon number 1 as the left-most parent carbon.

There is often many different ways to draw the same molecule.

For example, 2-methylpentane can be correctly drawn as either of the structures shown below.

There is no molecule called *4-methylpentane.*

The **parent chain is the longest, continuous chain of carbons atoms, NOT necessarily** the carbon chain that is drawn horizontally in a single line.

For the molecule shown below, you may be temped to use octane for the parent chain (shaded blue), and then name the molecule **3-propyloctane**.

The correct way to think about naming this molecule is shown below.

The name of this molecule is **4-ethylnonane**.

Summary for Naming Normal and Branched Alkanes

Step 1. Name the *parent chain*.

- For normal and branched alkanes, the ***parent chain is the longest, continuous chain of carbons atoms***.

Step 2. Name any alkyl group substituents.

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

- In order to assign "position numbers" to the substituents, the carbons ***in the parent chain*** are numbered. ***Begin numbering from the end of the parent chain that is nearest to a substituent***.

Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

- List the alkyl groups along with their position numbers, ***in alphabetical order***.
- Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) identical substituents are present.
- Alphabetize using the alkyl group name ***only***; **disregard** the Greek prefixes (di, tri, tetra).
- Place a ***comma*** *between position numbers, and* a ***dash*** between position *numbers* and *letters*.
- Write the parent chain name ***behind*** the list of alkyl groups.

Understanding Check: Give the correct IUPAC name for these molecules.

$$CH_3CHCH_3$$

$$CH_3CHCH_2CH_2CH_2CH_2CH_3 \qquad CH_3CH_2CHCH_2CHCH_2CH_2CH_3$$

$$CH_3 \qquad\qquad\qquad CH_3$$
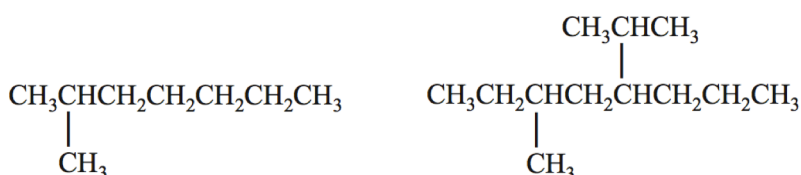
Understanding Check: Give the correct IUPAC name the alkane shown below.

$$CH_3 \quad CH_3$$
$$CH_3CH_2C\,CH_2CHCH_2CH_2CH_2CH_3$$
$$CH_3$$

Drawing the Structure of an Alkane from its Name

Example: Draw the ***condensed and skeletal*** structure for 2,2-dimethyl-4-propyloctane.
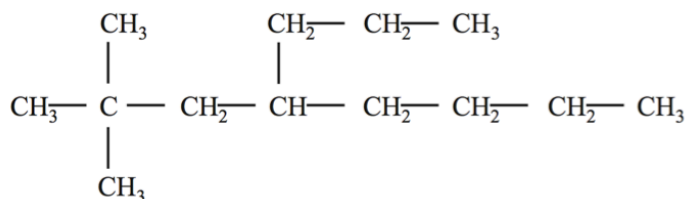
condensed structure   *skeletal structure*
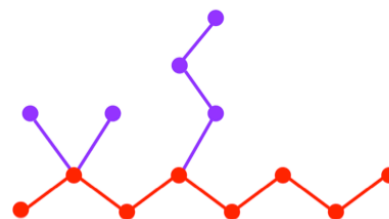
Understanding Check: Draw the ***condensed and skeletal*** structure for 6-isopropyl-2,3-dimethylnonane.

Cycloalkanes

Some alkanes contain carbon atoms bonded, not in a linear sequence, but in a "**ring**" pattern.

These alkanes are called _____.

- **Example** of a cycloalkane: *cyclohexane* (shown below).

| Line Bond Structure | Condensed Structure | Skeletal Structure |
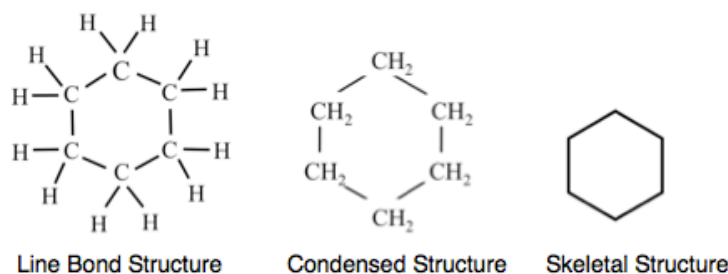
It is very common to see five- and six-carbon rings that occur in nature. The reason for this is that the bond angles in 5- and 6-carbon rings is fairly close to the 110° bond angles expected in molecules with AB_4 geometry.

In addition to the line bond, condensed, skeletal, and ball-and-stick representations, another structural representation called a "_____ - _____" is also used for cycloalkanes.

- Side-view structures contain information about the three-dimensional arrangement of the atoms.

The ball-and-stick model and a side-view structure for *cyclohexane* are shown below.

ball-and-stick model   side-view structure
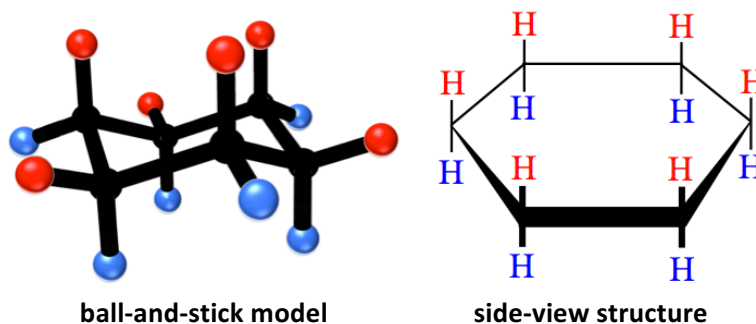
Note that in the ball-and-stick model (**left**), the ring of carbons (carbon atoms shaded black) is oriented horizontally. Each carbon is bonded to *two hydrogen atoms*. From each ring-carbon, one of these two bonds is oriented in a direction *pointing **above*** the ring structure (bonds to the red-shaded hydrogens), and the other bond is oriented in a direction *pointing **below*** the ring structure (bonds to the blue-shaded hydrogens).

It is convenient to express this three-dimensional information in the **side-view structural formula**. The actual bond angles are shown in the *ball-and-stick models* and are ***implied*** in the *side-view* representation.

In *side-view* structures, bold lines are used to indicate the perspective when viewing the ring. The ring is depicted as being oriented horizontally with the **bold edges** toward the viewer. The two bonds that are oriented upwards or downwards from the ring-carbons are drawn vertically. The hydrogen atoms in red font correspond to the hydrogens shown as red spheres in the ball and stick model; likewise the hydrogen atoms in the blue font correspond to the hydrogens shown as blue spheres in the ball-and-stick model.

Structural Representations of Cycloalkane Rings

	Cyclopropane	Cyclobutane	Cyclopentane	Cyclohexane
Line Bond Structure				
Condensed Structure				
Skeletal Structure				
Side-View Structure				
Ball-and-Stick Model				

Naming Cycloalkanes

Step 1. Name the *parent chain*.

For cycloalkanes, the ***parent chain is the* _____ *of carbon atoms*.

- The parent chain names for ring structures with 3 to 8 carbon atoms are shown on the right.

    Note that these names are based on the names used for the parent chains of branched alkanes, ***however* the term "_____" is used as a prefix.**

Common Error: A common mistake made by first-semester students is the failure to differentiate *cyclic* and *noncyclic* structures.

- For example, see the difference between hexane and cyclohexane below:

Cyclohexane

$CH_3—CH_2—CH_2—CH_2—CH_2—CH_3$
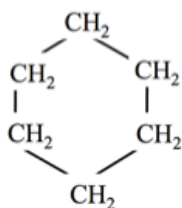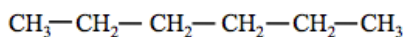
Hexane

Parent Chain Names for Cycloalkanes

Number of Carbon Atoms in Ring	Parent Chain Name
3	cyclopropane
4	cyclobutane
5	cyclopentane
6	cyclohexane
7	cycloheptane
8	cyclooctane

Step 2. Name any alkyl groups substituents.

The alkyl groups are named in the *same way* as we did for branched alkanes (methyl, ethyl, propyl, isopropyl, etc.).

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

We use the following rules for assigning position numbers to the ring-carbons.

- If there is *only* _____ *substituent*, a position number is not used.
    - Name the molecule by placing the alkyl group substituent name in front of the parent chain name; *no further steps are needed*.
    - For example, consider the molecule drawn *to the right* with a single, methyl group substituent attached to a six-carbon ring.

        We name this molecule **methylcyclohexane**.
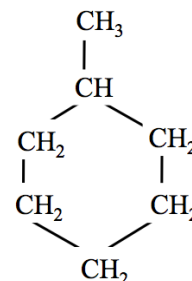
- If there is *more than one substituent*, assign position numbers to the alkyl groups.
    - For *identical substituents*, arbitrarily assign one of them to position number one. Then, beginning with carbon number **1**, number the other carbons in the direction (clockwise or counterclockwise) that gives the _____ sum of position numbers.
    - **Example:**

    1,3-dimethylcyclohexane   vs.   1,5-dimethylcyclohexane
            (correct)   (incorrect)
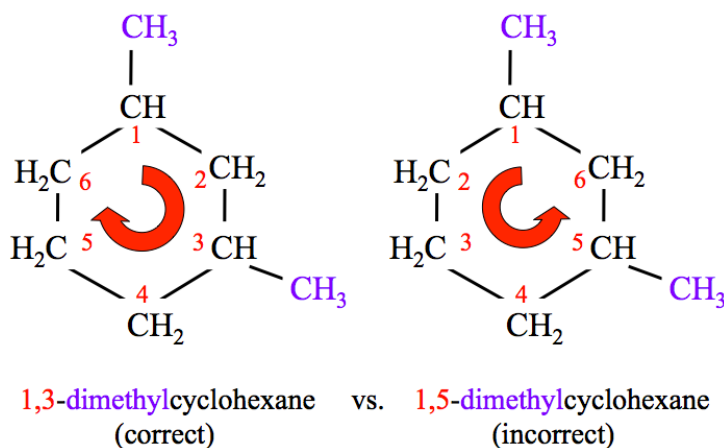
    - When substituents are *non identical*, the ring-carbon attached to the substituent that comes **first in alphabetical order is assigned position number 1.**
        - For example, the molecule drawn **below** has *non identical* substituents.

    We assign the position **number 1** to the ring-carbon that is bonded to the *ethyl group* because <u>e</u>thyl comes before <u>m</u>ethyl alphabetically.

    We number the ring-carbons in the **counter-clockwise direction** in order to result in the *smallest sum of position numbers*.
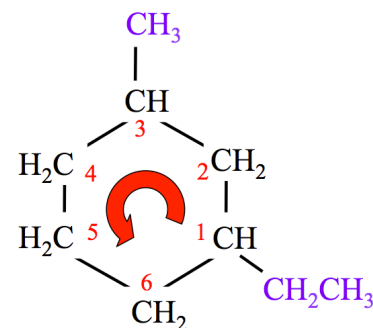
    1-ethyl-3-methyl

Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

- Step 4 is used in the exact same way for cycloalkanes as for branched alkanes.
- Let's name the cycloalkanes from our last two examples.
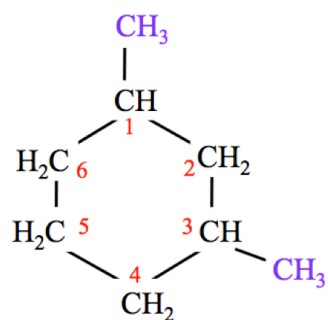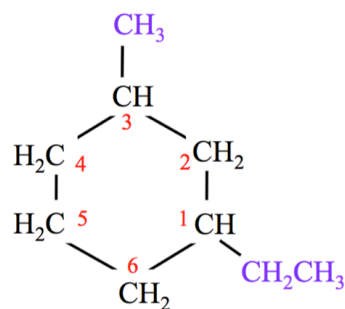
1,3-dimethylcyclohexane   1-ethyl-3-methylcyclohexane

Understanding Check:

The *cycloalkane* molecule shown below exists as a colorless gas at room temperature. What is the IUPAC system name for this molecule?
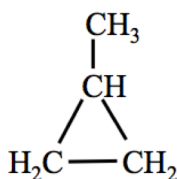
Understanding Check:

Draw the line bond, condensed, **and** skeletal structures of the following cycloalkanes:

    a. 1,1-dimethylcyclobutane

    b. 1-methyl-3-propylcyclopentane

    c. 1,4-diethylcyclohexane

Isomers

Isomers

isos | merós

equal | part
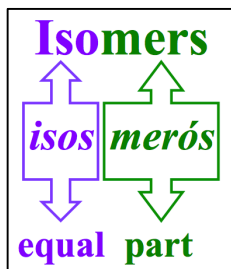
Isomers are molecules that have the _____ *molecular* _____, but differ in the way the atoms are arranged.

You will learn about two types of isomers:

    1) Constitutional Isomers

    2) Stereoisomers

Constitutional Isomers

Molecules that have the ***same molecular formula***, but ***different atomic connections*** are called

_____ _____.

Example: Consider the *three* constitutional isomers that have the molecular formula of C_5H_{12}.

$CH_3CH_2CH_2CH_2CH_3$

$$CH_3CHCH_2CH_3 \atop \qquad | \atop \qquad CH_3$$

$$CH_3 \atop | \atop CH_3CCH_3 \atop | \atop CH_3$$
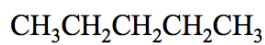
pentane
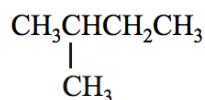
boiling point = 36°C

2-methylbutane

boiling point = 28°C
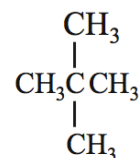
2,2-dimethylpropane

boiling point = 10°C

Understanding Check: Draw the constitutional isomers for C_4H_{10}

Understanding Check: Draw and **name** the *five* constitutional isomers of C_6H_{14}

Conformations

The infinite number of shapes that a molecule can take, because of the rotation around bonds, are called

_____.

Example: A *few* of the infinite conformations of *butane* resulting from rotation about the single bond between carbon number 2 and carbon number 3.
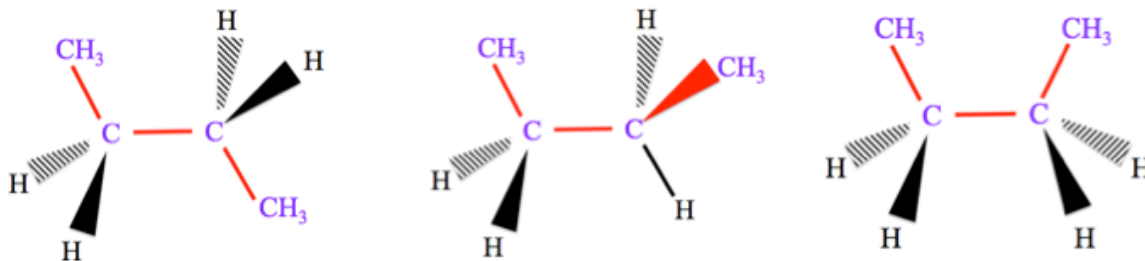
Common Error Warning: Do not confuse *conformations* with *constitutional isomers*!

The different *conformations* of a molecule have the *same molecular formula* and have the *same atomic connections*; whereas *constitutional isomers* have the *same molecular formula* yet **different** *atomic connections*.

Stereoisomers

In *cycloalkanes*, the free rotation around the carbon-carbon single bonds is _____ because hydrogens and/or substituents bonded to ring-carbons are too large to rotate through the center of the ring structure.

The restricted rotation results in the existence of a special type of _____.
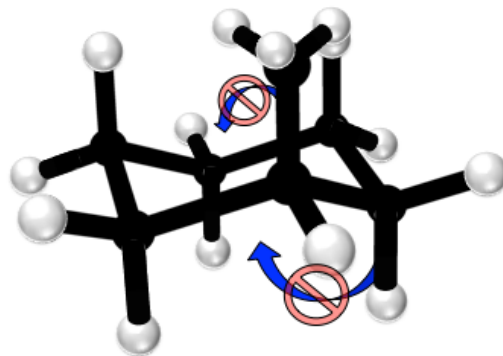
Stereoisomers are molecules that:
- have the *same* molecular formula
- have the *same* atomic connections
- have a *different* 3-dimensional shape
    > *So far the definition of stereoisomers is the same as conformations - but the next item makes them quite different.*
- **cannot** be converted from one to another without *breaking and reforming bonds*

It is **not** possible for one stereoisomer to take the shape of another stereoisomer by rotation around a bond.

Geometric Isomers

When *stereoisomers* exist because of *restricted bond rotation*, the stereoisomers are called
_____ *isomers*.

Examples:

trans-1,2-dimethylcyclohexane

cis-1,2-dimethylcyclohexane
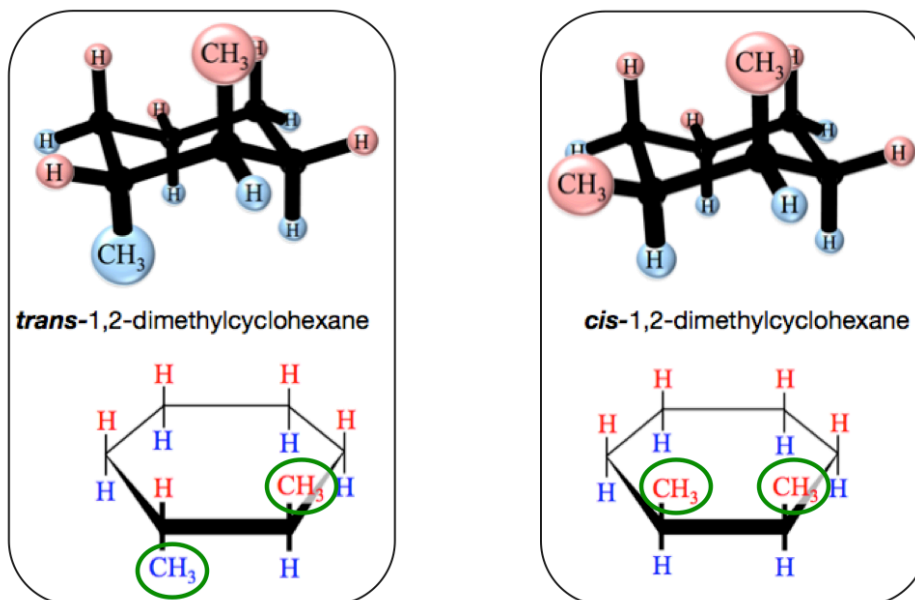
Geometric isomers come in *pairs* – one is the "_____-" and one is the "_____-" isomer.

When cycloalkanes have _____ *substituents*, *each on a different ring-carbon*, then there are two
geometric isomers.

For *cycloalkanes*, a *cis* geometric isomer has *both substituents* oriented in the same direction (either **both**
pointing above the ring structure or **both** *pointing below* the ring structure).

Conversely, a *trans* geometric isomer has the two *substituents* oriented in opposite directions (**one**
pointing above the ring structure and the **other** *pointing below* the ring structure).

two ways to draw *cis* cyclic compounds:
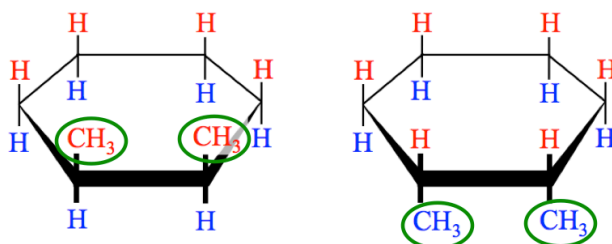
two ways to draw *trans* cyclic compounds:
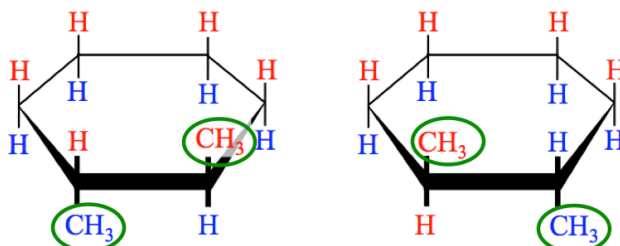
To visualize the cycloalkane geometric isomers, we must use *ball-and-stick representations* **or** draw **side view** structures; the three dimensional information in the **cis** vs. **trans** geometries **cannot** be visualized using our standard line bond, condensed, or skeletal structures.

Because alkyl group substituents cannot rotate through the center of the ring, the **trans** and **cis** isomers of cycloalkanes are **two different molecules**; they have slightly different physical properties (density, melting points, vapor pressure, etc.) and different chemical properties.

There are only slight differences in many properties because the isomers are very similar (but not identical).

- One important difference in the properties of some geometric isomers is their bioactivity.

Understanding Check

Using the templates below, complete the side view structures for the *cis* and *trans* isomers of 1,2 dimethylcyclopentane.
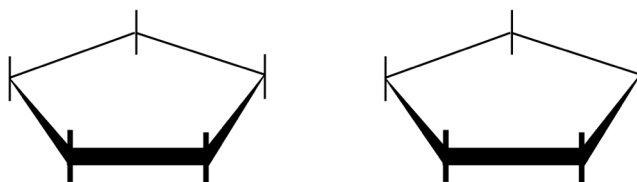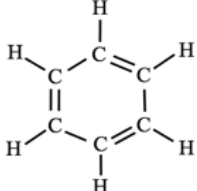
Understanding Check

Which of the following molecules have cis and trans isomers? There may be more that one correct selection.

   a) 1,2-dimethylcyclopentane

   b) 1-ethyl-2-propylcyclobutane

   c) methylcyclohexane

   d) 1,1-dimethylcylcohexane

Unsaturated Hydrocarbons

Review: Hydrocarbons can be categorized into the four subcategories:

Category	Defining Feature	Saturation	Example
alkane	all single bonds	saturated	ethane $CH_3 - CH_3$
alkene	at least one carbon-carbon **double** bond	unsaturated	ethene $CH_2 = CH_2$
alkyne	at least one carbon-carbon **triple** bond	unsaturated	ethyne $CH \equiv CH$
aromatic	alternating double and single bonds in a **cyclic** hydrocarbon	unsaturated	benzene

Unsaturated hydrocarbons contain one or more carbon-carbon _____ or _____ bonds.

Alkenes

_____ are molecules that consist *only of carbon and hydrogen atoms* and contain ***at least one carbon-carbon double bond***.
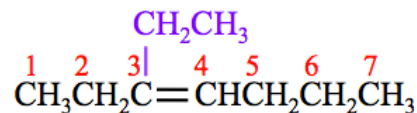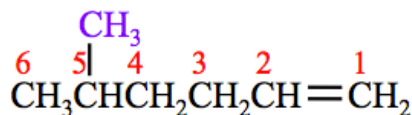
Systemic Method for Naming Alkenes:

Step 1. Find and name the *parent chain*.

The *parent chain is the longest, continuous chain of carbon atoms that* _____ *the double bond*.

The parent chain is named by combining a *numbering prefix* that specifies the number of carbon atoms in the parent chain, with the "-_____" suffix, which identifies the molecule as an **alkene**.

This parent chain *numbering prefixes* are the same as were used for *alkanes*, however we use the "**ene**" suffix.

- **Example:** If an alkene has three carbon atoms in the parent chain, the parent chain name is *prop**ene***.

For alkenes with ***more than three carbons***, the position of the double bond must be indicated by adding a *position number* to the parent chain name.

- Position number **1** is assigned to the carbon at the end of the parent chain that is **closest to the double bond.**

$$\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{CH_3}$$
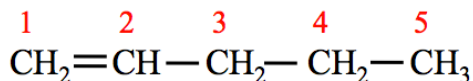
- If the double bond is between carbons number **1** and **2**, the number "**1**" is used as a prefix to the parent chain name. For example, in the molecule below, the parent chain is called **1**-pentene.

$$\overset{1}{CH_3}-\overset{2}{CH}=\overset{3}{CH}-\overset{4}{CH_2}-\overset{5}{CH_3}$$
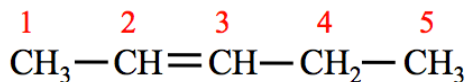
- If the double bond is between carbons number **2** and **3**, the number "**2**" is used as a prefix to the parent chain name. For example, in the molecule below, the parent chain is called **2**-pentene.

- If the double bond is between carbons number **3** and **4**, the number "**3**" is used as a prefix to the parent chain name...etc.

  Note that this is different from the method we used for numbering *alkanes*; for alkanes we assigned position number **1** to the carbon on the end of the parent chain that was closest *to a substituent*.

Step 2. Name any alkyl group substituents.

- **Alkyl group substituents** are named in the same way as you did for alkanes.

Step 3. Construct the name of the alkene by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

- This is done the same way as you did with alkanes.
- Remember to use a dash between position numbers and letters.

Example: What is the name of this alkene:
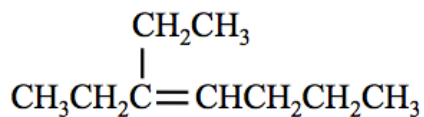
Step 1. Find and name the *parent chain*.

$$CH_3CH_2\overset{\overset{\displaystyle CH_2CH_3}{|}}{C}=CHCH_2CH_2CH_3$$

The *parent chain is the longest, continuous chain of carbon atoms that **contains the double bond**.*

- There are seven carbons in the parent chain.

Position number **1** is assigned to the carbon *at the end* of the parent chain that is **closest to the double bond.**

$$\overset{1}{CH_3}\overset{2}{CH_2}\overset{3}{\underset{|}{C}}\overset{|}{=}\overset{4}{CH}\overset{5}{CH_2}\overset{6}{CH_2}\overset{7}{CH_3}$$
(with CH$_2$CH$_3$ above carbon 3)

Since the double bond is between carbons number **3** and **4**, the number "**3**" is used as a prefix in the parent chain name.

> Parent chain name: **3-heptene**

Step 2. Name any alkyl group substituents.

Alkyl group substituents are named in the same way as we did for alkanes.

There is one substituent in this example: **ethyl**

Step 3. Construct the name of the alkene by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

The **ethyl** substituent is attached to carbon number **3**, use **3-ethyl.**

The name of this molecule is: **3-ethyl-3-heptene**

Example: What is the name of this alkene:
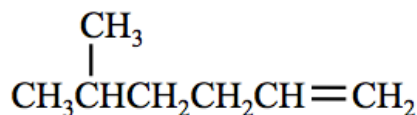
Step 1. Find and name the *parent chain*.

$$\overset{\overset{\displaystyle CH_3}{|}}{CH_3CH}CH_2CH_2CH=CH_2$$

The *parent chain is the longest, continuous chain of carbon atoms that **contains the double bond**.*

- There are six carbons in the parent chain.

Position number **1** is assigned to the carbon *at the end* of the parent chain that is **closest to the double bond.**

$$\overset{6}{CH_3}\overset{5}{CH}\overset{4}{CH_2}\overset{3}{CH_2}\overset{2}{CH}=\overset{1}{CH_2}$$
(with CH$_3$ above carbon 5)

Since the double bond is between carbons number **1** and **2**, the number "**1**" is used as a prefix in the parent chain name.

> Parent chain name: **1-hexene**

Step 2. Name any alkyl group substituents.

There is one substituent in this example: **methyl**

Step 3. Construct the name of the alkene by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

The **methyl** substituent is attached to carbon number **5**, use **5-methyl.**

The name of this molecule is: **5-methyl-1-hexene**

$$CH_3C = CHCH_3$$

with CH_3 above the first C
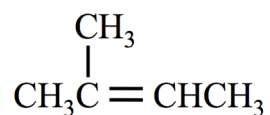
Understanding Check: Write the name of this alkene.
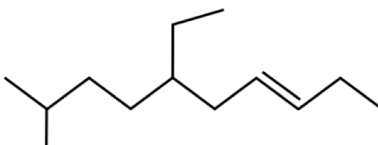
Understanding Check

Draw the **line bond**, **condensed**, **_and_** **skeletal structure** for each of these alkenes.

a) 2-methyl-1-butene

b) 3-ethyl-4-methyl-3-hexene

Geometric Isomers of Alkenes

*Unlike the case for single bonds, **there is no rotation around double bonds**.*

All other bonds to both double-bonded carbon atoms in alkenes are at 120° angles and *are on the same* _____ *as the double bond*.

- **Example:** Ethene
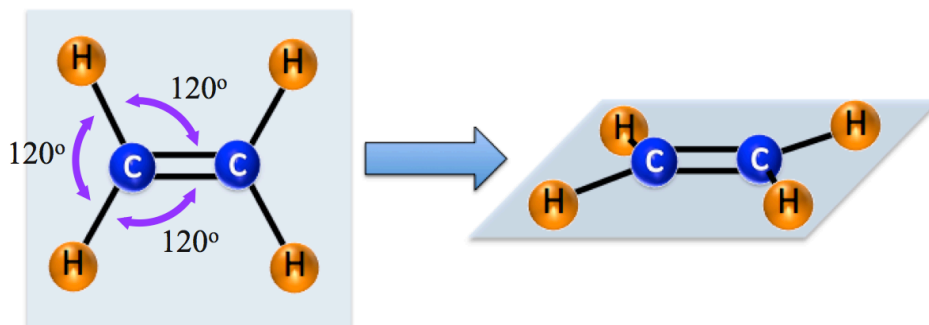
Because of the *geometry and lack of rotation around double bonded carbons*, **some alkenes can exist as** _____ _____ (*cis* and *trans*).

- **Example:** 2-butene
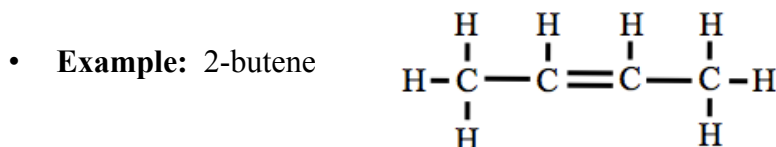
There are two possible geometric arrangements of the two methyl groups attached to the double bonded carbons.
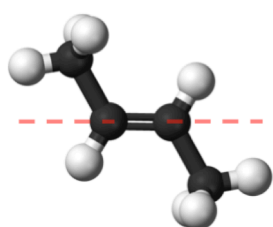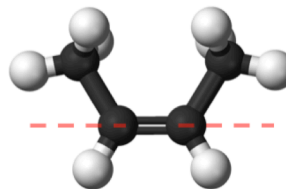
trans-2-butene   *cis*-2-butene

We identify the *cis* and *trans* isomers by noting the positions of alkyl groups on each of the double-bonded carbons relative to an imaginary line passing *along the double bond*.

When the alkyl groups are on _____ *sides* of the imaginary line, we have the *trans* geometric isomer.

When **both** of the alkyl groups are on the _____ *side* of the imaginary line, we have the *cis* geometric isomer.

Since the nature of double bonds does not allow free rotation, it is **not** possible for a *trans* isomer to rotate and thereby convert to the *cis* isomer (and vice versa).

I want to elaborate on the *inability for cis and trans isomers to interconvert* by contrasting **geometric isomers** and **conformations**. *Conformations* of a molecule arise from rotation around single bonds. An infinite number of conformations are possible for an **individual** molecule. In contrast, *geometric isomers* are two, distinct molecules that cannot interconvert by rotation around bonds.

Geometric Isomers of 2-Butene

Conformations of Butane
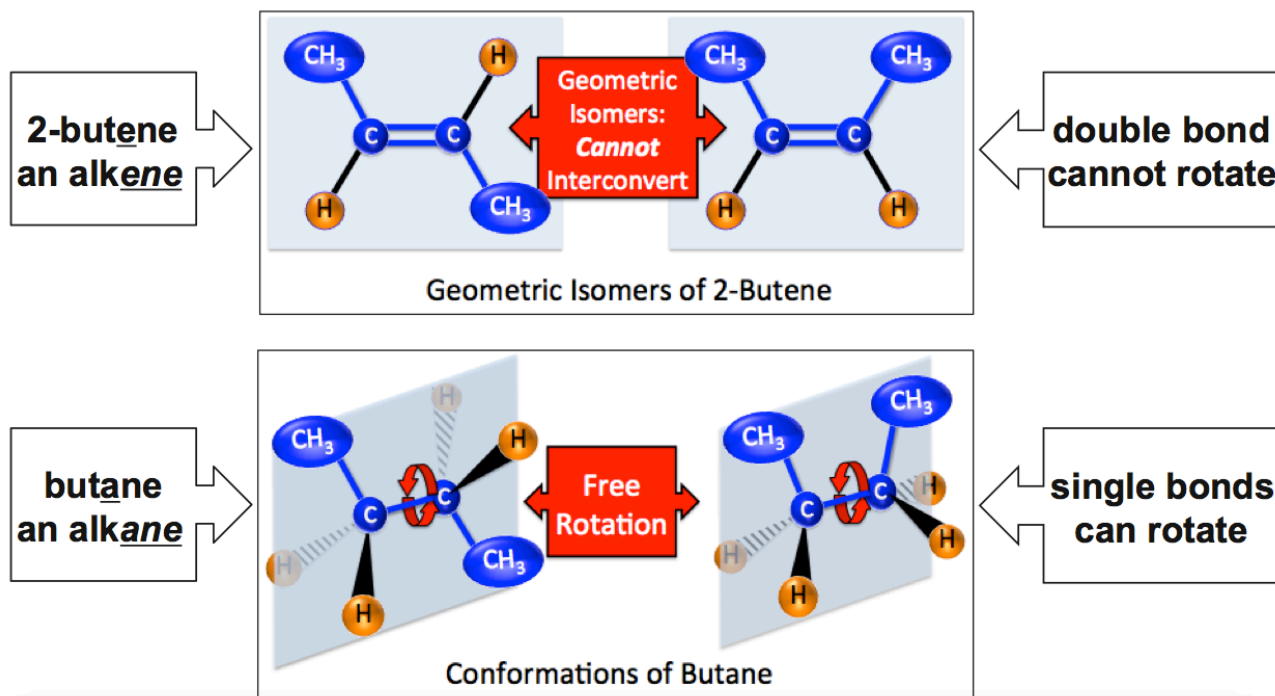
In order to differentiate *cis* vs. *trans* when using *condensed structures* for alkenes, the 120° bond angles around the double-bonded carbons are drawn as shown below.

trans-2-butene   **cis-2-butene**
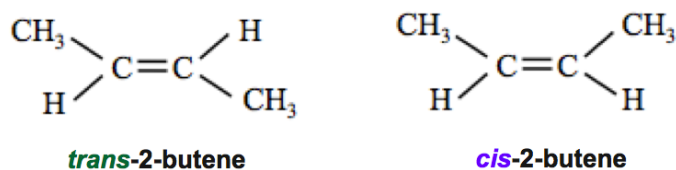
In *skeletal structures*, the bonds to the alkyl groups that emanate from the double-bonded carbons are oriented as shown below.

trans-2-butene   **cis-2-butene**

There will be *two correct ways* to draw **each *cis*** and **each *trans*** isomer.

- For example, the two **condensed structures** of *trans*-2-butene shown below are equivalent and equally correct representations of the isomer.

both are ***trans*-2-butene**

The two **condensed structures** of ***cis*-2-butene** shown below are equivalent.
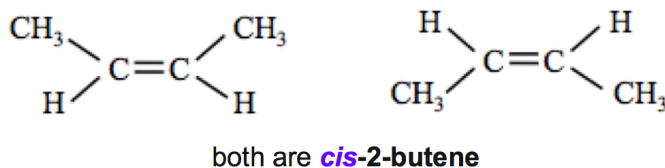
both are ***cis*-2-butene**

- The two **skeletal structures** of *trans*-2-butene shown below are equivalent and equally correct representations of the isomer.

both are ***trans*-2-butene**
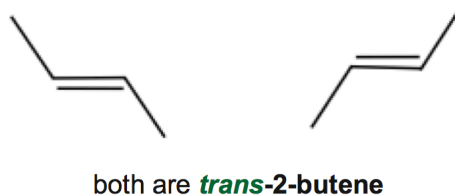
The two **skeletal structures** of *cis*-2-butene shown below are equivalent.
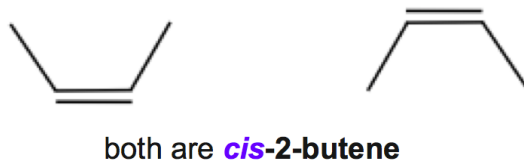
both are ***cis*-2-butene**

Alkynes

Alkynes are hydrocarbon molecules that contain *at least one carbon-carbon* _____ *bond*.
- Like the alk*ene*s, they are unsaturated hydrocarbons.

Naming Alkynes

Alkynes are named in the same way as you did for alkenes; the only difference is that we use the "_____"
suffix instead of the "**ene**" suffix.

    •   Example:

$$CH_3-C\equiv C-CH_2-CH_3$$

2-pentyne
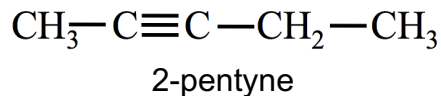
Alkyne Molecular Geometry

Alkynes involve a triple bond and the bond angles around the triple-bonded carbons are 180° as illustrated below.
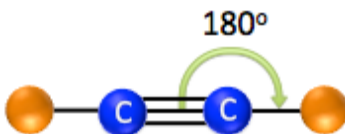
Each of the triple-bonded carbons can have only one other group single bonded to it (octet rule) and **this AB$_2$ geometry cannot result in geometric (*cis/trans*) isomers.**

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Aromatic Hydrocarbons

Aromatic hydrocarbons have alternating single and double bonds between the carbons that form the ring.

The smallest and simplest aromatic hydrocarbon that occurs is called _____.

- The line bond, condensed, and skeletal structures of **benzene** are shown below.

line bond structure   **condensed structure**   **skeletal structures**
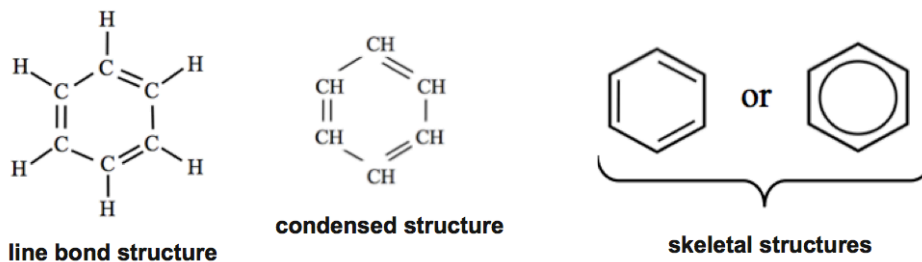
Naming Aromatic Hydrocarbons

Aromatic hydrocarbons are named using the same method that you used for cycloalkanes; **the ring structure is the parent chain.**

In this course, we will limit our naming of aromatic hydrocarbons to benzene and benzene rings with substituents.

- **Example:** The systemic name for the compound shown below is **methylbenzene**.
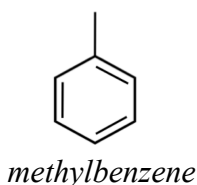
As was the case for cycloalkanes, we do not need to use a position number when there is only one substituent bonded to a ring structure.

methylbenzene

Note that sometimes book and journal authors combine (*hybridize*) skeletal and condensed structures when drawing cyclic compounds.

Example: Compare the skeletal and the skeletal/condensed hybrid structures of *methylbenzene*:
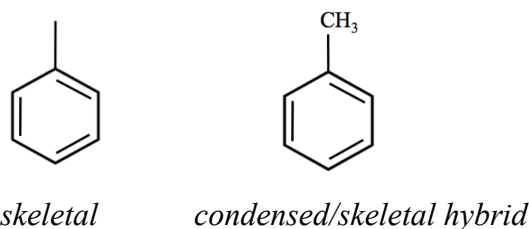
If you are using an online problem system and the question specifies a particular structure (i.e. line bond, condensed, skeletal), the auto-grader may not accept the hybrid as a correct response.

skeletal   *condensed/skeletal hybrid*

When cyclic compounds have *more than one substituent,* position numbers are included (you did so for cycloalkanes). **Examples:**

1,2-dimethylbenzene   1,3-dimethylbenzene   1,4-dimethylbenzene
(*ortho*-xylene)   (*meta*-xylene)   (*para*-xylene)
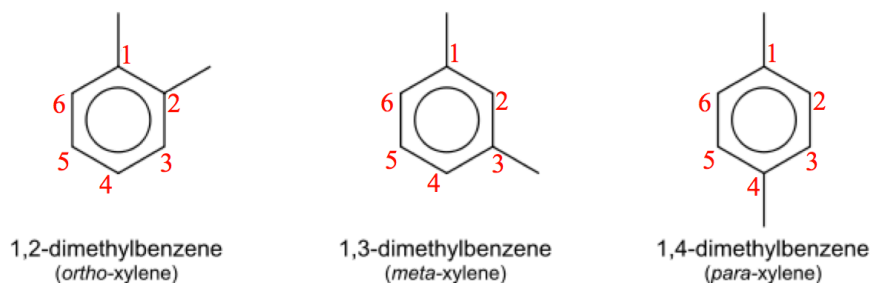
The common names are shown in parenthesis under the systemic names.

- When substituents are at positions number 1 and 2, then "***ortho-***" is used as a *prefix* in the common names.
- When substituents are at positions number 1 and 3, then "***meta-***" is used.
- When substituents are at positions number 1 and 4, then "***para-***" is used.

Some cyclic compounds have _____ *rings*.

Fused rings occur when neighboring rings *share carbon atoms*.

- For example, naphthalene, *shown on the right*, is an aromatic hydrocarbon that consists of *two fused rings*. The shared carbon atoms are highlighted red.
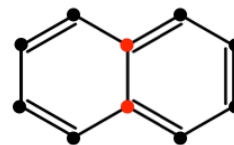
naphthalene

Aromatic hydrocarbons that contain fused rings are called **polycyclic aromatic hydrocarbons (PAHs)**.

- Some PAHs are shown in the table on the right.

Number of fused rings	Skeletal Structure	Name
3		Anthracene
4		Tetracene
4		Pyrene
4		Chrysene
5		Pentacene

Functional Groups

A _____ _____ is an **atom, group of atoms,** or **bond** that gives a compound a particular set of physical and chemical properties.

Organic compounds are categorized into various _____ by the functional group(s) that they contain.

You have already seen a couple examples of organic molecule *families* defined by the *type of carbon-carbon bond present*.

- When a carbon-carbon double bond (*functional group*) is present, the molecule is assigned to the *alkene* family.

- In the case of a carbon-carbon triple bond, we assigned the molecule to the *alkyne* family.

As an introduction to functional groups and families of organic compounds, in this video, I will introduce you to *three* organic families:

- **Alcohols**

- **Carboxylic Acids**

- **Esters**

The Alcohol Family

Alcohols contains one or more _____ (-OH) functional groups attached to a *hydrocarbon*.

The general form of an alcohol is shown below with the hydroxyl group highlighted in yellow.

$$\boxed{\text{Hydrocarbon}} - \ddot{\text{O}} - \text{H}$$
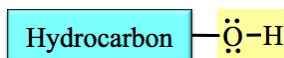
A specific example of an alcohol is ethanol. The condensed structural formula for ethanol is shown below.

$$CH_3CH_2 - OH$$
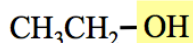
Ethanol is quite well known for being produced when carbohydrates, with the help of enzymes present in yeast, are used to make to beer, wine, and distilled adult beverages.

The Carboxylic Acid Family

Carboxylic acids contain a _____ *functional* group attached to a hydrocarbon.

Carboxyl groups contain both a *carbonyl group*, which is a carbon double bonded to an oxygen (**C=O**), *and* a *hydroxyl group* **(-OH)** that are connected to each other and the hydrocarbon (alkyl group) part.

$$\boxed{\text{Hydrocarbon}} - \overset{\overset{\displaystyle :O:}{\|}}{C} - \ddot{O} - H$$
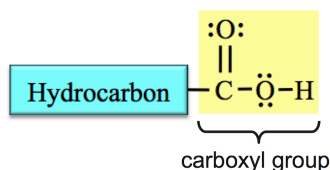
carboxyl group

A specific example of a carboxylic acid is *acetic acid*. The condensed structural formula for *acetic acid* is shown below.

$$CH_3 - \overset{\overset{\displaystyle O}{\|}}{C} - OH$$
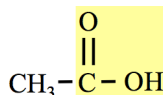
White vinegar is a mixture composed of 95% water and 5% acetic acid.

The Ester Family

Esters contain a _____ *functional* group that is bonded *between* *two* hydrocarbon parts.

Carboxylate groups contain both a *carbonyl group* (**C=O**), *and* an *oxygen atom.*

$$\boxed{\text{Hydrocarbon}} - \overset{\overset{\displaystyle :O:}{\|}}{C} - \ddot{O} - \boxed{\text{Hydrocarbon}}$$

carboxylate group
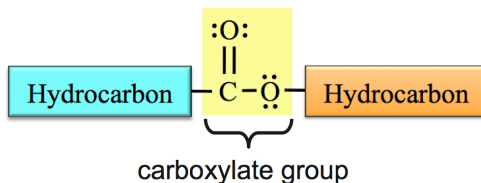
The boxes that represent hydrocarbons (alkyl groups) are shaded with different colors because the two hydrocarbon parts *are not always identical*.

Waxes are examples of esters.

- Waxes are produced in plants and animals; they are *esters* with relatively large hydrocarbon parts.
- The *skeletal* structural formula for one of the esters found in beeswax is shown below.

When drawing *condensed structures* of large molecules, such as the ester shown above, neighboring - CH$_2$ - groups can be further condensed in parenthesis as shown below:
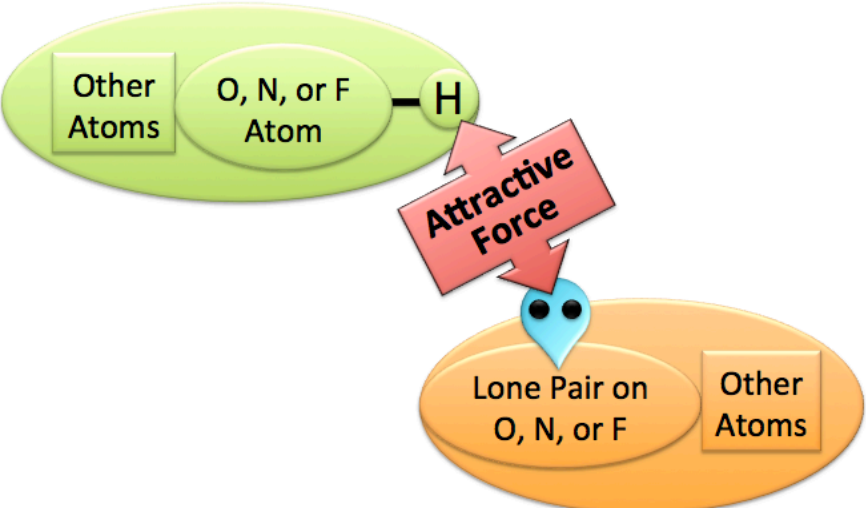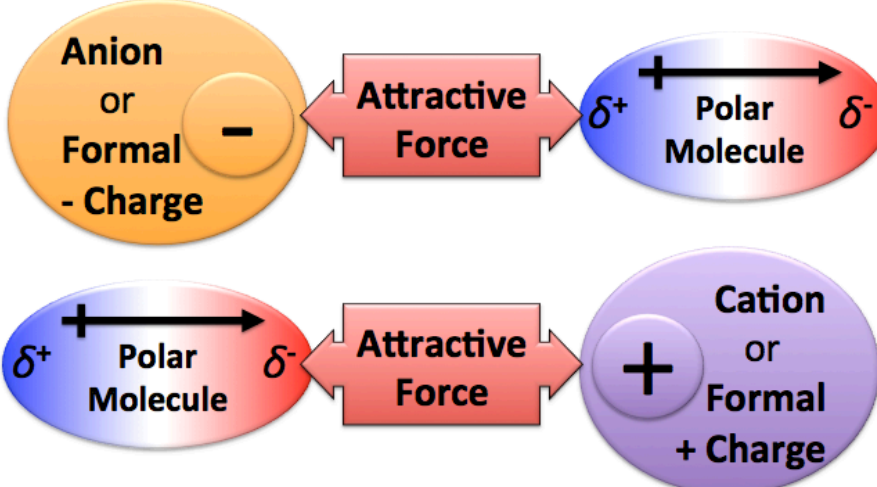
$$CH_3(CH_2)_{13}CH_2 \overset{\overset{\displaystyle O}{\|}}{C} - O - CH_2(CH_2)_{28}CH_3$$
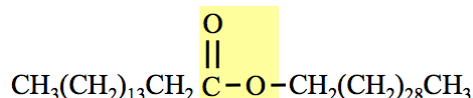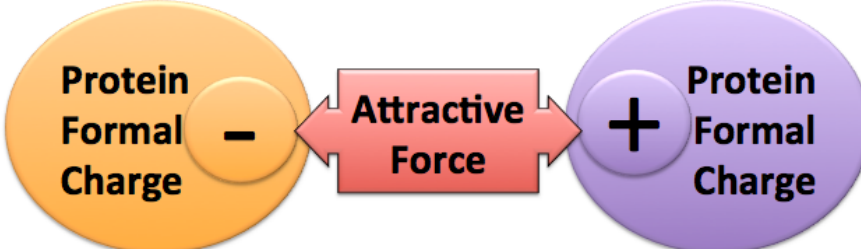
Summary of Organic Families and their Functional Groups

Organic Family	Functional Group	Description
Alkene	$C=C$ carbon-carbon double bond	Hydrocarbon with one or more *carbon-carbon double bonds*.
Alkyne	$C\equiv C$ carbon-carbon triple bond	Hydrocarbon with one or more *carbon-carbon triple bonds.*
Alcohol	-OH hydroxyl group	One or more hydroxyl groups bonded to a hydrocarbon
Carboxylic Acid	:O: ‖ —C–Ö–H carboxyl group	Carboxyl group bonded to a hydrocarbon
Ester	:O: ‖ —C–Ö— carboxylate group	Carboxylate group bonded *between* two hydrocarbons

Noncovalent Interactions Worksheet and Key

Summary of Noncovalent Interactions:

Noncovalent Interaction	Interaction Between:
Hydrogen Bonding Electrostatic attractive force between the partially positive charged hydrogen end of an O-H, N-H, or F-H bond and the negative charge of a lone pair on an O, F, or N.	
Dipole-Dipole Electrostatic attractive force between *two **polar** molecules*.	
London Dispersion Forces Electrostatic attractive force between ***any*** *two molecules*.	
Ion-Dipole Electrostatic attractive force between a *dipole* and *an ion or formal charge*. The partially positive charge of a dipole is attracted to a negatively charged ion *or* a negative formal charge. The partially negative charge of a dipole is attracted to a positively charged ion *or* positive formal charge.	
Salt Bridge Electrostatic attractive force between a negative formal charge and a positive formal charge in protein.	

Problems (see the key on the last two pages to check your work)

1) List **all** of the *noncovalent interactions* that can occur between the given pairs of molecules.

Molecules	Noncovalent Interaction(s) *Which noncovalent interactions occur between these pairs of molecules?*
Methane (CH_4) and Methane (CH_4)	

    H   H   H   H
    | | | |
H — C — C — Ö — H   H — C — C — Ö — H
    | | | |
    H H and H H	

H_2O and H_2O	
NH_3 and NH_3	

    •Ö•   •Ö•
    || ||
$CH_3C\,CH_2CH_3$ and $CH_3C\,CH_2CH_3$	

  :Ö—H   :Ö—H
    | |
$CH_3C\,CH_2CH_3$ and $CH_3C\,CH_2CH_3$	

HCl and HCl	
CO_2 and CO_2	
CCl_4 and CCl_4	

    H   H
    | |
H — C — Cl   H — C — Cl
    | |
    Cl and Cl	

2) If the given pairs of substances in the table below were mixed together, list **all of the noncovalent interactions** that could occur.

Choices:

(A) Hydrogen bonding

(B) Dipole-dipole forces

(C) London dispersion forces

(D) Ion-dipole forces

(E) Salt bridges

Compound Pairs	List of Noncovalent Interactions
NH_3 and H_2O	
Mg^{2+} and H_2O	
Cl_2 and H_2	
Acetic acid and H_2O $\ddot{O}$ $\parallel$ $CH_3C-\ddot{O}-H$ Acetic Acid	
SO_2 and H_2O	
SO_2 and H_2S	
ethane (CH_3CH_3) and methane (CH_4)	

Key

1) List **all** of the *noncovalent interactions* that can occur between the given pairs of molecules.

Molecules	Noncovalent Interaction(s)
Methane (CH_4) and Methane (CH_4)	London dispersions forces
and	hydrogen bonding, dipole-dipole forces, London dispersions forces
H_2O and H_2O	hydrogen bonding, dipole-dipole forces, London dispersions forces
NH_3 and NH_3	hydrogen bonding, dipole-dipole force, London dispersions forces
and	dipole-dipole forces, London dispersions forces
and	hydrogen bonding, dipole-dipole forces, London dispersions forces
HCl and HCl	dipole-dipole forces, London dispersions forces
CO_2 and CO_2	London dispersions forces
CCl_4 and CCl_4	London dispersions forces
and	dipole-dipole forces, London dispersions forces

2) If the given pairs of substances in the table below were mixed together, *list all of the noncovalent interactions* that could occur.

Choices:

(A) Hydrogen bonding

(B) Dipole-dipole forces

(C) London dispersion forces

(D) Ion-dipole forces

(E) Salt bridges

Compound Pairs	List of Noncovalent Interactions
NH_3 and H_2O	A, B, C
Mg^{2+} and H_2O	D (We will limit London dispersion forces to molecules and polyatomic ions; they are too small to be significant in monatomic **ions** in most applications)
Cl_2 and H_2	C
Acetic acid and H_2O Acetic Acid	A,B,C
SO_2 and H_2O	A,B,C,D (There is a formal charge of (1-) on an oxygen in SO_2; consider the line bond structure and you will see an oxygen that has *just one single bond*.)
SO_2 and H_2S	B,C,D
ethane (CH_3CH_3) and methane (CH_4)	C

Alkanes Worksheet and Key

1. Answer the following.

    a. What is the general formula for a ***non*cyclic alkane? C?H?

    b. If a ***non*cyclic alkane contains 15 carbon atoms, how many hydrogen atoms does it contain?

2. Draw the line bond structures of following types of hydrocarbons using *four* carbon atoms:

    a. **two *non*cyclic alkanes**

    b. **two** cycloalkanes

3. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for pentane.

    Molecular formula:

    Line bond structural formula:

    Condensed structural formula:

    Skeletal formula:

4. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for octane.
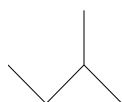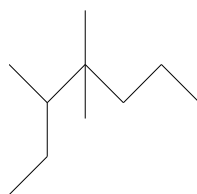
    Molecular formula:

    Line bond structural formula:

Condensed structural formula:

Skeletal formula:

5. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for 4-ethyl-2,3-dimethylheptane.

Molecular formula:

Line bond structural formula:

Condensed structural formula:

Skeletal formula:

6. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for 3,3-diethyloctane.

Molecular formula:

Line bond structural formula:

Condensed structural formula:

Skeletal formula:

7. What is the systematic name for the following structure?

8. What is the systematic name for the following structure?

9. There are 18 different alkane molecules that all have the molecular formula C_8H_{18}. Molecules with the same molecular formula, but different atomic connections (structural formulas) are called "constitutional isomers". See how many different alkanes, all with the same formula (C_8H_{18}) that you can draw. After you draw them, write their names. You can draw line bond, condensed, or skeletal structures (the key shows skeletal structures).

Alkanes Worksheet Key

1. Answer the following.

   a. What is the general formula for a **non**cyclic alkane? C_nH_{2n+2}

   b. If a **non**cyclic contains 15 carbon atoms, how many hydrogen atoms does it contain? **32**

2. Draw the line bond structures of following types of hydrocarbons using *four* carbon atoms:
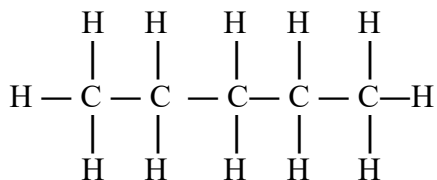
   a. **two** **non**cyclic alkanes
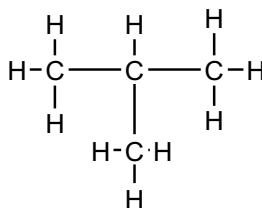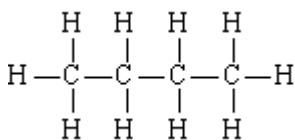
   b. **two** cycloalkanes
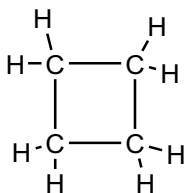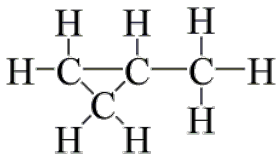
3. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal structure for pentane.
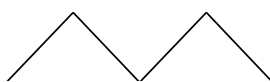
   Molecular formula: C_5H_{12}

   Line bond structural formula:

   Condensed structural formula: $CH_3CH_2CH_2CH_2CH_3$
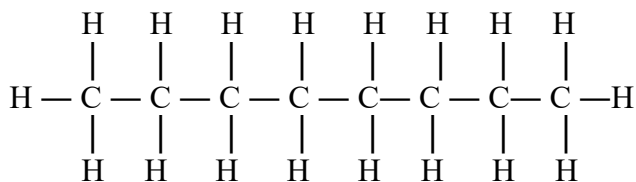
   Skeletal formula:

4. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for octane.
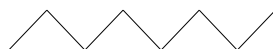
   Molecular formula: C_8H_{18}

   Line bond structural formula:

   $$
   \begin{array}{c}
   \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\
   | \quad | \quad | \quad | \quad | \quad | \quad | \quad | \\
   \text{H} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{C} - \text{H} \\
   | \quad | \quad | \quad | \quad | \quad | \quad | \quad | \\
   \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H}
   \end{array}
   $$

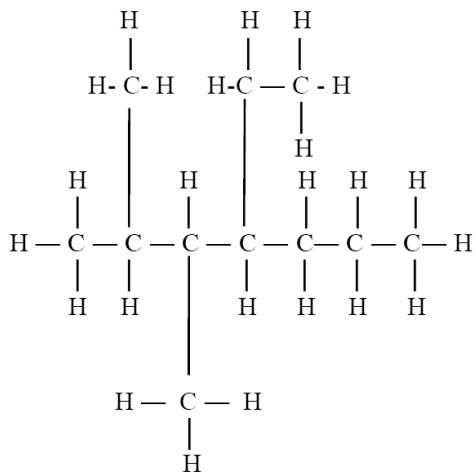   Condensed structural formula: $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
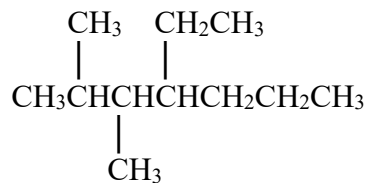   Skeletal formula:

5. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for 4-ethyl-2,3-dimethylheptane.
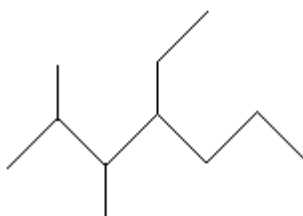
   Molecular formula: $C_{11}H_{24}$

   Line bond structural formula:

   Condensed structural formula:

   $$
   \begin{array}{c}
   \text{CH}_3 \quad \text{CH}_2\text{CH}_3 \\
   | \qquad | \\
   \text{CH}_3\text{CHCHCHCH}_2\text{CH}_2\text{CH}_3 \\
   | \\
   \text{CH}_3
   \end{array}
   $$

   Skeletal formula:

6. Give the molecular formula, the line bond structural formula, the condensed structural formula, and the skeletal formula for 3,3-diethyloctane.

Molecular formula: $C_{12}H_{26}$

Line bond structural formula:

```
         H   H
         |   |
     H — C — C — H
         |   |
             H
  H   H      H   H   H   H   H
  |   |      |   |   |   |   |
H—C — C — C — C — C— C — C— C —H
  |   |      |   |   |   |   |
  H   H      H   H   H   H   H
             H
             |
     H — C — C — H
         |   |
         H   H
```

Condensed structural formula:

```
        CH2CH3
         |
CH3CH2CCH2CH2CH2CH2CH3
         |
        CH2CH3
```

Skeletal formula:

7. What is the systematic name for the following structure?

2-methylbutane

8. What is the systematic name for the following structure?
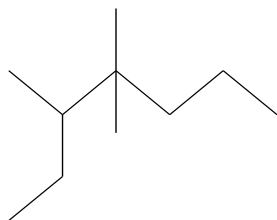
Note that this is the only "trick question" in this course; the parent chain is the *longest continuous chain of carbon atoms*, **NOT** always the chain that is drawn horizontally. The parent chain carbons are shown as black dots and the carbons in substituents (methyl groups) are shown as black squares in the drawing on the right.
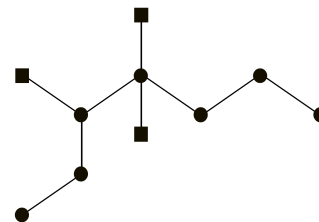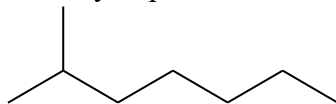
3,4,4-trimethylheptane

9. There are 18 different alkane molecules that all have the molecular formula C_8H_{18}. Molecules with the same molecular formula, but different atomic connections (structural formulas) are called "constitutional isomers". See how many different alkanes, all with the same formula (C_8H_{18}) that you can draw. After you draw them, write their names. You can draw line bond, condensed, or skeletal structures (the key shows skeletal structures).
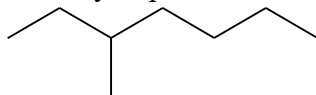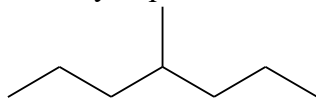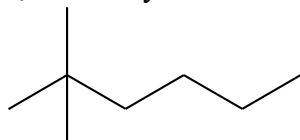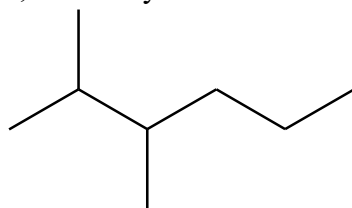
octane
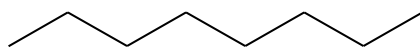
2-methylheptane

3-methylheptane

4-methylheptane

2,2-dimethylhexane
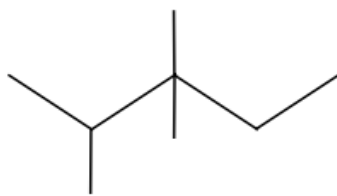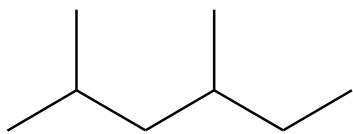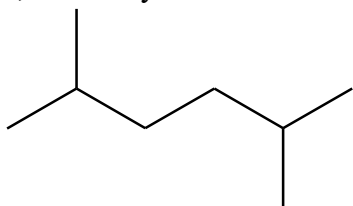
2,3-dimethylhexane

Continued on next page

2,4-dimethylhexane

2,3,3-trimethylpentane

2,5-dimethylhexane

2,3,4-trimethylpentane
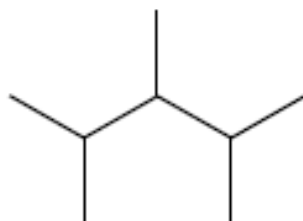
3,3-dimethylhexane
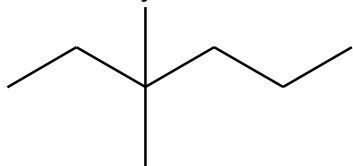
3-ethyl-2-methylpentane
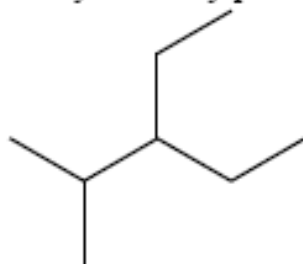
3,4-dimethylhexane
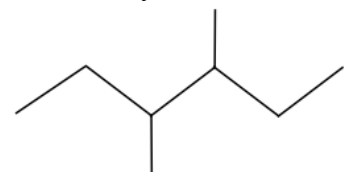
3-ethyl-3-methylpentane
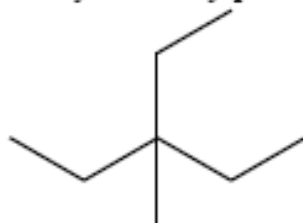
3-ethylhexane
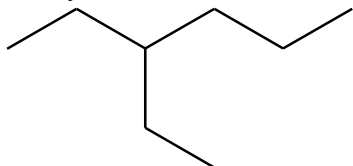
2,2,3,3-tetramethylbutane
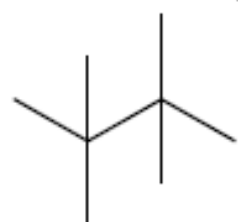
2,2,3-trimethylpentane
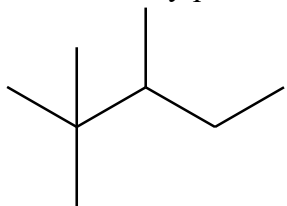
2,2,4-trimethylpentane
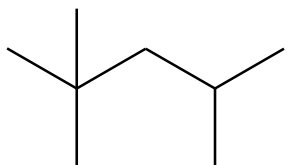
Alkenes and Alkynes Worksheet and Key

1. Draw the ***line bond*** structures for the following alkenes, cyclic alkenes, and alkynes:

a) noncyclic alkenes that contain 4 carbon atoms (three possible)

b) cyclic alkenes that contain 4 carbon atoms (four possible)

c) alkynes that contain 4 carbon atoms (two possible, neither of them are cyclic alkynes)

2. Draw the line bond structural formula, the condensed structural formula, and the skeletal structural formula for 1-pentene.

Line bond structure:

Condensed structure:

Skeletal formula:

3. Draw the line bond structural formula, the condensed structural formula, and the skeletal structural formula for 2-pentene.

   Line bond structure:

   Condensed structure:

   Skeletal formula:

4. Draw the line bond structural formula, the condensed structural formula, and the skeletal structural formula for 2-methyl-3-heptene.

   Line bond structure:

   Condensed structure:

   Skeletal formula:

5. Draw the line bond structural formula and the condensed structural formula for 3,3-diethyl-1-octyne.

   Line bond structure:

   Condensed structure:

6. What is the systemic name for the following structure?

7. What is the systemic name for the following structure?

$$CH_3C \equiv CCH_2CH_2CH_3$$

Alkenes and Alkynes Worksheet Key

1) Draw the **line bond** structures for the following alkenes, cyclic alkenes, and alkynes:

a) noncyclic alkenes that contain 4 carbon atoms (3 possible)

$$H-\overset{\overset{\displaystyle H}{|}}{C}=\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{C}-H$$

$$H-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{C}=\overset{\overset{\displaystyle H}{|}}{C}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-H$$

H-C-H

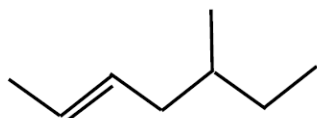$$H-\overset{\overset{\displaystyle H}{|}}{C}=\overset{|}{C}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-H$$
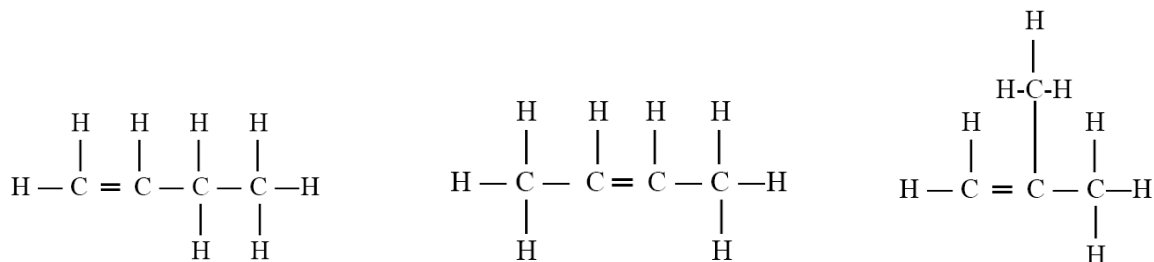
b) cyclic alkenes that contain 4 carbon atoms (4 possible)
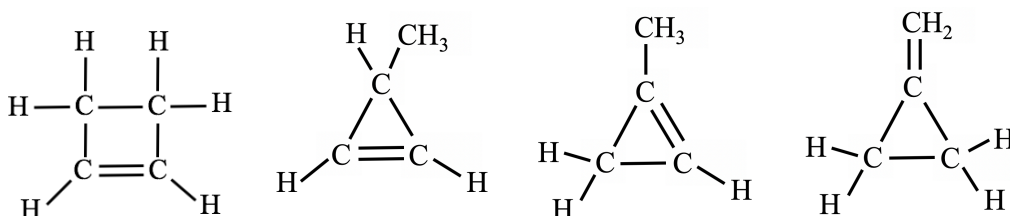
c) alkynes that contain 4 carbon atoms (2 possible, neither of them are cyclic alkynes)
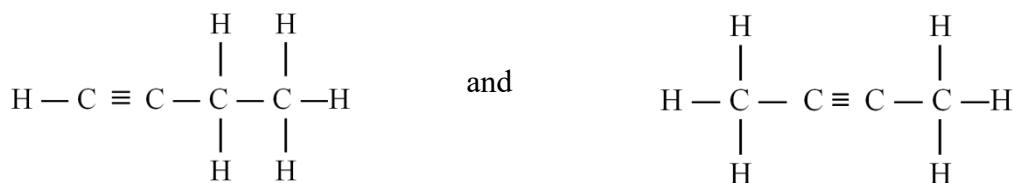
$$H-C\equiv C-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-H$$

and

$$H-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-C\equiv C-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-H$$

2. Draw the line bond structural formula, the condensed structural formula, and the skeletal structural formula for 1-pentene.

Line bond structure:

$$H-\overset{\overset{\displaystyle H}{|}}{C}=\overset{\overset{\displaystyle H}{|}}{C}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-H$$

Condensed structure: $CH_2=CHCH_2CH_2CH_3$

Skeletal structure:
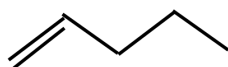
3. Draw the line bond structural formula, the condensed structural formula, and the skeletal structural formula for 2-pentene.

Line bond structure:

$$
\begin{array}{cccccc}
& H & H & H & H & H \\
& | & | & | & | & | \\
H - & C - & C = & C - & C - & C -H \\
& | & & & | & | \\
& H & & & H & H
\end{array}
$$

Condensed structure: $CH_3CH=CHCH_2CH_3$

Skeletal structure:
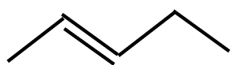
4. Draw the line bond structure, the condensed structural formula, and the skeletal structural formula for 2-methyl-3-heptene.

Line bond structure:

$$
\begin{array}{c}
H \\
| \\
H\text{-}C\text{-}H \\
\end{array}
$$

H-C-C-C=C-C-C-C-H

Condensed structure:

$$
\begin{array}{c}
CH_3 \\
| \\
CH_3CHCH=CHCH_2CH_2CH_3
\end{array}
$$
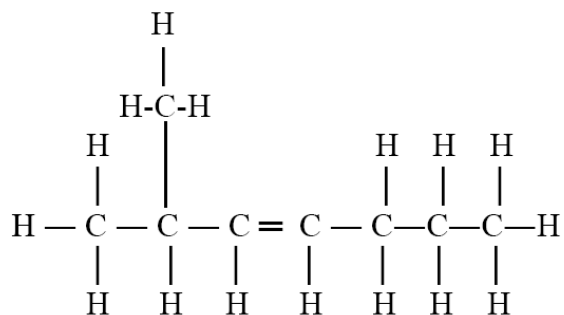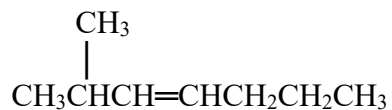
Skeletal structure:

5. Draw the line bond structural formula and the condensed structural formula for 3,3-diethyl-1-octyne.

Line bond structure:

$$
\begin{array}{c}
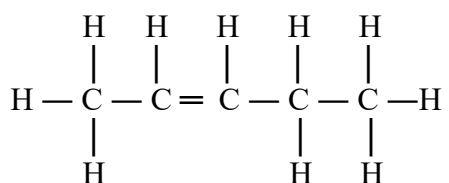\overset{\displaystyle H}{\underset{}{|}}\ \overset{\displaystyle H}{\underset{}{|}} \\
H-C-C-H \\
\overset{}{|} \\
H
\end{array}
$$

$$
H-C\equiv C-\underset{\displaystyle\begin{array}{c}|\\ CH_2CH_3\end{array}}{\overset{}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H
$$

H   H
| |
H — C — C — H
    |
    H
    H   H   H   H   H
    | | | | |
H—C≡C—C—C—C—C—C—C—H
    | | | | |
    H   H   H   H   H
    H
    |
H — C — C — H
    | |
    H   H

Condensed structure:

$$
\begin{array}{c}
CH_2CH_3 \\
| \\
CH\equiv CCH_2CH_2CH_2CH_2CH_3 \\
| \\
CH_2CH_3
\end{array}
$$
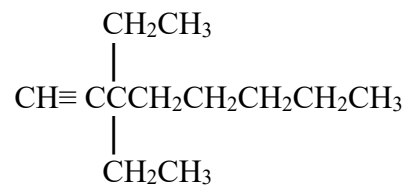
6. What is the systemic name for the following structure?

5-methyl-2-heptene

7. What is the systemic name for the following structure?

$$CH_3C\equiv CCH_2CH_2CH_3$$

2-pentyne

Naming and Drawing Alkenes Worksheet and Key

1) Draw and name the *cis* <u>and</u> *trans* condensed structure of:

```
      H    H    H    H    H
      |    |    |    |    |
H — C— C =  C— C — C—H
      |         |    |
      H         H    H
```
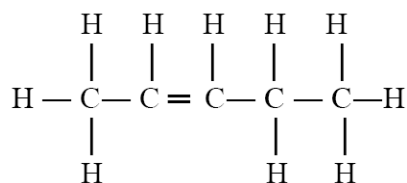
cis condensed structure:	*trans* condensed structure:
name:	name:

2. Name the following alkenes (include cis- or trans- for the alkenes that when appropriate)

a)

```
      H    H    H    H    H
      |    |    |    |    |
H — C=  C  — C— C — C—H
                |    |    |
                H    H    H
```

Name: _____

b)

$$CH_2 = CHCH_2CH_2CH_2CH_2CH_3$$

Name: _____

c)

$$CH_3CH\ CH_2CH_2\ CH = CHCH_2CH_3$$
$$|$$
$$CH_3$$
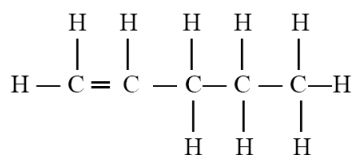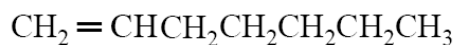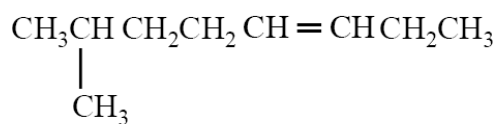
Name: _____

Be careful to correctly identify carbon #1……

d)

```
CH3           CH3
    \        /
     C = C
    /        \
   H           H
```

Name: _____

e)

$CH_3CH_2CH_2CH_2$ 　　　 H
　　　　　　　 C=C
　　　 H 　　　 $CH_2CH_2CH_3$
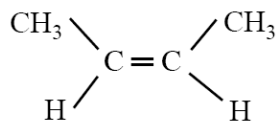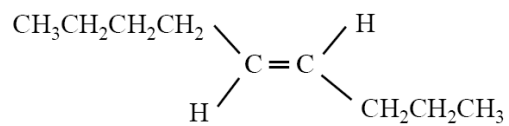
Name: _____

f)

Name: _____

3. Draw the line bond, condensed, and skeletal structure of the following alkenes.

a) 1-hexene

line-bond structure	condensed structure	skeletal structure

b) 4-isopropyl-2-methyl-1-nonene

line-bond structure	condensed structure	skeletal structure

c) cis-2-hexene

line-bond structure	condensed structure	skeletal structure

d) trans-2-pentene

line-bond structure	condensed structure	skeletal structure

e) cis-2-methyl-3-hexene

line-bond structure	condensed structure	skeletal structure

Key

1) Draw and name the *cis* <u>and</u> *trans* condensed structure of:

$$H - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - \overset{\overset{\displaystyle H}{|}}{C} = \overset{\overset{\displaystyle H}{|}}{C} - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - H$$

cis condensed structure:	*trans* condensed structure:
$$\overset{CH_3}{\diagdown}\underset{H \diagup}{C} = \underset{\diagdown H}{C}\overset{\diagup CH_2CH_3}{}$$	$$\overset{CH_3}{\diagdown}\underset{H \diagup}{C} = \underset{\diagdown CH_2CH_3}{C}\overset{\diagup H}{}$$
name: *cis*-2-pentene	name: *trans*-2-pentene

2. Name the following alkenes (include cis- or trans- for the alkenes that when appropriate)

a)

$$H - \overset{\overset{\displaystyle H}{|}}{C} = \overset{\overset{\displaystyle H}{|}}{C} - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - H$$

Name: _____1- pentene_____

b)

$$CH_2 = CHCH_2CH_2CH_2CH_2CH_3$$

Name: ____1- heptene_____ _____

c)

$$CH_3CH\,CH_2CH_2\,CH = CHCH_2CH_3$$
$$\underset{CH_3}{|}$$
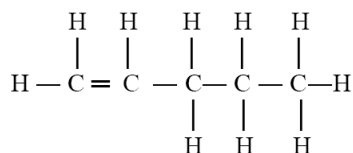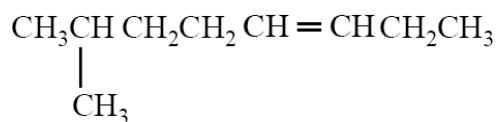
Name: _____7- methyl-3-octene _____
Note: Carbon #1 is the carbon nearest to the double bond

d)

$$\overset{CH_3}{\diagdown}\underset{H \diagup}{C} = \underset{\diagdown H}{C}\overset{\diagup CH_3}{}$$

Name: _____ *cis*-2-butene _____

e)

$CH_3CH_2CH_2CH_2$ H

           C=C

     H $CH_2CH_2CH_3$

Name: _____*trans*-4-nonene _____
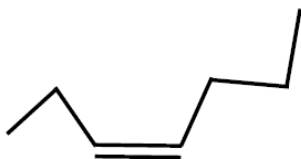
f)

Name: _____cis-3-heptene _____

3. Draw the line bond, condensed, and skeletal structure of the following alkenes.

a) 1-hexene

line-bond structure	condensed structure	skeletal structure

H H H H H H
| | | | | |
H — C = C — C— C — C— C—H
         | | | |
        H H H H
	$CH_2 = CHCH_2CH_2CH_2CH_3$	

b) 4-isopropyl-2-methyl-1-nonene

line-bond structure	condensed structure	skeletal structure

H
|
H — C — H
H   H H H H H H H
| | | | | | | |
H — C = C — C — C — C— C— C— C— C—H
     | | H H H H H
     H   H
     | |
  H— C—C—C—H
      | | |
     H H H
	CH_3
	|
	$CH_2 = CCH_2CHCH_2CH_2CH_2CH_2CH_3$
	|
	CH_3CHCH_3
		Note: There are several correct ways to draw many of these skeletal structures.

c) *cis*-2-hexene

line-bond structure	condensed structure	skeletal structure
H—C—C=C—C—C—C—H (with H atoms as shown) Note: cis/trans is not displayed in line-bond structures (only displayed in condensed and skeletal structures).	CH₃ / H C=C CH₂CH₂CH₃ / H (condensed structure as drawn)	(skeletal structure)

Line-bond structure:

```
     H   H   H   H   H   H
     |   |   |   |   |   |
 H — C — C = C — C — C — C — H
     |           |   |   |
     H           H   H   H
```

Note: cis/trans is not displayed in line-bond structures (only displayed in condensed and skeletal structures).

Condensed structure:

CH_3 and H on left carbon, $CH_2CH_2CH_3$ and H on right carbon, $C=C$

d) *trans*-2-pentene

line-bond structure	condensed structure	skeletal structure

Line-bond structure:

```
     H   H   H   H   H
     |   |   |   |   |
 H — C — C = C — C — C — H
     |           |   |
     H           H   H
```

Note: cis/trans is not displayed in line-bond structures (only displayed in condensed and skeletal structures).

Condensed structure:

CH_3 and H on left carbon, H and CH_2CH_3 on right carbon, $C=C$

e) *cis*-2-methyl-3-hexene

line-bond structure	condensed structure	skeletal structure

Line-bond structure:

```
         H
         |
     H — C — H
     H   |     H   H   H   H
     |   |     |   |   |   |
 H — C — C — C = C — C — C — H
     |   |         |   |
     H   H         H   H
```

Condensed structure:

CH_3

CH_3CH and H on left carbon, CH_2CH_3 and H on right carbon, $C=C$

Chapter 5 Lecture Notes: Gases, Liquids, and Solids

Educational Goals

1. Define and compare the terms **specific heat**, **heat of fusion**, and **heat of vaporization**. Know the equations that involve these concepts and be able to use them in calculations.

2. Understand the terms **energy** and **energy change**.

3. Know the definition of **pressure, vapor pressure,** and **atmospheric pressure** and be able to convert between pressure units of atm, Torr, and psi.

4. List the variables that describe a gas (P,V,n, and T) and be able to write and use the equations for the various **gas laws**.

5. Explain Dalton's Law of Partial Pressures and define **partial pressure**.

6. Understand the definitions of **density** and **viscosity**. Given the density, and either the mass or volume of a substance, be able to determine the volume or mass (respectively).

7. Know that a liquid in an open container will boil when its vapor pressure is equal to the atmospheric pressure.

8. Describe, compare, and contrast **amorphous solids** and **crystalline solids**.

9. Describe the makeup of the four classes of crystalline solids.

So far, you have learned about the underlying, nanometer scale, structure of matter. In chapter 5, you will use your new understanding of matter's nano-scale structure to better understand the macro-scale properties of the world that you can observe directly.

We defined chemistry as ***the study of matter and how it interacts with energy and with other matter***. In the previous chapters, you developed a model of matter. You learned that atoms consist of protons, neutrons, and electrons. You learned how these subatomic particles arrange themselves when they form atoms. Then you saw how atoms can combine to form ionic or covalent compounds. You learned how molecules and ions interact with each other through noncovalent interactions (hydrogen bonding, dipole-dipole forces, London forces, ion-dipole interactions, and salt bridges). In chapter 5 you will learn about *how matter interacts with energy*.

I will begin chapter 5 by discussing three phases of matter: solid, liquid, and gas. Throughout chapter 5, I will elaborate on the characteristics and properties of these three phases of matter.
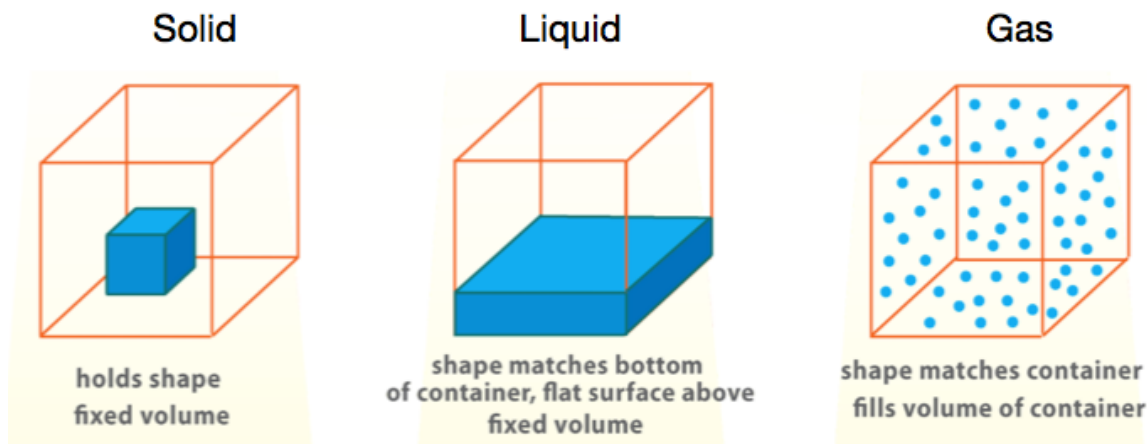
Matter

Matter is typically found in one of **three** different physical_____.

These three phases of matter are: **solid**, **liquid**, and **gas**.

At a given temperature:

- *solids* have fixed shapes and volumes
- *liquids* have variable shapes and fixed volumes
- *gases* have variable shapes and volumes.

A fourth, higher energy phase of matter that does not naturally occur at temperatures on earth is called the plasma phase. A plasma is similar to a gas, however it is composed of ions and unbound electrons.

Changing the _____ *of matter*, that is, converting matter between solid, liquid, and gas phases is considered a _____ *change* because the *chemical composition* **does not** change.

Examples of phase changes:

- *freezing* water to make ice
- *boiling* water to make steam
- *melting* iron

In order for a substance to change phases or temperature, _____ must be _____ or _____ from the substance.

Before we discuss the energetics of temperature and phase changes, let's consider what energy is and how chemical compounds can gain, lose, or store energy.

Energy

Energy can be defined as *the ability to do work*.

Energy can be found in **two** forms, _____ *energy* and _____ *energy*.

- *Potential energy* is _____ energy; it has the *potential* to do work.
  - An example of potential energy is the energy that is stored in the chemical bonds of propane. Consider propane fueled barbecues. If propane is mixed with the oxygen molecules in air and a spark is applied, a process called combustion uses the energy that was stored in propane molecules to generate heat. In this example, some of the potential energy in the propane and oxygen molecules is converted to the *kinetic energy* (motion) of the CO_2 gas and H_2O gas that are produced in the combustion process.

- *Kinetic energy* is *the energy of* _____. Whenever matter is moving, it has kinetic energy.
  - Kinetic energy can be thought of as the energy of the **motion of atoms or ions.**
  - You can think of _____ as being a measure of how _____ the atoms, ions, or molecules in a substance are moving.

More Kinetic Energy = More Atomic Motion = Higher Temperature

Keep in mind that although a substance is in the liquid or solid phase, the atoms within are moving. In the gas phase, it is easy to imagine the moving particles. Gas particles will move in almost perfectly straight lines until they collide with other particles or with the container walls. In liquids, the particles are much closer to each other than in gases, therefore the particles are colliding with other particles much more often than the particles in a gas. In chapter 3, I mentioned that a chemical bond between two atoms behaves like a spring connecting the atoms as illustrated to the right. Imagine hitting the molecular model on the right with a hammer and seeing the atoms and spring vibrate. That vibrational motion is how energy can be stored in chemical bonds.
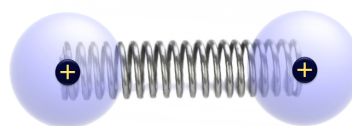
If a solid compound is at a *high temperature*, the atoms are vibrating at *high speeds*. If you touch this hot solid, the vibrating atoms will collide with your skin molecules causing the atoms in your skin to start vibrating at higher speeds, and you experience this as feeling "hot" or "getting burned." If the vibrating atoms in the solid transfer enough energy to the skin, chemical bonds can be broken and a burn injury occurs. When chemical bonds are broken, you can think of that as breaking the tiny springs holding the atoms together. We call this a chemical reaction; you will learn about chemical reactions in chapter 6.

Another way that molecular substances contain kinetic energy in the motion of atoms is by *spinning* (rotating). For example, water molecules can spin/rotate around an axis as shown on the right. The higher the temperature, the faster the spinning motion. Microwave ovens heat food because microwave electromagnetic radiation interacts with the electric dipole of water molecules causing the water molecules to spin faster.
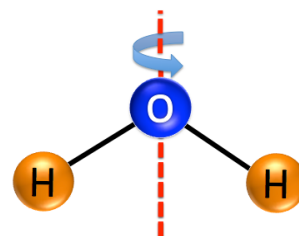
In the case of large molecules, in addition to the entire molecule spinning around an axis, kinetic energy can be present in the *rotation of groups* of atoms around single bonds (conformational changes).

Energy Changes

It is the _____ _____ that hold molecules together such that they exist in the solid or liquid phase instead of the gaseous phase.

Example: Hydrogen bonding holding water molecules together in an ice crystal.
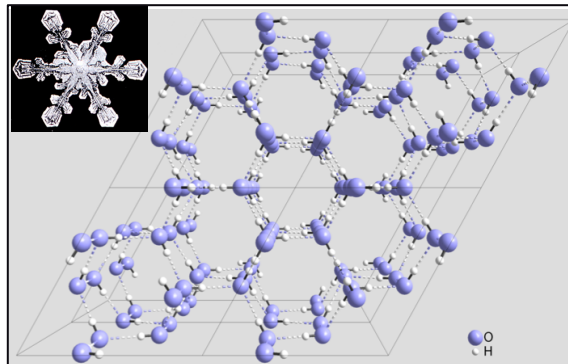
Whether a molecular compound exists in the gas, liquid, or solid phase is determined by a _____ between *noncovalent interactions* (working to keep the molecules close to one another) and *temperature* (kinetic energy working to distribute the molecules evenly in the container).

- If the *noncovalent interactions* are dominant, then the substance will exist in the solid or liquid phase.

- If the *temperature/kinetic energy* can **overcome** the noncovalent interactions, then the substance will exist in the gaseous phase.

Energy Units

Energy is **not** something that can be directly measured. For example, we calculate the energy of a moving object *by measuring its velocity*. We have thermometers to measure temperature, but there is no such thing as an "energometer." Classic, non-electronic thermometers work because the liquid (often mercury or colored-alcohol) in the bulb and the tube expands or contracts as the temperature increases or decreases. Upon an increase in temperature, expansion of liquid in the bulb causes an observable increase in the liquid level of the tube. The opposite process and observation happens for a decrease in temperature.

In electronic thermometers, the electrical current passing through the materials that compose their probe depends on temperature. These devices are calibrated so that the displayed temperature is related to the measured electrical current.

Optical (infrared) thermometers operate by measuring the amount of infrared (IR) light that is emitted from an object. The amount of IR light that an object emits depends on the object's temperature.
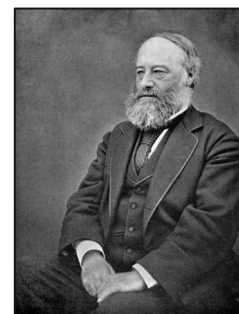
The *two energy units that you will use in this course* are the _____ **(cal)** and the _____ **(J)**.

- The Joule was named in honor of the English physicist and brewer, James Prescott Joule who, along with Lord Kelvin, developed the Kelvin absolute temperature scale.

The **calorie** energy unit is defined as the amount of energy required to raise the temperature of *one gram* of water by 1 °C.

The **Joule** energy unit is defined as the amount of energy required to pass a certain amount of current through a particular material for one second.

James Prescott Joule
(1818-1889)

The scientific community standardized these two measurements using the agreed upon conversion factor that _____ **is equal to *exactly*** _____.

4

Energy Unit Conversion Example: Convert 60.1 calories to Joules.

$$\frac{60.1 \text{ cal}}{} \left| \frac{4.184 \text{ J}}{1 \text{ cal}} \right. = 251 \text{ J}$$

Understanding Check: Convert 78 Joules to calories.

"Food Calories" vs. "calories"

Note that **nutritionists** use the "food **C**alorie" notation with *capital* "**C**" in the spelling and unit.

A food "**C**alorie" is equal to 1000 calories (1 Cal = 1000 cal = 1kcal).

- An apple contains about 120 Cal (=120,000 cal = 120 kcal).

Nutrition Facts
Serving Size 1 cup (228g)
Servings Per Container 2

Amount Per Serving
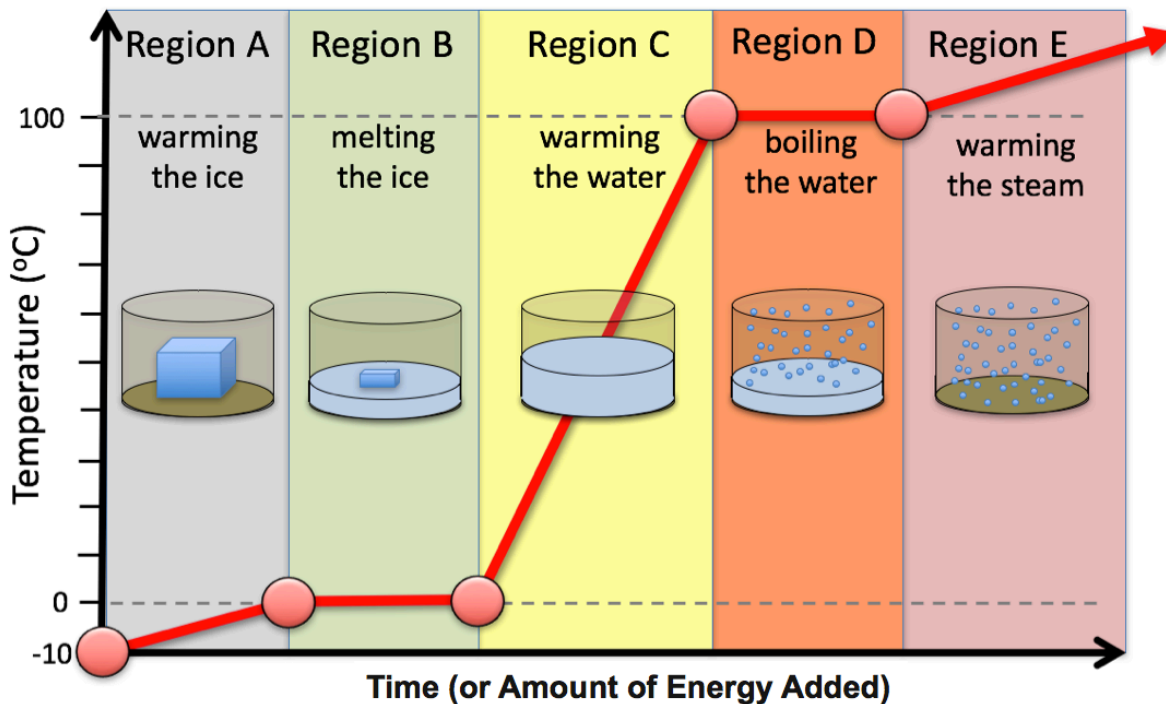**Calories** 250   Calories from Fat 110

Temperature Changes and Phase Changes

One of *two* things will happen if energy is added or removed from matter (assuming no chemical change takes place):

1) Change the _____ of the substance.

2) Change the _____ of the substance.

You can only do _____ of these at a time.

Region A | Region B | Region C | Region D | Region E

warming the ice | melting the ice | warming the water | boiling the water | warming the steam

Temperature (°C)

Time (or Amount of Energy Added)

I will discuss calculations that involve *temperature changes* or *phase changes*. Let's begin with *temperature changes*.

Calculations Involving Temperature Changes

The scientific community agreed that **energy** _____ to a substance is assigned _____ *values*, and that **energy** _____ from a substance is assigned _____ *values*.

The *amount of energy* that must be added (or removed) from **one gram** of a substance to result in a temperature change of **one ºC** is called the substance's _____ _____.

- We use the symbol "**S**" to represent specific heat.

- Since **specific heat** is the amount of *energy* transferred per **one gram** and **per 1 ºC** temperature change, its units will be either **cal/(g ºC)** or **J/(g ºC)**.

Specific Heats for Various Substances	
Substance	**Specific Heat (S)**
Water (H_2O liquid)	1.000 cal/(gºC)
Ice (H_2O solid)	0.500 cal/(gºC)
Steam (H_2O gas)	0.480 cal/(gºC)
Ethanol (liquid)	0.586 cal/(gºC)
Copper (solid)	0.0925 cal/(gºC)
Aluminum (solid)	0.0215 cal/(gºC)
Gold (solid)	0.0310 cal/(gºC)

There exists a mathematical relationship between the amount of energy transferred (heat) **to _or from_** a substance and the resulting temperature change.

The relationship between the *energy added or removed* from a substance and how much its temperature changes is:

$$Q = S \cdot m \cdot (\Delta T)$$

In this equation,

- "**Q**" is used to represent the *energy* added or removed from a substance (or heat).
- "**S**" is the *specific heat* of the substance.
- "**m**" is the *mass* of the substance.
- "**(ΔT)**" is the amount of the _____ *in temperature* (in ºC units) that occurs when the energy is added or removed from the substance.
  - In science, the Greek letter "**Δ**" is very often used as the phrase "*change in*."

(ΔT) is defined as the *final temperature* **minus** the *initial temperature* ($\Delta T = T_{final} - T_{initial}$).

To be consistent with the convention of assigning positive energy values for energy added to a substance and negative energy values for energy removed from a substance, (ΔT) is always defined as the final temperature minus the initial temperature $(\Delta T = T_{final} - T_{initial})$.

Note that if energy is ***added to a substance*** and a temperature change occurs, the final temperature will always be ***greater than*** the initial temperature and therefore ΔT $(= T_{final} - T_{initial})$ would be ***positive***. The mass (**m**) and specific heat (**S**) are both *always* positive, therefore when ΔT is also positive, the calculated energy (**Q**) will be ***positive***.

$$Q = S \cdot m \cdot (\Delta T)$$
$$(+) = (+) \bullet (+) \bullet \quad (+)$$

On the other hand, if energy is ***removed from a substance*** and a temperature change occurs, the final temperature will always be ***less than*** the initial temperature and ΔT $(= T_{final} - T_{initial})$ will be ***negative***; in this case the calculated energy (**Q**) will be ***negative***.

$$Q = S \cdot m \cdot (\Delta T)$$
$$(-) = (+) \bullet (+) \bullet \quad (-)$$

Example of a Calculation that Involves a Temperature Change

How much energy (calories) is required to be added to 7.00 grams of water that is initially at 37.0 °C in order to raise the temperature to 65.0 °C?

$$Q = S \cdot m \cdot (\Delta T)$$

$$\Delta T = T_{final} - T_{initial}$$
$$= 65.0\ ^\circ C - 37.0\ ^\circ C$$
$$= \mathbf{28.0\ ^\circ C}$$

$$Q = \left(\frac{1.000\ cal}{g\ ^\circ C} \right) (\ 7.00\ g\ )(\ 28.0\ ^\circ C\ ) = \mathbf{196\ cal}$$

Example of a Calculation that Involves a Temperature Change

Suppose that 3625 *calories of energy* is transferred to 245 grams of water that is originally at 22.4 °C:

a) What is the change in temperature (ΔT) of the water?

$$\frac{Q}{S \cdot m} = \frac{S \cdot m \cdot (\Delta T)}{S \cdot m}$$

$$(\Delta T) = \frac{Q}{S \cdot m} = \frac{3625\ cal}{\left(\dfrac{1.000\ cal}{g\ ^\circ C} \right) 245\ g} = \mathbf{14.8\ ^\circ C}$$

b) What is the final temperature (T_{final}) of the water?

$$\Delta T = T_{final} - T_{initial}$$
$$14.8\ ^\circ C = T_{final} - 22.4\ ^\circ C$$
$$T_{final} = \mathbf{14.8\ ^\circ C} + 22.4\ ^\circ C = \mathbf{37.2\ ^\circ C}$$

Understanding Check

1. How much energy (calories) is required to be added to 12.00 grams of ethanol that is initially at 24.0 °C in order to raise the temperature to 42.0 °C? (**NOTE:** You are warming *ethanol*, not water; use the specific heat of ethanol.)

2. How much energy must be added to 128 grams of ice that is initially at -54.0 °C in order to raise the temperature of the ice to its *melting point* (0.00 °C)? (**NOTE:** You are warming *ice*, not water. The specific heat of ice i*s **not** the same* as the specific heat of water; use the specific heat of *ice.*)

3. How much energy must be removed from 584 grams of water that is initially at 22.0 °C in order to lower the temperature of the water to its *freezing point* (0.00 °C)?

4. Suppose that 1250 calories of energy transferred to water that was originally at 22.4 °C, raises the temperature of the water to 34.8°C. What is the **mass** (**m**) of the water that was heated? **HINT:** Solve $Q = S \cdot m \cdot (\Delta T)$ for mass (**m**).

Phase Changes
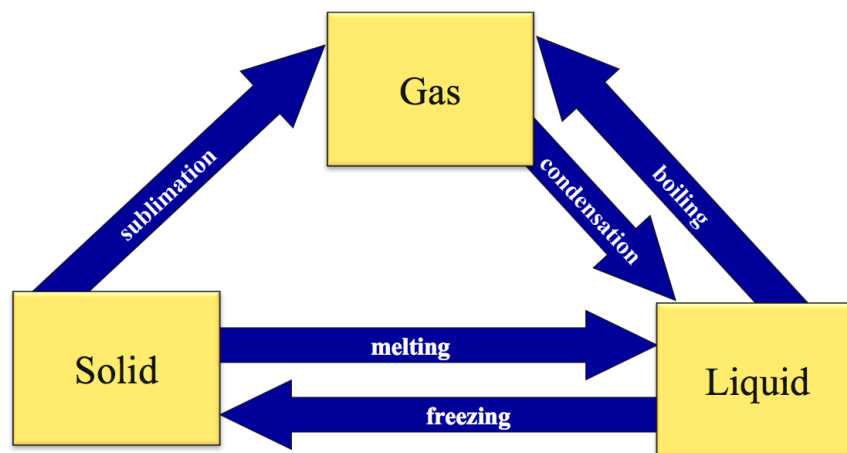
Adding a sufficient amount of energy to liquids will overcome the noncovalent interactions holding the particles together, to form a gas; we call this **boiling**. The reverse of this process, changing from gas to liquid, will occur if enough energy is removed from the gas; we call this **condensation**. *Adding* a sufficient amount of energy to solids will overcome the forces holding the molecules in place, to form a liquid; we call this **melting**. The reverse of this process, changing from liquid to solid, will occur if enough energy is removed from the liquid; we call this **freezing**. Under certain conditions, substances can be converted ***directly*** from the solid phase to the gas phase; we call this **sublimation**. You may have seen this with "dry ice" (solid CO_2 converting to gaseous CO_2 without forming liquid CO_2).

Calculations Involving Phase Changes

The amount of energy required to _____ **one gram** of a substance is called its _____ **of** _____ (abbreviated as H_{fus}).

- Heats of fusion for substances are determined _____; each substance has a unique heat of fusion.

Examples:

- The *heat of fusion* for ice is 79.7 cal/g and the *heat of fusion* for gold is 15 cal/g.

  Since these values are the energy that is required to melt one gram of the substance, the units will be either cal/g or J/g.

To do the opposite process, change from one gram of liquid to solid (*freezing*), the same amount of energy must be ***removed*** *from the substance*, and therefore the _____ of the *heat of fusion value* must be changed from ***positive*** to _____.

- For example, the amount of energy needed to be ***removed*** from water in order to convert it to ice is: **$(-H_{fus})$** = -79.7 cal/g.

The energy required to convert **one gram** of a substance from **liquid** *to* **gas** is called its _____ **of** _____ **(H_{vap})**.

- Heats of vaporization for substances are determined *experimentally*, vary from substance to substance, and are tabulated using energy units per gram.

To do get the energy required to do the opposite process, convert one gram of gas to a liquid (*condensation*), we change the ***sign*** of the *heat of vaporization value* (from ***positive*** to ***negative***) because energy is being remove from the substance.

The heat of fusion and vaporization values (shown in the table on the right) are the amounts of energy needed to melt or vaporize **one gram** of a substance.

We can use these values to calculate the **energy** needed to *melt* or *vaporize* any amount (mass) of the substance using the equation below.

Heats of Fusion and Heats of Vaporization of Some Substances

Substance	heat of fusion (H_{fus})	heat of vaporization (H_{vap})
H_2O	79.7 cal/g	540 cal/g
ethanol (ethyl alcohol)	26.05 cal/g	230 cal/g
2-propanol (rubbing alcohol)	21.37 cal/g	159 cal/g

$$\Delta E = (\text{mass}) \bullet (H_{fus} \text{ or } H_{vap})$$

ΔE, the "**change in energy**," is the amount of energy that was added to, or removed from the substance *in order to change the phase*.

- **ΔE** is defined as the final energy of the substance (after phase change) *minus* its energy before the phase was changed (**ΔE** = E_{final} - $E_{initial}$).

The unit for **mass** will be the gram (g) since the units for *heats of fusion* and *vaporization* in the table are calories *per* **gram**.

Example of a Calculation Involving a Phase Change

How much energy is required to melt 46.7 grams of *ice* that is originally at its melting point (0°C)?
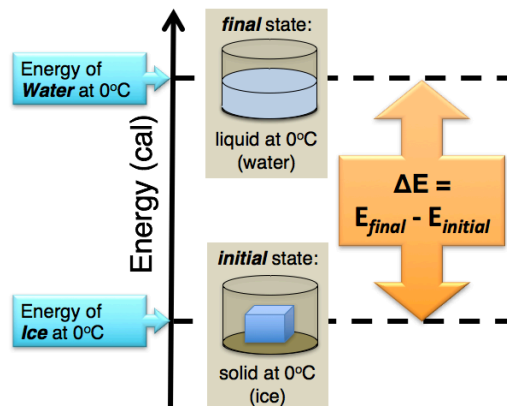
initial state: *final* state:

Phase Change

solid at 0°C   liquid at 0°C
(ice)   (water)

$$\Delta E = (\text{mass}) \bullet (H_{fus})$$

Substance	heat of fusion (H_{fus})	heat of vaporization (H_{vap})
H_2O	79.7 cal/g	540 cal/g
ethanol (ethyl alcohol)	26.05 cal/g	230 cal/g
2-propanol (rubbing alcohol)	21.37 cal/g	159 cal/g
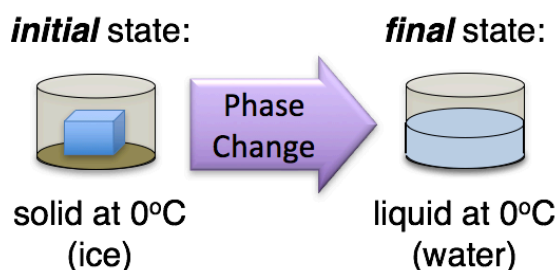
$$\Delta E = (46.7 \text{ g}) \left(\frac{79.7 \text{ cal}}{\text{g}} \right) = \textbf{3720 cal}$$
**or 3.72 x 10³ cal**

In order to convert ice to water, energy must be added such that the noncovalent interactions holding the H_2O molecules in their ice crystalline lattice positions are overcome. That is why the energy of water at 0°C is at a higher level than the energy of ice at 0°C.

The definition of **ΔE** as being equal to the **final** energy **minus** the **initial** energy, for example in the previous problem, ΔE = E_{final} (water) - $E_{initial}$ (ice), is consistent with the convention of assigning *positive energy* values when energy is <u>added</u> to a substance and *negative energy* values when energy is <u>removed</u> from a substance.

Energy of **Water** at 0°C

Energy (cal)

final state:

liquid at 0°C (water)

ΔE =
E_{final} - $E_{initial}$

initial state:

Energy of **Ice** at 0°C

solid at 0°C (ice)

Example of a Calculation Involving a Phase Change

Determine the amount of energy needed to be **removed** from 50.0 g of water (liquid) that is originally at 0 °C in order to freeze it.

initial state: **final** state:

liquid at 0°C   solid at 0°C
(water)   (ice)
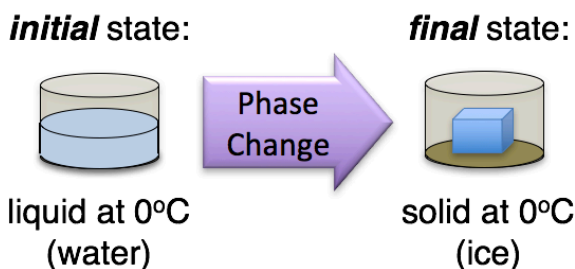
$$\Delta E = (\text{mass}) \cdot (-H_{fus})$$

$$\Delta E = (50.0 \text{ g}) \left(\frac{-79.7 \text{ cal}}{\text{g}} \right) = \textbf{-3990 cal}$$
$$\underline{\textbf{or}} \textbf{ -3.99 x 10}^3 \textbf{ cal}$$

Substance	heat of fusion (H_{fus})	heat of vaporization (H_{vap})
H_2O	79.7 cal/g	540 cal/g
ethanol (ethyl alcohol)	26.05 cal/g	230 cal/g
2-propanol (rubbing alcohol)	21.37 cal/g	159 cal/g

Understanding Check

1. How much energy (calories) is required to convert 35 grams of *water* (originally at its boiling point, 100 °C) into *steam*?

   - **NOTE:** You are converting from liquid to gas, use the heat of vaporization (H_{vap}) for H_2O.

2. How much energy must be removed from 224 grams of *liquid ethanol* (originally at its freezing point) in order to solidify it?

Gases

Properties of Gases

Except for the noble gases (He, Ne, Ar, Kr, Xe, and Ra), gases are composed of _____.

Compared to liquids and solids, particles in the gas phase are v*ery far apart from one another*.

- It is for this reason that gases have *low densities*.

Because of the relatively large distances between gas particles, most of the volume occupied by a gas is _____ *space*.

- Another word used for empty space is ***vacuum***.

Since a gas is mostly empty space, uncolored gases are invisible and colored gases are translucent (we can see light through them).

Gases completely fill their container (except for rare exceptions).

- In mixtures of gases (two or more types of gas particles), each gas is distributed *evenly* throughout the container (except for a few heavy, higher molecular weight gas molecules).

Gaseous particles travel at high speeds in all directions and will mix with other types of gas particles in a process called _____.

- ***Diffusion*** is the movement of one substance within another substance until it is _____ distributed.

Gases are easily ***compressed***.

- ***Compressibility*** is the ability to make the space a substance occupies become smaller.

Gas Pressure

One parameter that is used to describe gases is _____.

- In general, *pressure* is defined as the amount of _____ that acts upon a unit _____ *area*.
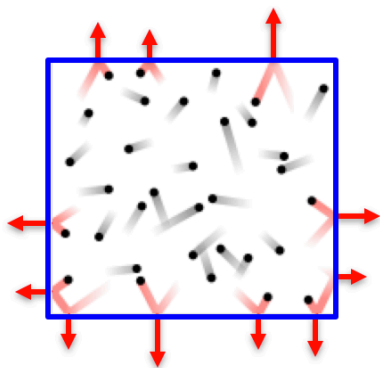
Each collision of a gas particle (shown as a sphere) with the wall of the container produces a force upon the wall (the force is represented as an arrow).

Gas pressure is caused by _____ of gaseous particles with the container walls or other surfaces.

The sum of the forces from all of the collisions divided by the container's inner surface area is the *pressure*.

The gas particles that surround the earth form the **earth's atmosphere** and are commonly referred to as **air.**

- Air is a _____ of gases.
  - The dry air (H_2O vapor excluded) nearest to the surface of the earth contains about 78% nitrogen, 21% oxygen, 1% argon, 0.04% carbon dioxide, and trace amounts of some other gases.
 - The percentage of H_2O vapor varies between 0.001% and 5% depending on local weather conditions.

_____ _____, sometimes referred to as "air pressure," is simply the pressure exerted by the air at a particular location.

Wherever there is air, atmospheric pressure exists.

Since the earth's gravity acts on the gas particles, air at lower elevations is more dense (more concentrated) than at higher elevations.

Since there are less gas particles present and therefore less collisions occurring at higher altitudes,

_____.

A plot of the relationship between the altitude and atmospheric pressure is shown on the right. Note that the pressure on top of Mt. Everest is equal to about half of the pressure that we experience near sea level. This means that there are about half as many molecules in a liter of air on top of Mt. Everest as there are at sea level; you would inhale half of the amount of oxygen in one breath as you would at sea level. Most mountaineers who climb above 8 km use oxygen tanks/masks so they can maintain safe blood oxygen levels.
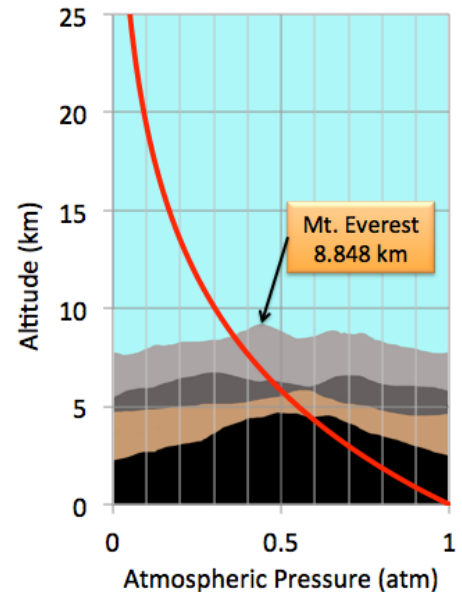
Measuring Pressure

The term "_____" is used for a device that measures pressure.

Devices used to measure atmospheric pressure are called _____.

- Italian physicist and mathematician Evangelista Torricelli is credited with the invention of the barometer in 1643.

Historically, the most common types of barometers involved a column of liquid "*supported*" by air. In order to minimize the size of the device, mercury - a very high-density liquid - is commonly used. An illustration of a *mercury barometer* is shown here. The collisions of gas particles in the air with the surface of the mercury force mercury **upward** in the column. This is balanced by the **downward** pull of gravity on the mercury in the column. Gravity is relatively constant; however, the pressure of the air varies with elevation and local weather conditions, therefore the height of mercury in the column will change as the air pressure changes.

An illustration of a mercury barometer.

The height of a column of mercury at sea level is about____ ___; this value will vary slightly depending on the weather.

Modern manometers include *mechanical* and *electronic* instruments. Microfabrication manufacturing technologies have enabled the use of miniaturized manometers in devices such as wristwatches and mobile phones.

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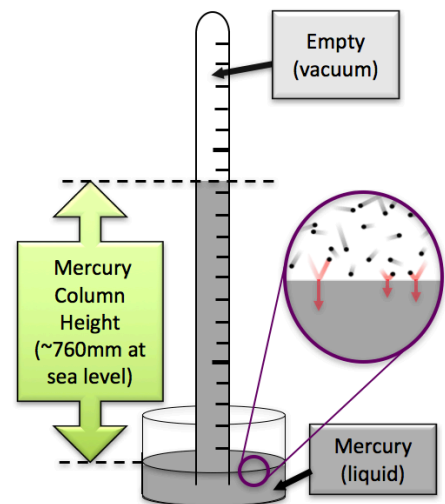
Units of Pressure

The *pressure units that we will use in this course* are **atmospheres (atm), pounds per square inch (psi), millimeters of mercury (mm Hg),** and **Torr**.

The relationships between these units are:

1 atm	=	760 mm Hg	(exact, infinite significant figures)
1 mm Hg	=	1 Torr	(exact, infinite significant figures)
1 atm	=	760 Torr	(exact, infinite significant figures)
1 atm	=	14.7 psi	(three significant figures shown here)

Pressure unit conversion example: Convert 757 mm Hg to atmosphere units (atm).

1 atm = 760 mm Hg (exact, infinite significant figures)

$$\frac{757 \; \cancel{mm \; Hg}}{} \; \left| \; \frac{1 \; atm}{760 \; \cancel{mm \; Hg}} \right. = 0.996 \; atm$$

Understanding Check: Convert 0.874 atm to Torr.

The Gas Laws

In all but extremely high pressure or very low temperature conditions, gases are very accurately and precisely described using only four parameters:

1) the **temperature** (**T**)

2) the **volume** of the container (**V**)

3) the **pressure** (**P**)

4) the amount of gas particles present (**moles**)

The *gas laws* are the mathematical _____ between the pressure, volume, temperature, and the number of moles of gas particles that are present in a *closed* container.

1) Boyle's Law

Robert Boyle, a 17th-century Irish natural philosopher, chemist, physicist, and inventor, studied the relationship between the _____ and _____ of a gas.

Boyle noticed that the pressure of a gas in a closed container is _____ *proportional* to the volume of the container.

- If two parameters are "inversely proportional," when one parameter (volume in this case) decreases, the other parameter (pressure in this case) increases. Furthermore, the increase and decrease (inverse relationship) follows a mathematical equation.

Graphs were not yet in use at the time of Boyle's work, however if the pressure is measured at several different volumes and the data points are plotted, the data points would fall upon the blue curve shown on the right.

The mathematical equation of the curve in this figure is:

$$P = (\text{Constant}) \times \left(\frac{1}{V}\right)$$
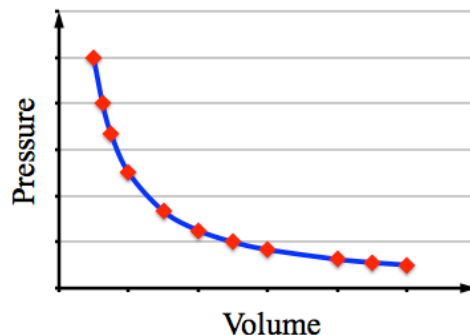
When observables such as pressure and volume are *inversely proportional*, a unique situation exists. In order to illustrate this important and useful situation, I will multiply both sides of *equation above* by (**V**) so that (**V**) cancels on the right-hand side of the equation to give:

$$P \times V = (\text{constant})$$

This equation tells us that no matter how the pressure and volume of a gas may be changed, the _____ **of the pressure and volume never changes** (is *constant*).

The implication of the "$P \times V = $ **(constant)**" equation is very useful in order to predict pressure and volume *changes* to a gas.

Compress Piston

Before Compression	After Compression
➤ Initial Pressure $= P_1$	➤ Final Pressure $= P_2$
➤ Initial Volume $= V_1$	➤ Final Volume $= V_2$
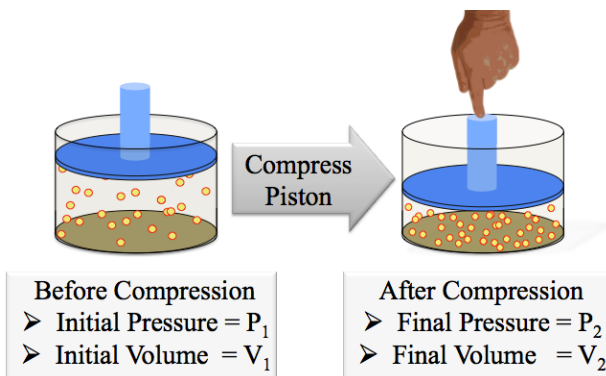
Since the product of the pressure and volume of a gaseous system is always constant, the initial and final pressures and volumes are related to each other in what is referred to as **Boyle's Law**.

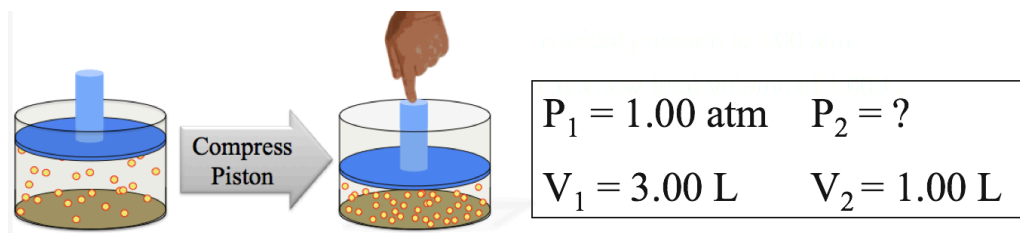> **Boyle's Law**
>
> $$P_1 \cdot V_1 = P_2 \cdot V_2$$

There are a couple of *important things to keep in mind* when using **Boyle's Law**:

1. Boyle's Law is only applicable *when the temperature **does not change** in the process*.
2. You can use **any** volume (or pressure) units, so long as the initial and final volume (or pressure) units *are the same* so that they will cancel.

Example:

The initial volume of the gas is 3.00 liters and the initial pressure is 1.00 atm.

The piston compressed (at constant temperature) to a new final volume of 1.00 L. What is the final pressure?

$$P_1 = 1.00 \text{ atm} \quad P_2 = ?$$
$$V_1 = 3.00 \text{ L} \quad V_2 = 1.00 \text{ L}$$

Solution: Use **Boyle's Law**: $\mathbf{P_1 \cdot V_1 = P_2 \cdot V_2}$

Boyle's Law contains four variables: P_1, V_1, P_2, and V_2. When any three of these variables are known, the fourth variable can be found using algebra.

- In this example, we know P_1, V_1, and V_2, and we wish to find the final pressure (P_2).

- To solve for $\mathbf{P_2}$, we divide **both sides** of the equation by $\mathbf{V_2}$:
$$\frac{\mathbf{P_1 \cdot V_1}}{\mathbf{V_2}} = \frac{\mathbf{P_2 \cdot \cancel{V_2}}}{\cancel{\mathbf{V_2}}}$$

- V_2 cancels on the right-hand side; we have isolated the unknown variable (P_2):
  - Insert the known values of P_1, V_1, and V_2, then solve for the final pressure (P_2):

$$P_2 = \frac{P_1 V_1}{V_2} = \frac{(1.00 \text{ atm})(3.00 \, \cancel{\text{L}})}{(1.00 \, \cancel{\text{L}})} = \mathbf{3.00 \text{ atm}}$$

Understanding Check

If 123 mL of gas that has a pressure of 782 Torr is compressed to a final volume of 63 mL, what would be the final pressure of the gas?

---

2) Charles' Law

Jacques Charles, a French inventor, scientist, mathematician, and balloonist, studied the mathematical relationship between the _____ and _____ of a gas.

Charles noticed that the volume of a gas in a closed container is _____ *proportional* to the temperature (at constant pressure).

- If two parameters are "*directly proportional*," this means that when one parameter increases, the other parameter increases *by the same factor*.

Charles found that if the volume is measured at several different temperatures and the data points are plotted, the data points would fall upon a straight line as shown on the right.

The mathematical equation of the line in this figure is:

$$V = (\text{Constant}) \times T$$
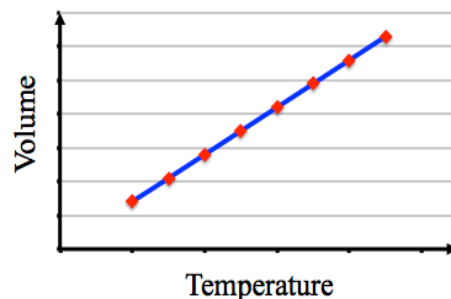
When observables such as volume and temperature are **directly proportional**, a unique situation exists. In order to illustrate this, I will divide both sides of *the equation above* by (**T**) so that (**T**) *cancels* on the right-hand side of the equation to give:

$$\frac{V}{T} = (\text{Constant})$$

This equation tells us that no matter how the volume and temperature of a gas may be changed, the _____ **of the volume to temperature never changes** (is *constant*).

Before Heating
Initial Volume = V_1
Initial Temperature = T_1

After Heating
Final Volume = V_2
Final Temperature = T_2
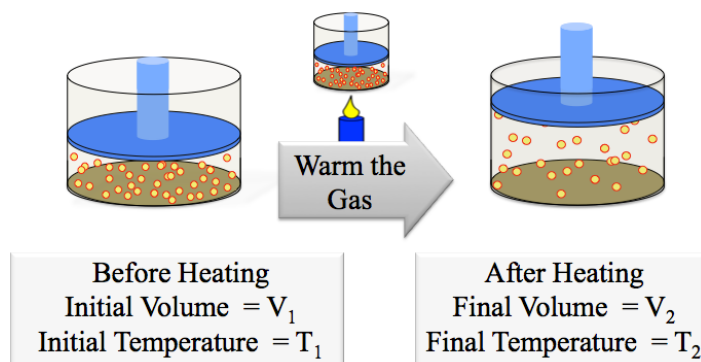
Since the ratio of the volume to temperature never changes, the initial and final volumes and temperatures are related to each other in what is referred to as **Charles' Law**.

Charles' Law
$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

We must use the *absolute temperature scale*, kelvin (___), _____ we are using the gas laws.

- The kelvin scale starts at zero (corresponding to zero kinetic energy) and includes only *positive values*. Celsius (°C) or fahrenheit (°F) scales cannot be used because they can have *negative* values. If a negative temperature value was used the equation for Charles' Law, then a *negative volume* would be calculated; this is problematic because a negative volume makes no sense.

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Example problem: The initial volume of gas in a cylinder with a piston is 7.20 liters. The gas is heated from 265 K to 428 K (at constant pressure). What is the final volume?
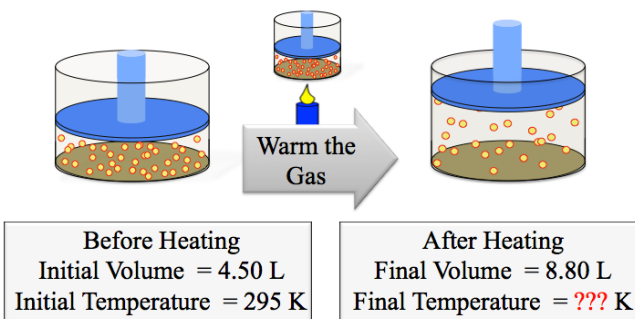
Solution: Use **Charles' Law**:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

Charles' Law contains four variables, V_1, T_1, V_2, and T_2. When any three of these variables are known, the fourth variable can be found using algebra.

Before Heating	After Heating
Initial Volume = 7.20 L	Final Volume = ???
Initial Temperature = 265 K	Final Temperature = 428 K
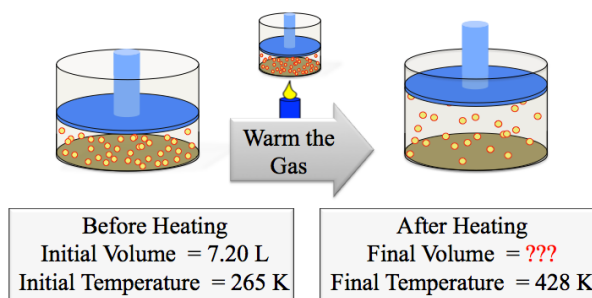
- In this example, we know V_1, T_1, and T_2; we wish to find V_2:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

- To solve for V_2, we multiply both sides of the equation by T_2:

$$\frac{T_2 \cdot V_1}{T_1} = \frac{V_2 \cdot \cancel{T_2}}{\cancel{T_2}}$$

- T_2 cancels on the right-hand side; we have isolated the unknown variable (V_2).
   - Insert the known values of V_1, T_1, and T_2 then solve for the final volume (V_2):

$$V_2 = \frac{T_2 \cdot V_1}{T_1} = \frac{(428 \cancel{K}) \cdot (7.20 \text{ L})}{(265 \cancel{K})} = \textbf{11.6 L}$$

There are a couple of *important things to keep in mind* when using **Charles' Law**:

1. Charles' Law is only applicable ***when the pressure does not change in the process***
2. Temperature must be entered into the Charles' Law equation in **kelvins**.
   - If you are given the initial and/or final temperature in °C or °F, **convert to K** *before* using Charles' Law.

Understanding Check

The initial volume of gas in a cylinder with a piston is 1.80 liters. The gas is ***cooled*** from 125 °C to 22 °C (at constant pressure). What is the final volume?

- CAUTION: Which temperature units must be used in gas law calculations?

I want to show you another example problem that involves some algebra that you may not have seen before.

Example problem: The initial volume of a gas in a cylinder with a piston is 4.50 L and the initial temperature is 295 K. When the gas is heated, its volume increases to 8.80 L (at constant pressure), what is the final temperature?

Solution: Because the volume and temperature are changing (at constant pressure) we use *Charles' Law*:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

Warm the Gas

Before Heating	After Heating
Initial Volume = 4.50 L	Final Volume = 8.80 L
Initial Temperature = 295 K	Final Temperature = ??? K

The variable that we wish to solve for, T_2, is in the *denominator* of the fraction. There is a mathematical shortcut called "cross-multiplication" that allows us to simplify the equation.

If $\dfrac{A}{B} = \dfrac{C}{D}$ $\qquad \dfrac{A}{B} \bowtie \dfrac{C}{D}$, then $A \cdot D = B \cdot C$

When we apply this to our equation for Charles' law, the variable we wish to solve for, T_2, is *no longer in the denominator* of the equation.

$$\text{Since} \quad \frac{V_1}{T_1} = \frac{V_2}{T_2} \quad \text{, then} \quad V_1 \cdot T_2 = T_1 \cdot V_2$$

- To solve for T_2, we divide both sides of the equation by V_1: $\qquad \dfrac{\cancel{V_1} \cdot T_2}{\cancel{V_1}} = \dfrac{T_1 \cdot V_2}{V_1}$

$$T_2 = \frac{T_1 \cdot V_2}{V_1} = \frac{(295 \text{ K}) \cdot (8.80 \cancel{\text{ L}})}{(4.50 \cancel{\text{ L}})} = 577 \text{ K}$$

3) Gay-Lussac's Law

Joseph Luis Gay-Lussac and Guillaume Amonton studied the relationship between the temperature and pressure of a gas.

They noticed that the pressure of a gas in a fixed-volume container is _____ *proportional* to the temperature.

Because the pressure and temperature of a gas are directly proportional, the *ratio of the pressure to temperature never changes* (is *constant*).

$$\frac{P}{T} = (Constant)$$

Since the *ratio* of pressure to temperature never changes *when a gas undergoes a change (at constant volume),* the initial and final pressures and temperatures are related to each other in what is referred to as **Gay-Lussac's Law**.

Gay-Lussac's Law
$\dfrac{P_1}{T_1} = \dfrac{P_2}{T_2}$

There are a couple of *important things to keep in mind* when using **Gay-Lussac's Law**:

1. It is only applicable *when the volume does not change in the process*.

2. Temperature must be entered in kelvins.
   o If you are given the initial and/or final temperature in °C or °F, **convert to K**.

The math and concepts involved in solving Gay-Lussac's Law problems are identical to those of Charles' Law, so instead of showing you an example, I will have you go directly to an Understanding Check problem.

Understanding Check

The initial pressure of gas in a container is 15.7 atm. The gas is **_heated_** from 292 K to 525 K. The container's volume does not change. What is the final pressure?

---

4) The Combined Gas Law

How do we predict the behavior of a gas if **all three parameters**, temperature, volume, and pressure, **undergo changes**?

By mathematically combining the three previous gas laws, we get the "_____ **gas law**."

Combined Gas Law
$\dfrac{P_1 \cdot V_1}{T_1} = \dfrac{P_2 \cdot V_2}{T_2}$

Understanding Check: A gas in a cylinder with a piston has an initial pressure of 1.00 atm and an initial volume of 10.0 liters. The gas is cooled from 298 K to 265 K ___and___ the piston is compressed to give a final volume of 7.0 L. What is the *__final pressure__*?

5) Avogadro's Law

If you were to add more gas to a cylinder below a piston, the volume would increase.

Amadeo Avogadro studied the mathematical relationship between the amount of gas particles present and the volume of the gas.

Avogadro noticed that the _____ of a gas is *__directly proportional__* to the number of _____ of gas particles (at constant pressure and temperature). Because the volume and number of moles of a gas are *directly proportional*, the **ratio of the volume to the number of moles never changes**.

The initial and final number of moles present and volumes are related to each other in what is referred to as **Avogadro's Law**.

$$\text{Avogadro's Law}$$
$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$

"n_1" and "n_2" represent the initial and final *number of moles of gas particles*, respectively.

Understanding Check: 0.56 moles of gas are contained in a cylinder with a piston and the volume of gas is 4.0 L. If 2.00 moles of gas are *__added__* to this cylinder (at constant pressure and temperature), what is the final volume?

6) The Ideal Gas Law

In order for a gas to obey the gas laws perfectly, it could not experience *any* noncovalent interactions *and* have an infinitely small volume; this **hypothetical gas** is called an "_____ **gas**."

- No **real gas** perfectly obeys the gas laws, **HOWEVER**, the gas laws are **very reliable** in predicting the properties (P,V,T, and n) of gaseous systems at all **but** extremely high pressure **or** extremely low temperature conditions.

By mathematically combining *Avogadro's Law* and the *Combined Gas Law*, we get an equation that shows the relationship between pressure, volume, temperature, and the amount of a gas present (moles). We call this relationship the **ideal gas law**.

$$\text{Ideal Gas Law}$$
$$P \cdot V = n \cdot R \cdot T$$

In the **ideal gas law** equation, **n** represents the *number of moles* of gas particles that are present, and **R** is called the _____ _____.

The **gas constant** (**R**) is just a number that does not change; its value is a consequence of nature. The value of **R** was determined experimentally.

- In this course, we will use the value of **R** rounded to *three significant figures*:

$$R = 0.0821 \left(\frac{L \cdot atm}{K \cdot mole} \right)$$

We applied the previous five gas laws to systems where *a _____ occurred*.

- For example, when a gas was at an initial state (with P_1 and V_1), and then the pressure and volume were changed (at constant temperature), we used *Boyle's Law* to predict either P_2 or V_2 of the final state.

Unlike the previous gas laws, the **ideal gas law** is used to predict a property (**P**, **V**, **T**, or **n**) of a gaseous system at any time; ___ _____ *in the system will be involved*.

The *ideal gas law* involves *four variable parameters*: **P**, **V**, **T**, or **n**; when three of these four variables are known, we can use the *ideal gas law* to predict the value of the fourth, unknown variable.

Example: What is the volume of 1.00 moles of a gas at a pressure of 1.00 atm and a "comfortable" room temperature of 295 K?

Solution: Use the *ideal gas law*:

> Variables:
> **P = 1.00 atm**
> **V = ???**
> **n = 1.00 mole**
> **T = 295 K**

$$R = 0.0821 \left(\frac{L \cdot atm}{K \cdot mole} \right)$$

Ideal Gas Law

$$P \cdot V = n \cdot R \cdot T$$

- In this example, we know P, T, and n; we wish to solve the ideal gas law equation for the volume (**V**):

$$P \cdot V = n \cdot R \cdot T$$

- To solve for **V**, we divide both sides of the equation by **P**:

$$\frac{P \cdot V}{\cancel{P}} = \frac{n \cdot R \cdot T}{P}$$

- **P** cancels on the left side of the equation; we have isolated the unknown variable (**V**):

$$V = \frac{n \cdot R \cdot T}{P}$$

- Insert the known values of P, T, n, and R, and then solve for the volume (**V**):

$$V = \frac{(1.00 \ \cancel{mole}) \cdot \left(0.0821 \ \frac{L \cdot atm}{\cancel{K} \cdot \cancel{mole}} \right) \cdot (295 \ \cancel{K})}{(1.00 \ \cancel{atm})} = 24.2 \ L$$

Because the gas constant has units of (**L•atm/K•mole**), when using the ideal gas law, the pressure must have **atm** units, the temperature must have **K** units, and the volume must have **L** units.

- If you are given **P**, **V**, or **T** in any other units, you must first convert them to units that match the gas constant's units.

Understanding Check

A gas in a 3.80 L container has a pressure of 8.63 atm and a temperature of 295 K. How many moles of gas are present?

---

7) Dalton's Law

The *identity* of a gas does not need to be known when using the gas laws. The gas laws work quite well whether the gas is CO_2, N_2, argon, or any other gas.

The reason for this is related to the gas laws' ability to precisely predict the behavior of gases in all but extremely high pressure or low temperature conditions. Under most conditions, **real gases** behave very similar to **ideal gases.** This is true because gas particles are far apart from other particles most of the time, and they are moving so fast that when they approach each other and/or collide, they do not experience noncovalent interactions for significant amounts of time.

Another simplification in describing gases results from this situation. ***Not only are the gas laws applicable to any single type of gas, they work just as well for mixtures of gases***.

John Dalton was the first person to report that the gas laws applied equally well to gas mixtures.

Dalton's Law states that the _____ *pressure of a mixture of gases* in a container is equal to the _____ of the pressures that each gas in the mixture would exert **if that gas were alone in the container**.

Example: a sample of argon in a one-liter container has a pressure of 1.20 atm, a sample of N_2 in a one-liter container has a pressure of 1.80 atm, and a sample of CO_2 in a one-liter container has a pressure of 0.90 atm. If these three samples were combined in a one-liter container, the total pressure would be the sum of the pressures that *each gas exerted* when it was alone in the container.

Combine the Gas Samples

Argon	N₂	CO₂	Mixed Gases
P = 1.20 atm	P = 1.80 atm	P = 0.90 atm	P = 3.90 atm
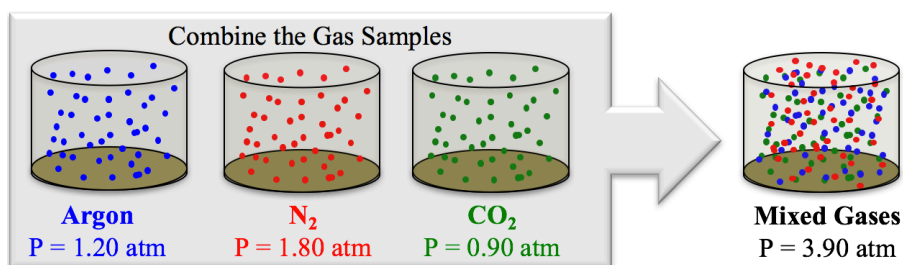
- Total pressure of the mixture = 1.20 atm + 1.80 atm + 0.90 atm = 3.90 atm

For Dalton's Law to be applicable, the temperature and volume of the gases must not change.

The amount of pressure exerted by an individual gas in a mixture is called that gas's _____ _____.

For the mixture described in this example:

The *partial pressure* of Ar = 1.20 atm
The *partial pressure* of N_2 = 1.80 atm
The *partial pressure* of CO_2 = 0.90 atm

Understanding Check

A sample of O_2 gas in 20.0 liter container has a pressure of 625 Torr. In another 20.0 L container, a sample of neon (Ne) gas has a pressure of 127 Torr. If the two gas samples are combined in a 20.0 L container, what would be the pressure of the gas mixture?

Liquids

The major difference between liquids and gases is that the particles are much _____

_____.

- *Noncovalent interactions* therefore play a very important role in determining the properties of liquids.

Consider how much closer H_2O molecules are to each other in the liquid phase vs. the gas phase.

- At its normal boiling point (100 °C and 1 atm pressure), the volume of H_2O gas is about 1600 times greater than the volume of an equal mass of H_2O in the liquid phase.
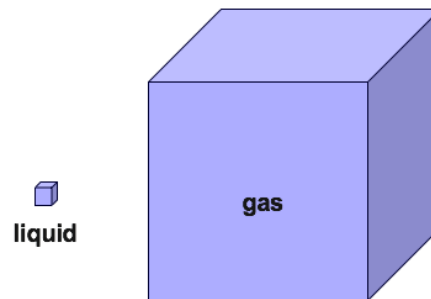
Properties of Liquids: Viscosity

You have probably noticed a difference in the way syrup and water behave when you pour them. We often say that syrup is "thicker" than water because it flows more slowly than water. The technical way to make this statement is, "syrup is more *viscous* than water."

Viscosity is a measure of a substance's _____ *to* _____.

The nanometer scale explanation for the existence of viscosity is that molecules in a liquid need to "slide" past the molecules that surround them in order for the liquid to flow. Noncovalent interactions attract the molecules to each other and impede their ability to slide past each other.

- The _____ the noncovalent interactions, the _____ *viscous* a liquid is.

Temperature (kinetic energy) aids molecules in overcoming noncovalent interactions in order to more easily slide past each other, therefore a liquid's viscosity is temperature dependent.

- With very few exceptions, the _____ the _____, the _____ a substance's viscosity.
- You may have observed this if you compared hot and cold syrup's ability to flow (viscosity).

Properties of Liquids: Vapor Pressure

Consider a glass of water that is at room temperature of (~22 °C).

Water slowly **evaporates** even though it is at a temperature less than its boiling point (100 °C).

You can think of temperature as a measure of the _____ *kinetic energy* of a substance.

- I use the word "*average*" because not every molecule in a sample has the *exact same amount* of kinetic energy.

Because of random collisions between the water molecules, individual molecules in the glass are *constantly gaining **and** losing energy*.

The *total* energy and the *average* energy of the water **do not change**; the water molecules simply *exchange* energy with each other.

In random events such as collisions of molecules, there is a ***probability distribution*** of molecular kinetic energies as shown below.
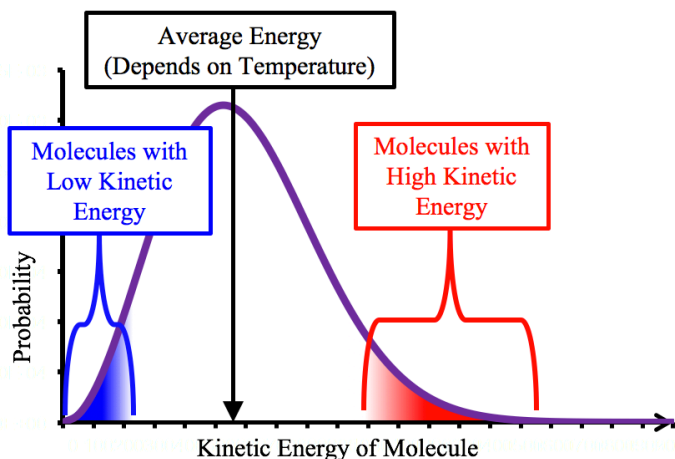
The horizontal axis shows the molecular kinetic energies.

The vertical axis is the probability of a molecule having a particular kinetic energy.

The probability distribution (shown as a purple curve) has a *maximum height* at the *most probable kinetic energy*.

Except at extremely low temperatures, the ***average kinetic energy*** of the molecules is *very close to the center (peak) of the distribution* (indicated by the black arrow).

The average energy depends on the temperature.

Because of the shape of the histogram, ***a relatively small number of molecules*** have *very low kinetic energy (*as indicated by the blue shaded area under the curve) or *very high kinetic energy* (as indicated by the red shaded area under the curve). These low-probability ends of histogram curves are called "tails." When thinking about the system on the nanometer scale, it is as if each molecule is at its own temperature. Since thermometers are on the macro-scale size, they interact with many millions of molecules and therefore measure the average energy/temperature.

Consider the molecules in the ***high energy tail*** (shaded red) of the histogram.
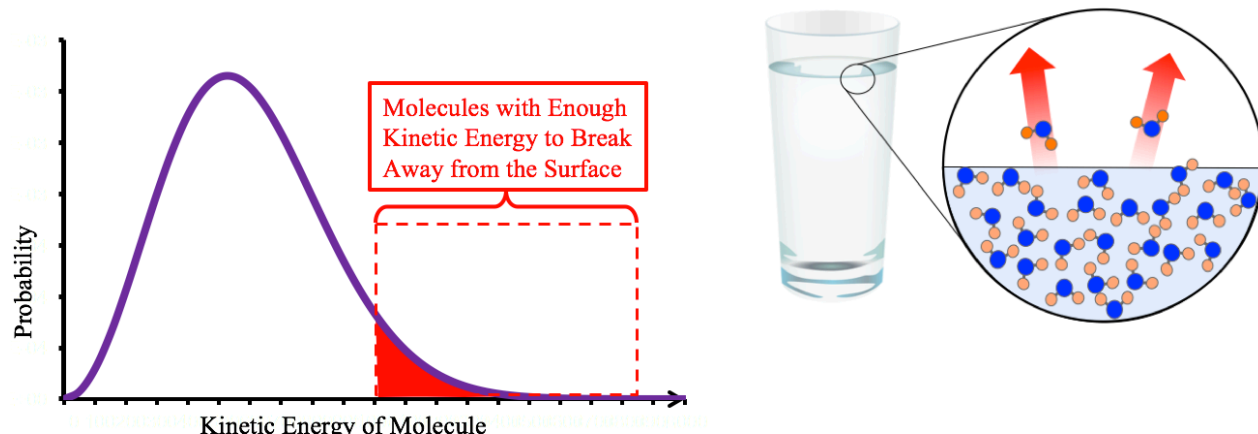
- When some of these molecules happen to be *on the surface of the water*, they have enough kinetic energy to "**break free**" from the *noncovalent interactions* holding them to their neighboring molecules.

- We call this process _____.

If a piston were brought into contact with the surface of the liquid, the molecules that are escaping the liquid's surface would exert an *upward force* on the piston.

The total force from the molecules breaking free from the liquid (per surface area unit) is referred to as the _____ _____ of a substance.

- The greater the vapor pressure, the _____ the evaporation rate.

The Temperature Dependence of the Vapor Pressure

At higher temperatures, a greater number of molecules have enough energy to break free of the surface as indicated by the amount of area (shaded red) under the higher temperature histogram (dashed curve).
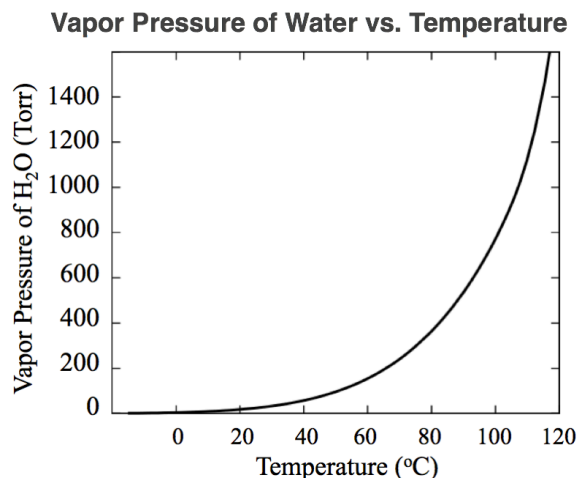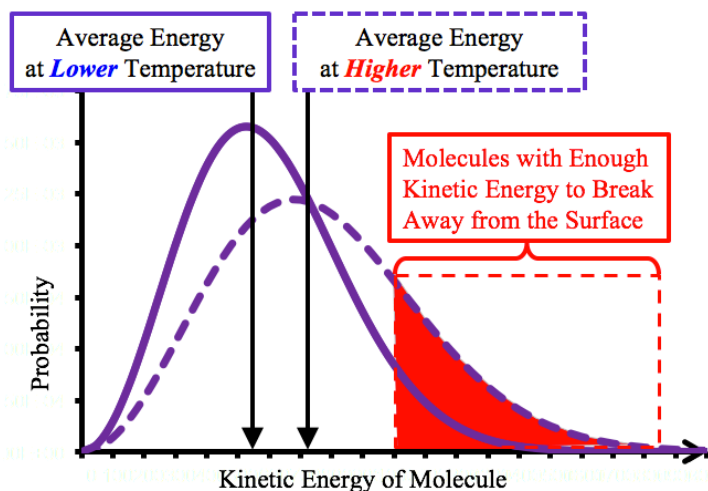
The **vapor pressure** of a substance _____ *with* _____ .

Properties of Liquids: Boiling Points

The boiling point of a liquid in an *open container* is the temperature at which its vapor pressure equals the _____ pressure.

In *closed containers*, liquids boil when their vapor pressure equals the pressure of the gas _____ them.

The temperature at which a liquid boils at 1 atm pressure is called its _____ *boiling point*.

- It is no coincidence that the *normal boiling point of water* is exactly 100 $^{\circ}$C; the Celsius scale is based on the *normal boiling point* and *freezing point* (0 $^{\circ}$C) of water.

Consider the graph of the vapor pressure of water vs. temperature shown below.
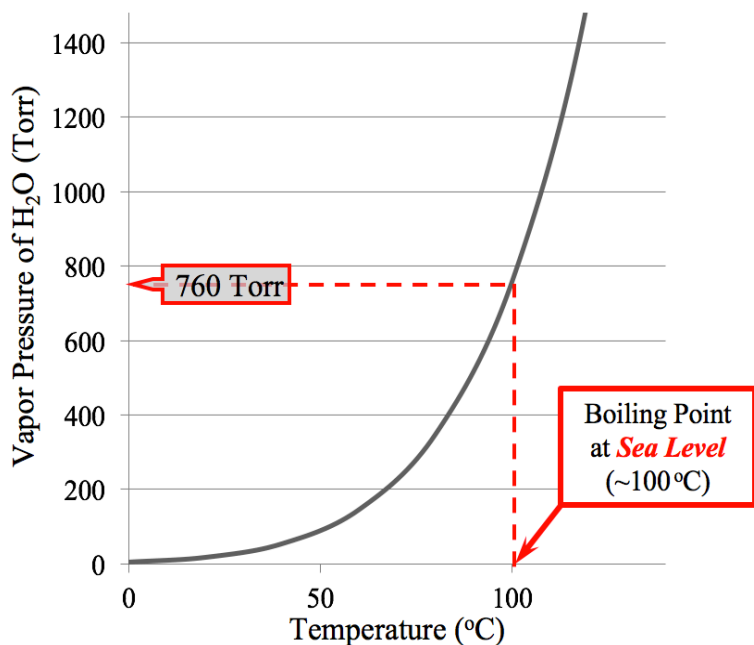
The dashed line indicates that the vapor pressure of water at 100 $^{\circ}$C is equal to 760 Torr (1 atm).

This is why water will boil at 100 $^{\circ}$C in an open container at sea-level where the atmospheric pressure is 760 Torr (1 atm).

You may have heard that it takes more time to cook food (in boiling water) at higher elevations.

- This is true because water will boil at a lower temperature as the elevation increases (because the atmospheric pressure decreases).

For example, if you were to cook food in boiling water while in Denver, Colorado (elevation 5280 ft) where the air/atmospheric pressure is about 625 Torr, water boils at about 93°C, as indicated by the blue dashed lines in graph shown in the figure on the right.

- It would take longer to cook food in boiling water at this elevation than it would at sea level.
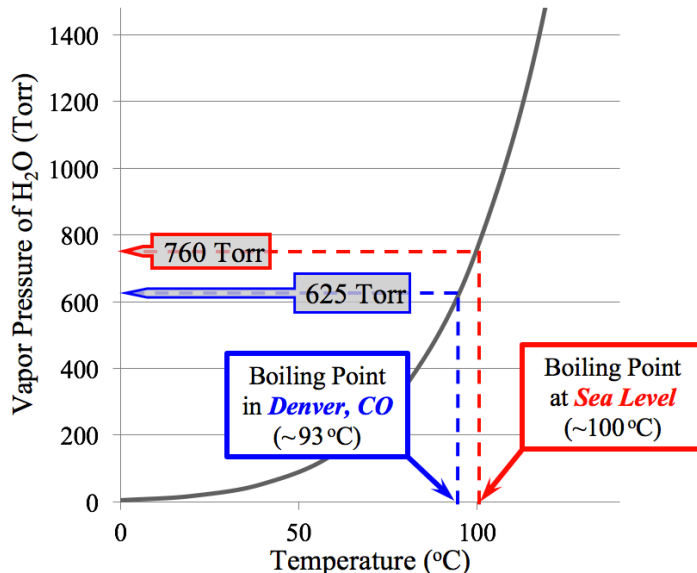
Understanding Check

In pressure cookers, the water is boiled at a pressure of about 1500 Torr. Use the graph (**shown in the video**) to **estimate** the temperature at which food is cooked in a pressure cooker.

Now that you understand the details of **evaporation**, let's conclude this subsection on liquids by considering what happens in a capped water bottle.

In **closed containers**, liquid phase molecules are not only evaporating, gaseous H_2O molecules are also colliding with the liquid's surface, losing energy, and re-entering the liquid phase (**condensation**). These processes are illustrated below.
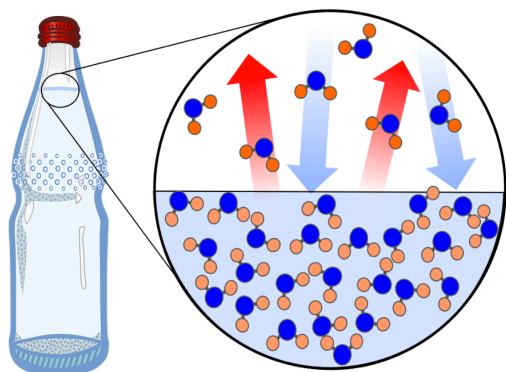
The upward arrows represent **evaporation** and the downward arrows represent **condensation**.

If the bottle is **open**, the H_2O vapor that leaves the bottle does not return to the liquid phase in the bottle.

Once the bottle is **capped**, the amount of vapor increases until there are so many H_2O molecules in the gas phase that they are colliding with the surface and re-entering the liquid (**condensing**) at the **same rate** that they are evaporating.

Solids

The major difference between solids and liquids is that the atoms, ions, or molecules that make up a solid *cannot move away from their neighboring particles*, whereas the particles that make up liquids are able to do so.

- It is for this reason that you are not able to pour solids.

- Although solid phase particles are not able to overcome the *noncovalent interactions* holding them next to neighboring particles, they do contain *kinetic energy* in the form of *vibrations* and, in some cases, *conformational* changes.

Classification of Solids

Solids can be classified based on whether or not the arrangement of particles is _____.

- In _____ *solids*, the atoms, ions, or molecules are arranged in an *ordered*, three-dimensional pattern called a *crystal lattice*.
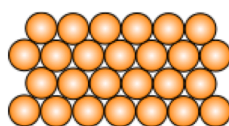
Illustration of a Crystalline Solid

- In _____ *solids*, the particles *are not* arranged in an *ordered* pattern.

  - The word *amorphous* is from the Greek "a," *without*, and "morphé," *form*.
  - An example of an amorphous solid is rubber.
  - The molecules in amorphous solids are held to each other by noncovalent interactions.
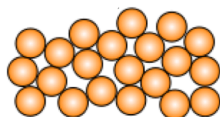
Illustration of an Amorphous Solid

Types of Crystalline Solids

The four types of **crystalline solids**, along with their descriptions and some examples, are listed below.

Type	Description	Examples
Ionic Solids	Composed of cations and anions that are arranged in a lattice pattern such that the attraction of unlike charge is maximized and the repulsion of like charge is minimized (ionic bonding).	Table Salt (NaCl) Baking Soda (NaHCO$_3$)
Molecular Solids	Composed of molecules that are arranged in a lattice pattern such that the attraction of intermolecular forces are maximized.	Ice Table Sugar (Sucrose)
Covalent Network Solids	The entire bulk of the solid is composed of atoms that **are all** *covalently bonded to their neighbors*.	Diamond Silica
Metallic Solids	The nuclei and their core electrons are in lattice positions, and the valence electrons are dispersed *throughout the entire crystal*.	Gold Aluminum

I have discussed the first two types of crystalline solids listed in the table in previous chapters: *ionic solids* and *molecular solids*.

I will now introduce you to two *other types* of crystalline solids: **covalent network solids** and **metallic solids**.

Covalent Network Solids

In **covalent network solids**, the entire bulk of the solid is composed of atoms that **are all** *covalently bonded to their* _____.

- The covalent bonding pattern *extends throughout the entire crystal*.

Very few substances exist as covalent networks.

Diamond is a material that exists as a *covalent network*.

Pure diamond is composed of carbon atoms that are each covalently bonded to *four* other carbon atoms.

This bonding pattern (AB_4 geometry class, $110°$ bond angles) is shown on the right.
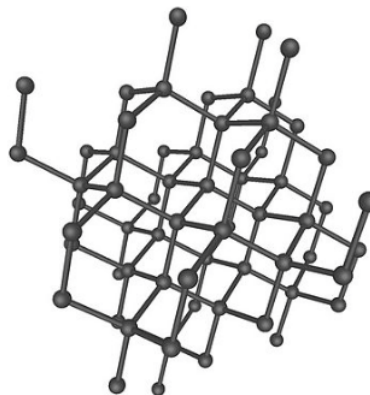
Another example of a **covalent network solid** is quartz.

- Quartz is composed of silicon (Si) and oxygen atoms.

A Quartz Crystal
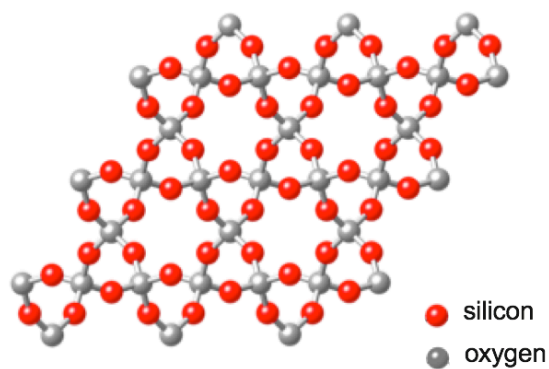
The Covalent Network Bonding Pattern of Quartz

- silicon
- oxygen

Metallic Solids

You have learned about two types of *chemical bonds*: **ionic bonds** and **covalent bonds**. I have not yet presented a model of how metal atoms are held together in the solid state.

There is *one other type of **chemical bonding*** called

_____ **bonding**.

- Metal atoms form crystals.
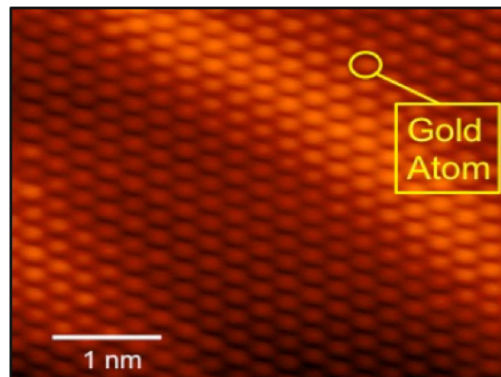
An Atomic Force Microscope Image of the Surface of Solid Gold
(Each bright spot is a gold atom.)

Image source: Virginia Technical Institute, Physics Dept. Showcase (with permission)
Author: Prof. Chenggang Tao

In metallic bonding, the *nuclei* and their *core electrons* are arranged in a lattice pattern, and the _____ *electrons* are dispersed ***throughout the*** _____ *crystal*.

The image below is a two-dimensional model that illustrates how the nuclei, core electrons, and valence electrons are arranged in metals.
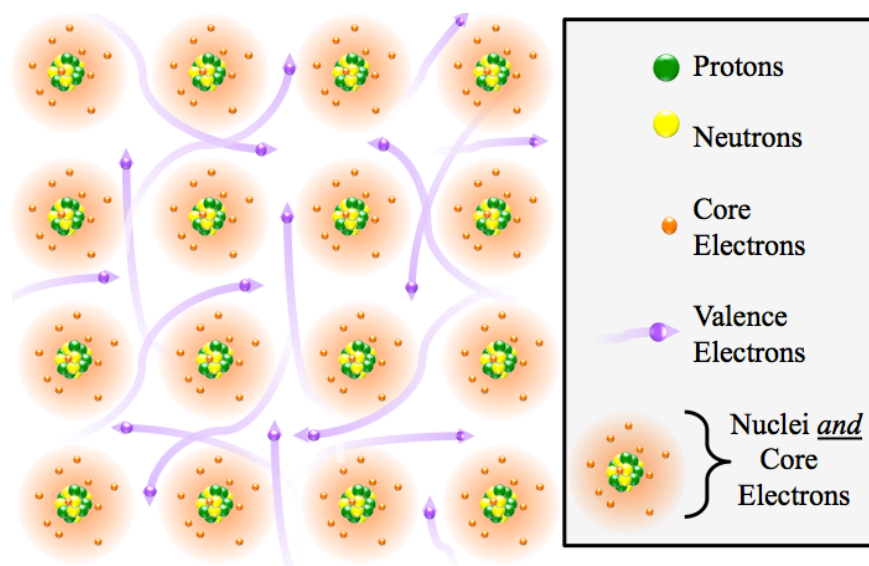
The mobile valence electrons in metallic bonding are sometimes referred to as a "***sea of electrons***."

Each metal nucleus <u>with</u> its ***core electrons*** has an overall _____ *charge and is called a "cationic center."*

The _____ *attraction* between the **negative charge of the** *sea of electrons* and the *positive cationic centers* is responsible for holding the particles together in metals.

A model of the positive "cationic" centers and the sea of electrons (purple shaded area) is shown on the right.
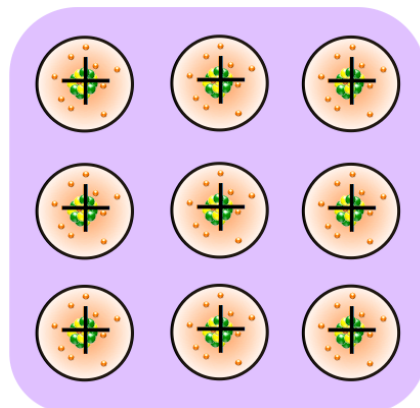
Properties of Metallic Substances

Metallic substances are solid *at room temperature* with one exception; mercury exists as a liquid.

Metallic solids are _____.

- *Malleable* substances can be hammered or beaten into thin sheets.

The reason metals can be flattened without breaking (shattering), can be visualized in the cationic centers/sea of electrons model as shown below.
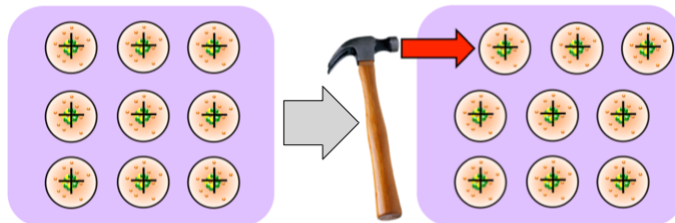
When a layer of cationic centers is shifted by hammering, the sea of electrons is still present to hold the solid together.

The opposite of "*malleable*" is "*brittle*." *Brittle* substances shatter when hammered or crushed.

- *Ionic compounds* are brittle because shifting the ion positions would put cations next to other cations and anions next to other anions and result in a strong electrostatic repulsion.
- *Covalent networks* are brittle because the covalent bonds can be broken when hammered or crushed.

Metallic solids are _____.

- *Ductile* substances can be drawn or pulled through a series of increasingly smaller holes to produce wire.

Metallic substances are good **conductors of electricity.**

- The relative ability for electrons to move through a substance is called its electrical _____.
- The opposite of electrical conductivity is electrical *resistance*.
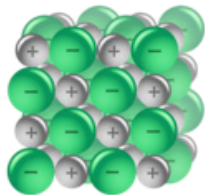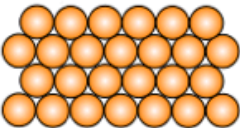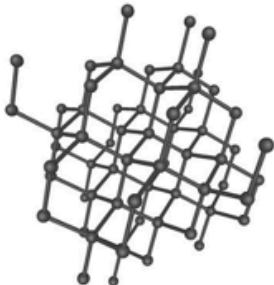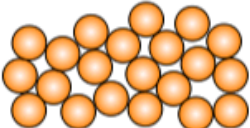
The reason metals are good conductors of electricity can be visualized in the cationic centers/sea of electrons model.

Connect a Battery or other Electrical Power Source
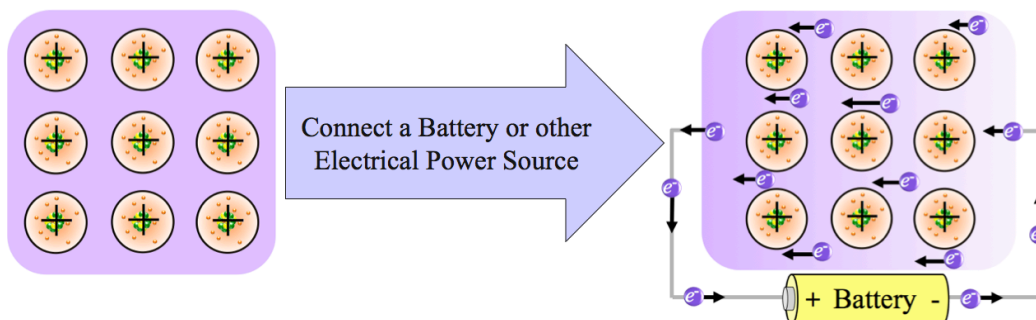
+ Battery -

When the positive and negative terminals of a battery (or other power source) are connected to opposite sides of a metal, the *mobile valence electrons* will be attracted (and move) to the positive terminal of the battery. The negative terminal will supply new electrons that will also move through the metal toward the positive terminal of the battery. This is called an electrical circuit. The rate of electron flow depends on the resistance of the material in the circuit and the voltage of the battery or power source.

Summary of Solids

Type	Description	Example(s)	Structural Model
Ionic Solids (Crystalline)	Composed of cations and anions that are arranged in a lattice pattern such that the attraction of unlike charges is maximized and the repulsion of like charges is minimized (ionic bonding).	Table Salt (NaCl)	
Molecular Solids (Crystalline)	Composed of molecules that are arranged in a lattice pattern such that the noncovalent interactions are maximized.	Ice Table Sugar (Sucrose)	
Covalent Network Solids (Crystalline)	The entire bulk of the crystalline solid is composed of atoms that **are all** *covalently bonded to their neighbors.*	Diamond	
Metallic Solids (Crystalline)	The nuclei and their core electrons are in lattice positions and the valence electrons are mobile and dispersed throughout the entire crystal.	Gold, Aluminum	
Amorphous Solids	The particles **are not** arranged in an ordered pattern.	Natural and Synthetic Rubbers	

Calculations for Temperature and Phase Change Worksheet

The heat of fusion of ice is 79.7 cal/g.
The heat of vaporization of water is 540 cal/g.

Report the answer using the correct number of significant figures!

1. How much energy is required to melt 100.0 grams of ice?

Answer: 7970 cal

2. How much energy is required to vaporize 234.5 g of water?

Answer: 1.3×10^5 cal

3. If 30.6 calories are required to vaporize 25 g of a substance, what is the heat of vaporization of that substance?

Answer: 1.2 cal/g

4. How much energy is removed from 500.0 g of water when the temperature is lowered by 1.10 °C?

Answer: -550 cal (or -2.30×10^3 J)

5. How much energy is required to raise the temperature of 1000.0 g of water from 23.00 °C to 26.00 °C?

Answer: 3.00×10^3 cal (or 1.26×10^4 J)

6. The specific heat of copper is (0.0924 cal/g°C), how much energy is required to raise the temperature of 10.0 g of copper by 100.0 °C?

Answer: 92.4 cal

7. If 25.6 J of energy raised 786 g of a substance from 20.0°C to 35.0°C, what is the specific heat of the substance (S)?

Answer: 2.17×10^{-3} J/g °C

Gas Laws Worksheet

Charles's Law (temperature, volume)

1) A 550.0 mL sample of nitrogen gas is warmed from 77 °C to 86 °C. Find its new volume if the pressure remains constant.

564 ml

2) A gas occupies 1.00 L at 0.00°C. What is the volume at 333.0 °C?

2.22 L

Boyle's Law (pressure, volume)

3) Convert 338 L at 63.0 atm to its new volume at 1.00 atm.

21300 L   or   2.13 x 10⁴ L

4) A tank of nitrogen has a volume of 14.0 L and a pressure of 760.0 mm Hg. Find the volume of nitrogen when its pressure is changed to 400.0 torr while the temperature is held constant.

26.6 L

5) What pressure (mm Hg) is required to compress 196.0 liters of air at 1.00 atmosphere into a cylinder whose volume is 26.0 liters?

5730 mmHg

Gay-Lussac's Law (temperature, pressure)

6) A gas has a pressure if 0.0370 atm at 50.0 °C. What is the pressure at 0.00 °C?

.0313 atm

7) If a gas in a closed container, with an original temperature of 25.0 °C, is pressurized from 15.0 atmospheres to 16.0 atmospheres, what would the final temperature of the gas be?

318 K

Use the <u>combined gas law</u> to solve the following problems:

8) If I initially have a gas at a pressure if 12 atm, a volume of 23 liters, and a temperature of 200.0 K, and then I raise the pressure to 14 atm and increase the temperature to 300.0 K, what is the new volume of the gas?

30. L

9) A gas takes up a volume of 17 liters, has a pressure of 2.3 atm, and a temperature of 299 K. If I raise the temperature to 350 K and lower the pressure to 1.5 atm, what is the new volume of the gas?

31 L

Ideal Gas Law

10) Calculate the pressure, in atmospheres, exerted by each of the following:
a. 250 L of gas containing 1.35 moles at 320 K.

.14 atm

b. 4.75 L of gas containing 0.86 moles at 300. K.

4.5 atm

11) Calculate the volume, in liters, occupied by each of the following:
a. 2.00 moles of H_2 at 300. K and 1.25 atm.

39.4 L

b. 0.425 moles of ammonia gas (NH_3) at 0.724 atm and 37°C

14.9 L

12) Determine the number of moles contained in each of the following gas systems:
a. 1.25 L of O_2 at 1.06 atm and 250. K

.0646 moles

b. 0.80 L of ammonia gas (NH_3) at 0.925 atm and 27°C
.030 moles

Chapter 6 Lecture Notes: Chemical Reactions

Educational Goals

1. Define the term "**chemical reaction**."

2. Given the **reactants** and **products** in a chemical reaction, *write* and *balance* chemical equations.

3. Use **stoichiometric calculations** to determine the **theoretical yield** and **percent yield** of a reaction.

4. Identify **redox reactions** and determine which species is oxidized and which is reduced.

5. Understand and identify the four *general types* of reactions.

6. Identify combustion, hydrogenation of alkenes, hydrolysis of esters, hydration of alkenes, and dehydration of alcohol reactions.

7. Given the reactants for **combustion, hydrogenation of alkenes, hydrolysis of esters, hydration of alkenes,** or **dehydration of alcohol reactions**, be able to *predict* and *draw* structural formulas of the products.

8. Describe the difference in energy changes (ΔG) for **spontaneous** and nonspontaneous reactions, and list the factors that affect the **rate** of a chemical reaction.

In chapter 5 you learned about *physical changes*. In chapter 6 you will learn about **chemical changes** that occur in processes called *chemical reactions*.   Chemical reactions occur in nature and in man-made events. A series of chemical reactions occurs in plants as they convert carbon dioxide and water molecules into the carbohydrate molecules that we eat and oxygen molecules that we breathe. Chemical reactions are used for propulsion in automobile engines and rocket thrusters. Some chemical reactions occur very quickly, as in explosions, and some reactions very slowly, as in the rusting of a nail. Chemistry is the study of how matter interacts with energy and/or other matter; *one way this happens is in chemical reactions*.

A chemical reaction is a process in which **chemical bond(s)** are *broken* **and/or** *new bonds are made*, such that one or more _____ _____ are formed.

Example: One of the rocket engines in the space shuttle uses a chemical reaction in which oxygen gas and hydrogen gas are changed into gaseous H_2O molecules.

- To describe the chemical reaction, we say, "oxygen gas **reacts** with hydrogen gas to produce gaseous H_2O."

A Rocket Thruster

Scientists often write a ***chemical*** _____ to describe a ***chemical reaction***.

- Chemical equations are similar to mathematical addition equations, except in chemical equations an arrow ($\rightarrow$) is used *instead of* an equal (=) sign.

- For example, the **"unbalanced"** ***chemical equation*** for the reaction of oxygen and hydrogen to produce H_2O vapor is:

$$H_2 + O_2 \rightarrow H_2O$$
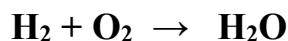
When writing chemical equations, we often indicate the _____ of each reactant and product in parenthesis after its chemical formula.

- One of the following states is used: gas ***(g)***, liquid ***(l)***, solid ***(s)***, or aqueous ***(aq)***.
  - Aqueous ***(aq)*** indicates that the substance is ***dissolved in water***.

- For our rocket fuel example, we write:

$$H_2\ (g) + O_2\ (g) \rightarrow H_2O\ (g)$$
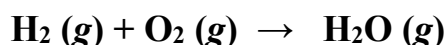
The substances on the ***left-hand side*** of the reaction arrow ($\rightarrow$) are referred to as the _____.

The substances on the ***right-hand side*** of the reaction arrow are referred to as the _____.

In the rocket fuel chemical reaction, we began with two *reactants* (O_2 and H_2), and ended with one *product* (H_2O).

Antoine Lavoisier and his wife, Marie-Anne Pierette Paulze, and Mikhail Lomonosov are credited for proposing and verifying the **law of conservation of mass**.

Antoine Lavoisier (1743-1794) and his wife, Marie-Anne Pierette Paulze (1758-1836)

- This law states that ***matter is neither created nor destroyed in a chemical reaction, only the chemical bonding changes.***
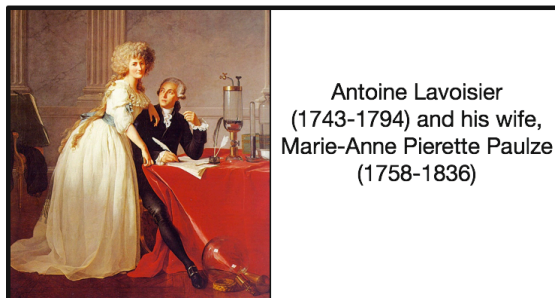
The *law of conservation of mass* requires that the _____ ***number of atoms of each element*** appear ***on*** _____ _____ ***of the chemical equation***; when this is applied to a chemical equation, we say that the equation is "_____."

In our rocket fuel chemical equation, we need to have at least <u>***two***</u> H_2O molecules on the right-hand side to "balance" the two oxygen atoms on the left-hand side (in O_2).

We use a _____ and re-write the equation as:

$$H_2\ (g) + O_2\ (g) \rightarrow 2\,H_2O\ (g)$$
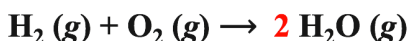
The **coefficients** indicate the **multiples** of each reactant and each product needed in order to have a *balanced equation*.

- If no coefficient appears for a substance, this implies that the coefficient is "___."

Because I added a coefficient of "**2**" to H_2O, the *oxygen atoms* are now *balanced*; there are *two oxygen* atoms ***on each side*** of the equation.

Is this equation completely balanced now?

$$H_2 \ (g) + O_2 \ (g) \ \rightarrow \ \textbf{2 H}_2\textbf{O} \ (g)$$
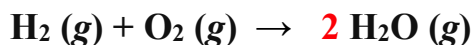
The equation is not yet balanced.

There are two hydrogen atoms on the reactant side (on the left) of the equation and the two H_2O molecules on the product side (right-hand side) contain a total of four hydrogen atoms (two hydrogens for _each_ H_2O).

We need to use _another coefficient_ to balance the equation.

- We need **two** H_2 molecules on the **reactant side** in order to balance the chemical equation:

$$\textbf{2 H}_2 \ (g) + O_2 \ (g) \ \rightarrow \ \textbf{2 H}_2\textbf{O} \ (g)$$
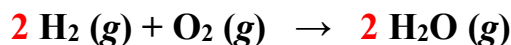
In this reaction, it takes _____ H_2 molecules to **react** with _____ O_2 molecule to **produce** _____ H_2O molecules.

I told you that a chemical reaction is a process in which **chemical bond(s)** are _broken **and/or**_ new bonds are made such that one or more **new substances** are formed.

- Consider how this occurred in our reaction of rocket fuel.

In order to produce <u>two</u> H_2O molecules, _two_ H-H bonds and the O-O double bond must break and _**four**_ <u>new</u> O-H bonds must be made.
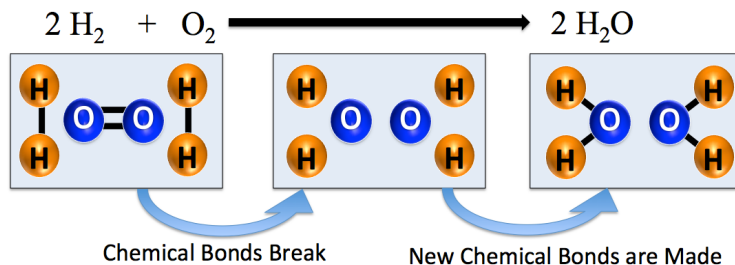
The exact order of bond breaking and making in chemical reactions is called the **reaction mechanism**. The details of the particular reaction mechanism for our reaction of rocket fuel and many other chemical reactions are not completely known and remain an active area of research in academia and industry.

Observational Evidence of Chemical Reactions

When reactants are converted into new substances, several macro-scale observations may present evidence that a chemical reaction has occurred.

1) A _____ _change_ is evidence of a chemical reaction.

Many substances absorb visible light and therefore appear with a particular color. As a colored reactant is converted to product(s), the color of the reactant disappears. Chemical reactions _**always**_ involve the formation of _one or more **new substances**_ called _**product(s).**_ If a product absorbs visible light, a new color will appear.

This is the basis of the color change seen in the chemical reaction that occurs when a nail "rusts."

$$4 \ Fe \ (s) + 3 \ O_2 \ (g) \rightarrow 2 \ Fe_2O_3 \ (s)$$
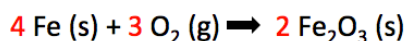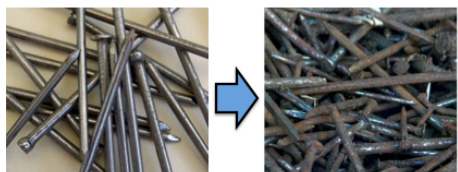
The reactants are iron metal and oxygen gas. Although iron metal does not absorb visible light, it does reflect it, and therefore has a "silver" appearance. The iron metal nail reacts with O_2 in the air to form Fe_2O_3 (rust). Fe_2O_3 absorbs all colors of visible light, a bit more strongly in the blue region, and therefore has a dark brown/red color.

2) The **formation of a** _____ _____ is evidence of a chemical reaction.

- **Example:** Epoxy adhesives involve a chemical reaction of two *liquid reactants* that form a **new**, *solid product* substance.
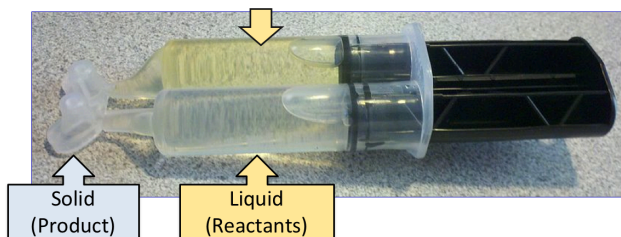

Solid (Product)   Liquid (Reactants)

- Another example of a reaction in which a *new phase is formed* is the reaction of aqueous acetic acid (white vinegar) with sodium bicarbonate (baking soda).
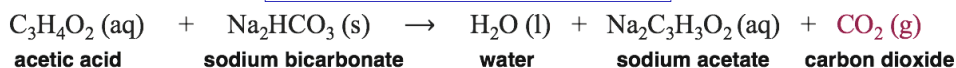

$$C_3H_4O_2 \ (aq) \ + \ Na_2HCO_3 \ (s) \ \longrightarrow \ H_2O \ (l) \ + \ Na_2C_3H_3O_2 \ (aq) \ + \ CO_2 \ (g)$$

acetic acid   **sodium bicarbonate**   **water**   **sodium acetate**   **carbon dioxide**

3) Observation of a _____ *change* is evidence of a chemical reaction.

- **Example:** A "thermite" reaction.

$$2 \ Al \ (s) + Fe_2O_3 \ (s) \longrightarrow Al_2O_3 \ (s) + 2 \ Fe \ (l)$$

Originally at room temperature.

Products are very hot.
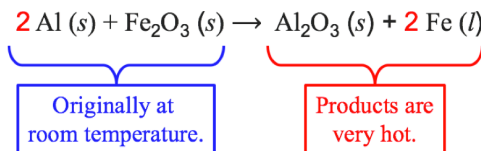
4) Observation of the *emission of* _____ is evidence of a chemical reaction.

- Examples of this are the thermite reaction that I just discussed and a chemical reaction that occurs in fireflies.
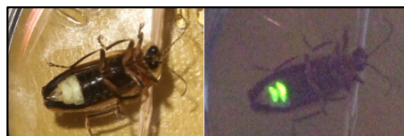
In a series of two reactions, a molecule called firefly luciferin is converted to oxyluciferin.

luciferin   oxyluciferin   + LIGHT
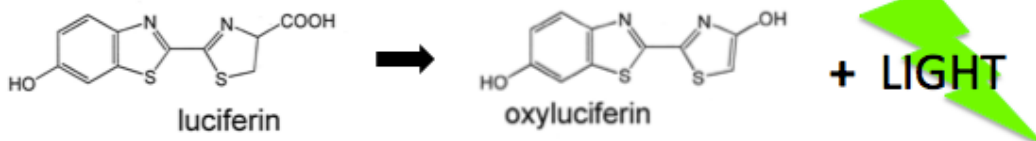
5) Observation of *a new* _____ is evidence of a chemical reaction.

- An example of the detection of a new odor from a chemical reaction is "*rotting*."

6) The *appearance of a* _____ is evidence of a chemical reaction.

- **Example:** The burning (combustion) of methane (CH_4), in natural gas.

$$CH_4\ (g)\ +\ 2\ O_2\ (g)\ \longrightarrow\ CO_2\ (g)\ +\ 2\ H_2O\ (g)$$
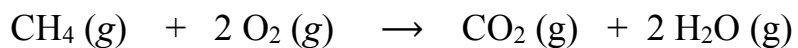
Understanding Check

Answer the following questions about the chemical equation shown below:

$$2\ H_2 + S_2 \rightarrow 2\ H_2S$$
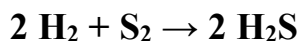
a. What are the reactants?

b. What is the product?

c. What is the number "2" in front of the H_2 (and H_2S) called?

d. Is the reaction balanced?

e. Why is there not a coefficient for S_2?

f. How many hydrogen **atoms** are needed to produce **two** H_2S molecules?

g. How many sulfur **atoms** are needed to produce **two** H_2S molecules?

h. How many hydrogen **molecules** are needed to produce **two** H_2S molecules?

i. How many sulfur **molecules** are needed to produce **two** H_2S molecules?

Balancing Chemical Equations

Matter is neither created nor destroyed in a chemical reaction.

- Therefore, the same _____ of atoms of each element appear on **both** _____ of a *balanced chemical equation*.

I introduced you to the *law of conservation of mass* and the need to balance chemical equations in the previous video.

- Some *students* are able to balance chemical equations "*in their heads*" by inspection of the unbalanced equation. This approach often involves trial and error placement of coefficients.

- Other students prefer a systematic, methodical approach.

In this video, I will provide you with a systematic method for balancing equations.

Whether you use the inspection (trial and error) approach _or_ the systematic method, the end result is the _same_ balanced equation.

There are ***three steps*** involved in the *systematic balancing method*:

Step 1: Make a table that lists the elements that are present and count all atoms on each side of the *unbalanced* equation.

- If **H_2 or O_2** is present, list these elements last.

- A polyatomic ion may be counted as one "element" *if it appears on __both__ sides of the equation.*

Step 2: Balance an element in the table by adding *coefficient(s)* to the equation (start with the first element on the list).

Step 3: Recount each atom and update the table, then repeat **Steps 2 and 3** for all elements as needed until the equation is balanced.

We will go right to an example problem where we will use these steps.

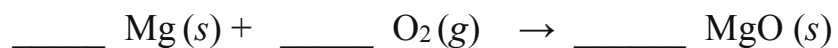**Take notes here – fill in the table and coefficients while watching the video.**

Example: Balance the equation for the following reaction:

_____ H_2 (g) + _____ O_2 (g) → _____ H_2O (g)
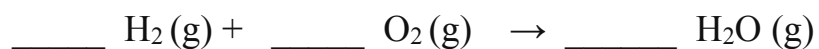
Amount on Reactant Side	Element	Amount on Product Side
	O	
	H	

Take notes here – fill in the table and coefficients while watching the video.
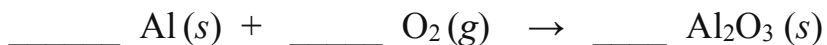
Example: Balance the following chemical equation:

_____ Mg (s) + _____ O_2 (g) → _____ MgO (s)

Amount on Reactant Side	Element	Amount on Product Side
	Mg	
	O	

Next, I want to show you and example problem that illustrates the short-cut that you can use when the same **polyatomic ion** appears on the reaction side **and** product side of the equation.

When I gave you the three steps involved in the systematic balancing method, I gave you a couple of instructions for performing "**Step 1**" that will save time and make balancing a bit simpler.

Step 1: Make a table that lists the elements that are present and count all atoms on each side of the *unbalanced* equation.

- If **H₂ or O₂** is present, list these elements last.
- A polyatomic ion may be counted as one "element" *if it appears on* <u>both</u> *sides of the equation.*

Let's take a look at how this *second instruction* works.

Take notes here – fill in the table and coefficients while watching the video.

Example: Balance the following chemical equation.

_____ Al (s) + _____ FeSO₄ (aq) → _____ Al₂(SO₄)₃ (aq) + _____ Fe (s)
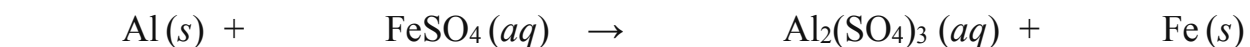
Amount on Reactant Side	Element	Amount on Product Side
	(SO_4)	
	Al	
	Fe	

Step 1: Make a table that lists the elements that are present and count all atoms on each side of the *unbalanced* equation.

- If **H₂ or O₂** is present, list these elements last.

When **H₂** or **O₂** are present, we list hydrogen and oxygen last because **H₂** and **O₂** *consist of only one type of element*, and therefore when a coefficient is added to these molecules, it will not change the number of atoms of other elements that have already been balanced.

Take notes here – fill in the table and coefficients while watching the video.

Example: Balance the following chemical equation.

$$\_\_\_\_ \; C_3H_8 \,(g) \; + \; \_\_\_\_\_ \; O_2 \,(g) \; \rightarrow \; \_\_\_\_\_ \; CO_2 \,(g) \; + \; \_\_\_\_\_ \; H_2O \,(g)$$
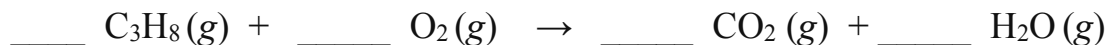
Amount on Reactant Side	Element	Amount on Product Side
	C	
	H	
	O	

Sometimes two coefficients must be _____ applied in order to balance an element.

Take notes here – fill in the table and coefficients while watching the video.

Example: Balance the following chemical equation.

$$_____ \; Al \,(s) \; + \; \_\_\_\_\_ \; O_2 \,(g) \; \rightarrow \; \_\_\_\_ \; Al_2O_3 \,(s)$$

Amount on Reactant Side	Element	Amount on Product Side
	Al	
	O	

Common Errors to Avoid When Balancing Chemical Equations

When you are asked to balance an equation, *for example*:

$$\underline{\qquad} \; N_2 \; + \; \underline{\qquad} \; O_2 \rightarrow \underline{\qquad} \; N_2O$$

Avoid making the following mistakes:

1. **Do not change** the ***formula*** of a reactant or product:

$$N_2 + O_2 \rightarrow N_2O_2$$
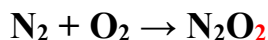
- By ***changing*** the product from N_2O to N_2O_2, you are not balancing the equation *for the given reaction*. The formation of N_2O_2 may or may not occur, however *it is not the reaction whose equation you were asked to balance*.

2) **Do not** add ***new*** reactants or products.

$$N_2 + O_2 \rightarrow N_2O + O$$
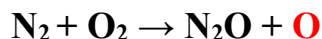
- By adding a new product (**O**), you are not balancing the equation for *the reaction that you were asked to balance*.

3) **Do not** use ***multiples of the coefficients*** when writing the balanced equation.

We ***would not*** write: $4\,N_2 + 2\,O_2 \rightarrow 4\,N_2O$

- Although the equation above is balanced, the convention for balancing equations is to use the ***lowest set*** of coefficients. To get this set, we divide each coefficient by the greatest common factor of all coefficients. The greatest common factor of the coefficients in our equation is **2**, so the correct balanced equation is written as:

$$2\,N_2 + O_2 \rightarrow 2\,N_2O$$
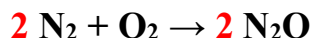
4) When chemical reactions are described in ***words***, you should identify the following ***diatomic molecules*** that are referred to by ***their element's names***:

$$H_2, \; N_2, \; O_2, \; F_2, \; Cl_2, \; Br_2, \; \text{and} \; I_2$$
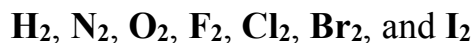
When uncombined with other elements in compounds, these elements exist as *diatomic molecules*.

- These elements are highlighted in the periodic table shown below.
- Except for H_2, these substances can be remembered by the upside-down "**L**" pattern seen in their periodic table positions.

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt									

When describing our example reaction, $2\,N_2 + O_2 \rightarrow 2\,N_2O$, *in words*, we would say,

"***nitrogen*** reacts with ***oxygen*** to produce (or form) dinitrogen monoxide."

- Note that oxygen ***also*** exists as O_3, however O_3 is called "ozone."

Understanding Check
Balance the following chemical equations:

a. $Fe + O_2 \rightarrow Fe_2O_3$

b. $H_2 + Cl_2 \rightarrow HCl$

c. $Ag + H_2S \rightarrow Ag_2S + H_2$

d. $CH_4 + O_2 \rightarrow CO_2 + H_2O$

e. $HgO \rightarrow Hg + O_2$

f. $Co + H_2O \rightarrow Co_2O_3 + H_2$

Understanding Check
Write ***balanced chemical equations*** for each of the following *equation descriptions*. You **do not** need to include the *states* of the reactants or products.

IMPORTANT NOTE: Before attempting to balance the equations, you must first convert the ***compound names*** into the correct ***chemical formulas***. If you begin to struggle with that, you may wish to go back to chapter 3 and re-work the naming problems.

a. Aluminum metal ***reacts with*** copper(II) chloride ***to produce*** aluminum chloride <u>and</u> copper metal.

b. Lead(II) nitrate reacts with sodium bromide to produce lead(II) bromide and sodium nitrate.
   - HINT: Since you have the same polyatomic ion (nitrate) on both sides of the equation you can use the shortcut that was listed in Step #1 of our balancing method.

c. Zinc metal reacts with oxygen gas to produce zinc oxide.
   - Oxygen is one of the *diatomic molecules* that are referred to by their *element's name*.

d. Aluminum sulfate reacts with barium iodide to produce aluminum iodide and barium sulfate.

e. At temperatures reached during baking, sodium bicarbonate (baking soda) decomposes (reacts) to produce sodium carbonate, carbon dioxide, and dihydrogen monoxide.
   - Bicarbonate is a *polyatomic ion* (**not** the same as the carbonate polyatomic ion).

f. Sodium metal reacts with water to produce sodium hydroxide and hydrogen gas.

g. Lead(IV) sulfide reacts with oxygen gas to produce lead(IV) oxide and sulfur dioxide.

Stoichiometric Calculations for Chemical Reactions

Stoichiometry is the calculation of the _____ of reactants and/or products in a chemical reaction.

The calculated values allow us to predict how much product(s) will be produced from a given amount of reactant(s), or conversely, how much reactant(s) will be needed in order to produce a desired amount of product.

Before we do *stoichiometric calculations* with chemicals, let's do a similar problem with something with which we are all familiar - *food*!!!

I will use the formation of a grilled cheese sandwich as an *analogy* to a chemical reaction.

2 Slices of Bread   +   1 Slice of Cheese   ⟶   1 Sandwich

If this was an actual chemical reaction we would say, "two slices of bread *react with* one slice of cheese *to produce* one cheese sandwich."

> *Question #1:* Suppose you want to make as many cheese sandwiches as possible for lunch. If you have 20 slices of bread, how many slices of cheese do you need? _____
>
> *Question #2:* If you have an *unlimited* supply of cheese slices, how may sandwiches can you make from the 20 slices of bread? _____

When we do stoichiometry calculations for real reactions, the first thing that we need to have is a balanced chemical equation. For the sandwich analogy, the balanced equation is shown below.

$$2\ B\ +\ C\ \rightarrow\ B_2C$$
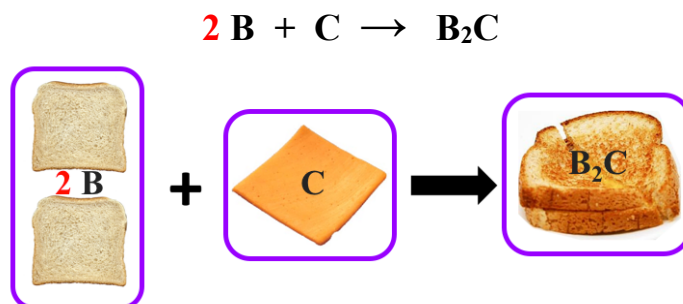
B represents a slice of bread, **C** represents a slice of cheese, and a sandwich "compound" is therefore a "**B₂C.**"

The _____ between the amounts of reactants used and/or products formed can be found from the _____ in the balanced chemical equations.

- It is for this reason that coefficients are sometimes referred to as "**stoichiometric coefficients**."

We treat **stoichiometry problems** like **unit conversation** problems.

- In **Question #1**, you converted from **units** of "slices of bread" to **units** of "slices of cheese."

  Question #1: Suppose you want to make as many cheese sandwiches as possible for lunch. If you have 20 slices of bread, how many slices of cheese do you need? **10 slices of cheese**

$$\frac{20 \text{ slices of bread}}{} \left| \frac{1 \text{ slice of cheese}}{2 \text{ slices of bread}} \right. = 10 \text{ slices of cheese}$$

- In **Question #2**, you converted from **units** of "slices of bread" to **units** of "sandwiches."

  Question #2: If you have an *unlimited* supply of cheese slices, how may sandwiches can you make from the 20 slices of bread? **10 sandwiches**

$$\frac{20 \text{ slices of bread}}{} \left| \frac{1 \text{ sandwich}}{2 \text{ slices of bread}} \right. = 10 \text{ sandwiches}$$

I used the formation of a cheese sandwich analogy because you are quite familiar with making sandwiches; now we will move on to work on **real chemical reactions**.

The coefficients in the balanced equation represent the ratios in which reactants are consumed and products are made in a chemical reaction.

- For example, consider the reaction for the combustion of methane.

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O$$
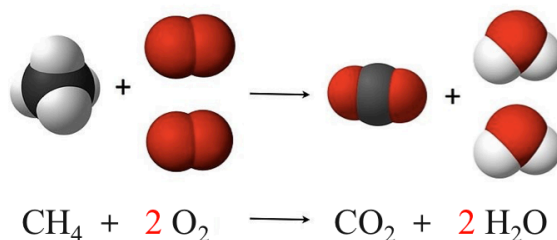
- Use the balanced chemical equation to answer these questions:

    1) How many H_2O molecules are produced from 1 CH_4 molecule? _____

    2) How many O_2 molecules are needed to produce 2 H_2O molecules? _____

    3) How many CH_4 molecules are needed to react with 2 O_2 molecules? _____

In practice, scientists and technicians usually work with very large numbers of particles, not just a few molecules or ions.

It is more practical to consider the coefficients to represent the ratios in which _____ **of substances** are used and produced in a chemical reaction.

    1) How many **moles** of H_2O are produced from **1 mole** of CH_4? **2 moles**

    2) How many **moles** of O_2 are needed to produce **2 moles** of H_2O? **2 moles**

    3) How many **moles** of CH_4 are needed to react with **2 moles** of O_2? **1 mole**

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Your understanding of the coefficients in chemical equations will help you to construct **conversion factors** and use them in stoichiometric calculations.

Example: For the combustion of methane reaction, how many moles of H_2O can be produced from 2.84 moles of methane (CH_4)? Assume you have an unlimited supply of O_2.

- We will approach stoichiometry problems *just as we did with* _____ _____ *problems using our factor-label method*.

- In this problem, we are converting from units of "**moles of CH_4**" to units of "**moles of H_2O.**"

Implied Coefficient   Implied Coefficient

$$1\,CH_4\,(g) \;+\; 2\,O_2\,(g) \rightarrow 1\,CO_2\,(g) + 2\,H_2O\,(g)$$

$$\frac{2.84 \text{ moles } CH_4}{} \left| \frac{2 \text{ moles } H_2O}{1 \text{ mole } CH_4} \right. = \textbf{5.68 moles } H_2O$$
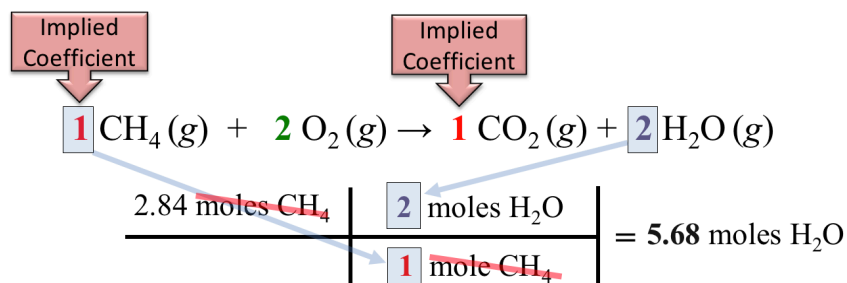
In some stoichiometry problems, like the example problem just completed, you will be given a certain amount of one reactant and an *unlimited supply* of the other reactant(s), and then asked to calculate how much *product* could be made.

In other stoichiometry problems, you may need to calculate how much of one reactant *would be needed* to react with a given amount of *another reactant* as in the example that follows.

Example: For the combustion of methane reaction, how many moles of O_2 will be needed to react with 6.93 moles of CH_4?

- In this problem, we are converting from units of "**moles of CH_4**" to units of "**moles of O_2.**"

- Get the relationship between **moles of CH_4** and **moles of O_2** *from the* **coefficients** *in the chemical equation*.

Implied Coefficient   Implied Coefficient

$$1\,CH_4\,(g) \;+\; 2\,O_2\,(g) \rightarrow 1\,CO_2\,(g) + 2\,H_2O\,(g)$$

$$\frac{6.93 \text{ moles } CH_4}{} \left| \frac{2 \text{ moles } O_2}{1 \text{ mole } CH_4} \right. = \textbf{13.9 moles } O_2$$
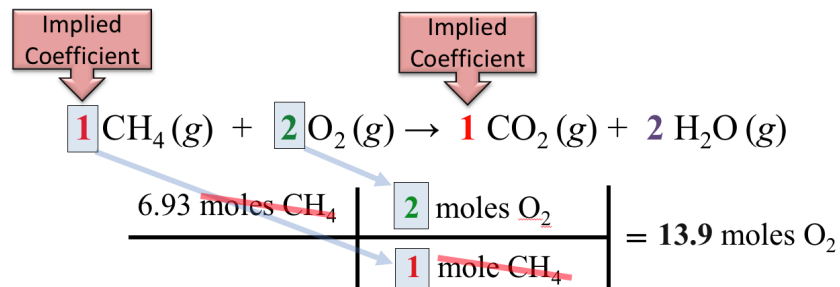
Sometimes stoichiometry problems involve the calculation of how much of **one reactant** *would be needed* to **produce** a specified amount of *product*.

Example: For the combustion of methane reaction, how many moles of O_2 will be needed to *produce* 1.74 moles of H_2O? Assume that there is an unlimited supply of CH_4.

- In this problem, we are converting from units of "**moles of H_2O**" to units of "**moles of O_2.**"

$$CH_4\,(g) \;+\; 2\,O_2\,(g) \rightarrow \quad CO_2\,(g) + 2\,H_2O\,(g)$$

$$\frac{1.74 \text{ moles } H_2O}{} \left| \frac{2 \text{ moles } O_2}{2 \text{ moles } H_2O} \right. = \textbf{1.74 moles } O_2$$

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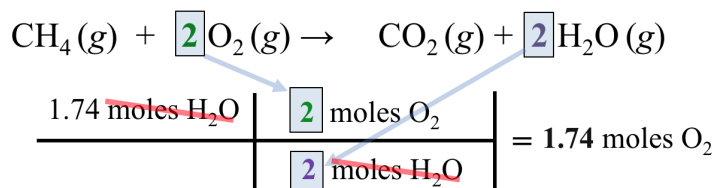
In a combustion reaction, *propane* (C_3H_8) reacts with *oxygen* to produce CO_2 and H_2O.

$$C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O\ (g)$$
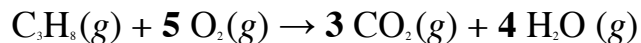
a) How many moles of H_2O can be produced from 1.32 moles of propane (C_3H_8)?
   - Assume there is an unlimited supply of O_2.

b) How many moles of O_2 will be needed to react with 12.6 moles of C_3H_8?

c) How many moles of O_2 will be needed to *produce* 0.843 moles of H_2O?
   - Assume there is an unlimited supply of C_3H_8.

In the previous stoichiometry problems, we were given the number of moles of a particular product or reactant and asked to calculate the number of moles of another product or reactant involved in the reaction. We did so by using the ratios of the substances' coefficients as conversion factors. This process is shown in the schematic diagram below.
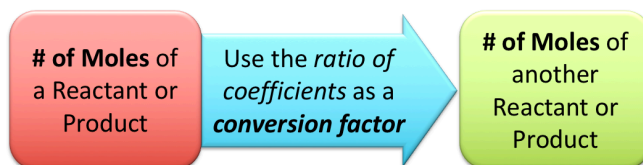
We cannot *directly* measure the number of moles on a balance in the lab.

In practice, we usually know the **number of** _____ of a reactant or product and wish to determine the **number of grams** of another reactant needed **or** the **number of grams** of a product in a reaction.

Because the coefficients that we use as conversion factors in stoichiometric calculations are the **ratios of moles**, we must **first convert all masses (grams) to moles,** do the stoichiometric calculations, and then convert the calculated number of moles for the substance of interest into grams. This **three-step process** is shown in the schematic diagram below.

15
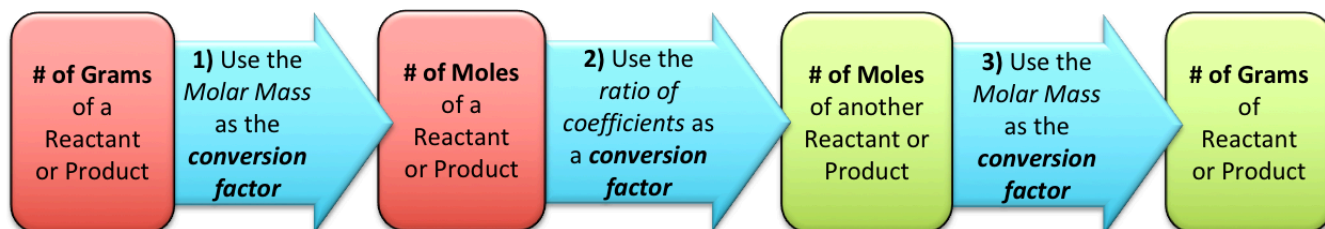
Example: For the combustion of *propane*: $C_3H_8\,(g) + 5\,O_2(g)\;\rightarrow\;3\,CO_2\,(g) +\;4\,H_2O\,(g)$

How many **grams** of H_2O can be produced from 29.0 **grams** of propane (C_3H_8)?

- Assume you have an unlimited supply of O_2.

29.0 grams of propane (C_3H_8)	**1)** Use the *Molar Mass* as the *conversion factor*	**# of moles** of propane (C_3H_8)	**2)** Use the *ratio of coefficients* as a *conversion factor*	**# of moles** of H_2O	**3)** Use the *Molar Mass* as the *conversion factor*	**# of grams** of H_2O

Step # 1:
Convert from grams of C_3H_8 to moles of C_3H_8.
- Use the *molar mass* of C_3H_8:

$$\frac{29.0\ \text{grams}\ C_3H_8}{} \times \frac{1\ \text{mole}\ C_3H_8}{44.11\ \text{grams}\ C_3H_8}$$

$$= 0.657\ \text{moles}\ C_3H_8$$

Step #2:
Convert from moles of C_3H_8 to moles of H_2O.
- Use the *ratio of coefficients* as a *conversion factor*

$$\frac{0.657\ \text{moles}\ C_3H_8}{} \times \frac{4\ \text{moles}\ H_2O}{1\ \text{mole}\ C_3H_8}$$

$$= 2.63\ \text{moles}\ H_2O$$

Step #3:
Convert from moles of H_2O to grams of H_2O.
- Use the *molar mass* of H_2O:

$$\frac{2.63\ \text{moles}\ H_2O}{} \times \frac{18.02\ \text{grams}\ H_2O}{1\ \text{mole}\ H_2O}$$

$$= 47.4\ \text{grams}\ H_2O$$

Alternative Solution: You may feel comfortable enough to use the short cut where all three of the conversions above are combined into one equation:

Step # 1	Step # 2	Step # 3

$$\frac{29.0\ \text{grams}\ C_3H_8}{} \times \frac{1\ \text{mole}\ C_3H_8}{44.11\ \text{grams}\ C_3H_8} \times \frac{4\ \text{moles}\ H_2O}{1\ \text{mole}\ C_3H_8} \times \frac{18.02\ \text{grams}\ H_2O}{1\ \text{mole}\ H_2O} = 47.4\ \text{grams}\ H_2O$$

Example: For the combustion of *propane*: $C_3H_8 (g) + 5\,O_2(g) \rightarrow 3\,CO_2 (g) + 4\,H_2O\ (g)$

How many **grams** of O_2 will be needed to **produce** 50.0 grams of H_2O?

- Assume that you have an unlimited supply of C_3H_8.

| 50.0 grams of H_2O | **1)** Use the Molar Mass as the *conversion factor* | # of moles of H_2O | **2)** Use the ratio of coefficients as a *conversion factor* | # of moles O_2 | **3)** Use the Molar Mass as the *conversion factor* | # of grams of O_2 |

Step # 1:
Convert from grams of H_2O to moles of H_2O.
- Use the **molar mass** of H_2O:

$$\frac{50.0 \text{ grams } H_2O}{} \times \frac{1 \text{ mole } H_2O}{18.02 \text{ grams } H_2O}$$

$= 2.77$ **moles H_2O**

Step #2:
Convert from moles of H_2O to moles of O_2.
- Use the *ratio of coefficients* as a *conversion factor*

$$\frac{2.77 \text{ moles } H_2O}{} \times \frac{5 \text{ moles } O_2}{4 \text{ moles } H_2O}$$

$= 3.46$ **moles O_2**

Step #3:
Convert from moles of O_2 to grams of O_2.
- Use the **molar mass** of O_2:

$$\frac{3.46 \text{ moles } O_2}{} \times \frac{32.00 \text{ grams } O_2}{1 \text{ mole } O_2}$$

$= 111$ **grams O_2**

Alternative Solution: You may feel comfortable enough to use the short cut where all three of the conversions above are combined into one equation:

Step # 1   Step # 2   Step # 3

$$\frac{50.0 \text{ grams } H_2O}{} \times \frac{1 \text{ mole } H_2O}{18.02 \text{ grams } H_2O} \times \frac{5 \text{ moles } O_2}{4 \text{ moles } H_2O} \times \frac{32.00 \text{ grams } O_2}{1 \text{ mole } O_2} = 111 \text{ grams } O_2$$

Understanding Check

For the combustion of *propane*: $C_3H_8 (g) + 5\,O_2(g) \rightarrow 3\,CO_2 (g) + 4\,H_2O\ (g)$

How many **grams** of O_2 will be needed to **react with** 70.0 **grams** of C_3H_8?

Energy Changes in Chemical Reactions

All chemical reactions involve changes in _____.

Some reactions _____ *energy* as heat, light, electricity, and/or mechanical energy (work).

The energy that is released in a chemical reaction comes from _____ *energy* contained in the

_____.

Examples of reactions that produce heat and light are combustion reactions (burning).

- We call reactions that release energy, in the form of heat, _____ **reactions**.

Combustion reactions can also produce *mechanical energy; another way to state this is, "combustion reactions can do work."*

- For example, when combustion occurs in the cylinder/piston system of an internal combustion engine, a sudden increase in the number of moles of gas present (produced in the reaction) causes a large increase in pressure within the cylinder, which then moves the piston. The piston is coupled to a shaft that rotates and ultimately rotates the wheels. Examples of reactions that release electrical energy are the reactions that occur in various types of batteries.

Some reactions must continuously _____ *energy* in order to occur.

- **Example:** The *formation* of hydrogen and oxygen gas (at room temperature) from water.

$$2\ H_2O\ (l)\ \longrightarrow\ 2\ H_2\ (g)\ +\ O_2\ (g)$$
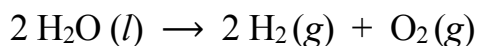
- Note that this is the ***reverse*** of the rocket fuel reaction that I discussed earlier. The conversion of oxygen and hydrogen to H_2O releases energy; so it makes sense that the ***reverse reaction***, converting H_2O to hydrogen and oxygen would require energy.

- The conversion of water to hydrogen and oxygen gas can be done by adding electrical energy to water in a process called **electrolysis**.

In a battery that is submerged in water, H_2O (*l*) is converted to O_2 (*g*) at one terminal and H_2 (*g*) at the other terminal.
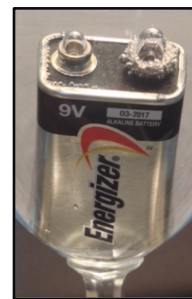
Spontaneity of Chemical Reactions

Recall the important law that is central to understanding nature: **matter tends to exist in the lowest possible energy state**.

We applied this law to understand why light is emitted from atoms and why most substances exist as molecules or ions instead of as isolated atoms.

This is a *universal law,* therefore it also applies to chemical reactions.

Chemical reactions can occur when the *total energy of the products* is less than the *total energy of the reactants*.

When a chemical reaction can continue to occur *without an external input of energy*, we say the reaction is

_____.

Let's examine the concepts of reaction energy and spontaneity by examining a reaction that we are now familiar with - the combustion of propane gas.

$$C_3H_8\,(g) \;+\; 5\,O_2\,(g) \;\longrightarrow\; 3\,CO_2\,(g) \;+\; 4\,H_2O\,(g)$$
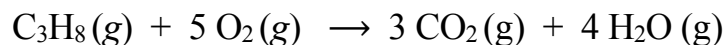
Many of us have used propane gas in outdoor lanterns and barbecues. We know that once we use a spark or match to start the reaction, that the combustion reaction continues to occur *without an external input of energy*. It is therefore a ***spontaneous reaction***.

Let's think about the change in energy (ΔE) in the combustion of propane.

The **total energy** (E) is the sum of ***kinetic energy*** (E_k) and ***potential energy*** (E_p).

$$\mathbf{E = E_k + E_p}$$

A particle's ***kinetic energy*** comes from its ***motion***.

Potential energy is stored in a substance's _____ ***bonds*** (and noncovalent interactions).

- _____ chemical bonds (or noncovalent interactions) _____ energy.

- _____ new chemical bonds (or noncovalent interactions) _____ energy.

For the combustion of propane reaction, in the ***reactants***, ***potential energy*** is stored in C-C bonds, C-H bonds, and the O-O bonds.

During the reaction, chemical bonds in the reactants are broken and new chemical bonds (C-O and O-H) are formed in the products.

$$C_3H_8\,(g) \;+\; 5\,O_2\,(g) \;\longrightarrow\; 3\,CO_2\,(g) \;+\; 4\,H_2O\,(g)$$
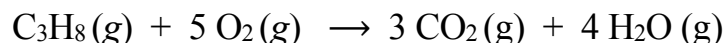
In the ***products***, ***potential energy*** is stored in C-O bonds, and O-O bonds.

We all know, from our familiarity with the combustion of propane gas, that energy is ***released*** in this reaction.

- The ***amount* of energy released** in the reaction is equal to the _____ in ***potential energy*** (ΔE_p) between the products ($E_{p\ products}$) and reactants ($E_{p\ reactants}$):

$$\textbf{Energy Released } (\Delta E_p) = (E_{p\ products}) - (E_{p\ reactants})$$

This ***released energy*** does not just vanish into a hole in the universe! Energy is never created or destroyed, it only changes its form.

The energy released in the reaction is converted to ***kinetic energy in the products***, and then is often transferred to surrounding matter such as air (or the items cooking on the grill).

In the case of similar reactions that happen in *internal combustion engines*, some of the energy that is released goes into mechanical work (moving the car), and the remainder goes into warming of the engine, and then finally into warming of the air that contacts the car's engine and radiator. The ratio of energy that goes into *moving the car* to the total energy released by the reaction is called the **engine efficiency**. In the case of reactions that occur in batteries, most of the energy released in a reaction goes into kinetic energy of electrons moving through an electrical circuit; the remainder of the energy goes into warming the battery and surroundings.

The field of study called **thermodynamics** often deals with calculating the energy changes in chemical reactions. These energetic calculations are useful for predicting how chemical systems will behave under various conditions because matter tends to exist in the lowest possible energy state. For example, the combustion of propane reaction occurs *because the bonding arrangement of atoms in the products is at a lower energy than that of the reactants.*

Energy calculations are only useful when they involve properties (variables) that can be directly measured (such as temperature, moles of each substance, volume, and pressure).

When using the temperature and pressure as variables in energy calculations, we refer to the calculated energy as "_____ _____" abbreviated with the symbol "**G.**"

- The details of the difference between *total energy* (**E**) and *free energy* (**G**) are beyond the scope of this course.

- For *our purposes*, you can consider the *free energy* (**G**) and *total energy* (**E**) to be _____.

- **Matter tends to exist in the lowest possible *free energy* state, therefore chemical reactions will occur when the total *free energy* of the products is less than the total *free energy* of the reactants**.

Let's consider the *combustion of propane* in terms of *free energy* (**G**).

$$C_3H_8\,(g) \;+\; 5\,O_2\,(g) \;\longrightarrow\; 3\,CO_2\,(g) \;+\; 4\,H_2O\,(g)$$
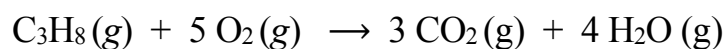
The figure shown below illustrates the difference in *free energy* between the products and the reactants for this reaction.

This figure is an *energy level diagram*, similar to the energy level diagrams that you saw in chapter 3, with higher energy toward the top.

The amount of free energy present in the reactants *alone* (**G**$_{reactants}$) is indicated by the upper dashed line (blue in the video).

The amount of free energy contained in products *alone* (**G**$_{products}$) is indicated by the lower dashed line (green in the video).

The _____ *in free energy* (**ΔG**) for reaction is equal to the difference in free energy between the products (**G**$_{products}$) and the reactants (**G**$_{reactants}$):

$$\Delta G = \left(G_{products}\right) - \left(G_{reactants}\right)$$

Reactants:

$$C_3H_8\,(g) + 5\,O_2\,(g)$$

$$\Delta G = G_{products} - G_{reactants}$$

Products:

$$3\,CO_2\,(g) + 4\,H_2O\,(g)$$

Free Energy of **Reactants**

Free Energy (G)

Free Energy of **Products**

Note the use of our convention of defining **change (Δ)** as the final state (products only) *minus* the initial state (reactants only).

The free energy of the products for the combustion of propane is **less than** the free energy of the reactants as indicated by their positions in the energy level diagram.
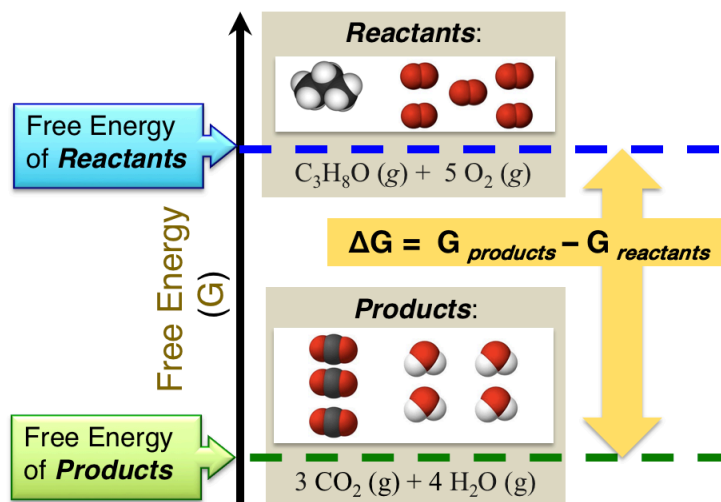
When the *free energy* of the *products* of a reaction is *less than* the free energy of the *reactants*, we say that the reaction is **exergonic**.

> Chemical reactions will occur spontaneously when the *free energy* of the product(s) is less than the *free energy* of the reactant(s).

$$\Delta G = (G_{products}) - (G_{reactants})$$

When the *free energy* of the *products* of a reaction is *less than* the free energy of the *reactants*, the *change in free energy* (**ΔG**) will have a _____ *value*.

Summary of Spontaneity of Reactions

When a chemical reaction can continue to occur *without an external input of energy*, we say the reaction is *spontaneous*.

The following statements are true for *spontaneous reactions*:

- The *free energy* (**ΔG**) the *products* of the reaction is *less than* the *free energy* of the *reactants*.
- The sign of **ΔG** is *negative*.

Understanding Check

Determine if the following reactions are **spontaneous** or **non-spontaneous**.

1. $2 H_2 (g) + O_2 (g) \rightarrow 2 H_2O (g)$, $\Delta G = -54,640$ calories (per mole of product formed)

2. $2 H_2O (l) \rightarrow 2 H_2 (g) + O_2 (g)$, $\Delta G = 56,670$ calories (per mole of products formed)

3. The rusting of an iron nail: $4 Fe + 3 O_2 \rightarrow Fe_2O_3$
   (HINT: Have you ever observed a rusty nail?)

Rates of Chemical Reactions

Knowing if the value of **ΔG** is negative or positive allows us to predict whether or not a reaction is spontaneous, however it does not give us any information about *how quickly a reaction happens*.

Some reactions happen *very quickly*, for example, the explosions of fireworks.

Some reactions happen so *slowly* that you cannot tell that the reaction is occurring even when viewed for a few hours, for example the rusting of a nail.

To understand the factors that determine and influence how quickly chemical reactions happen, we must consider the energy during *the process* of converting reactants to products. We will do so using a graph of the free energy *as the reaction progresses*.

Let's consider a generalized chemical reaction where **molecule A** *reacts* with **molecule B** to *produce* **molecule C** and **molecule D**:

$$A + B \rightarrow C + D$$

$$A + B \rightarrow C + D$$
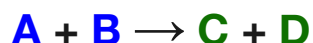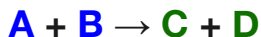
We plot the free energy (G) on the vertical axis. The horizontal axis indicates the *progress of the reaction* (process of converting reactants to products). The **curve** (purple in the video) represents the free energy during the reaction process.

We begin on the **left** where we have the *reactants only*.
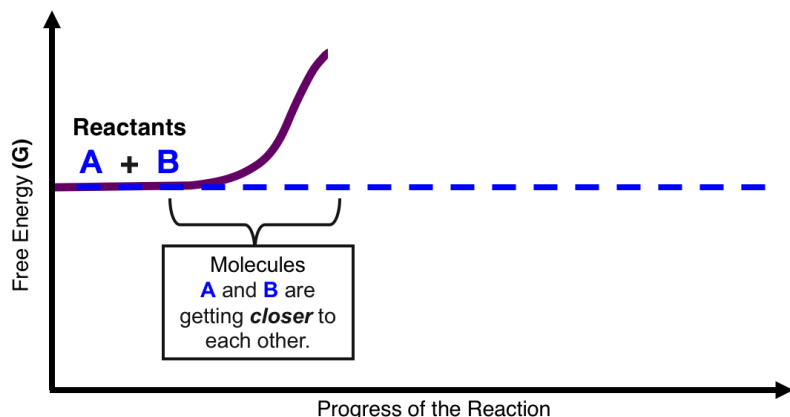
The free energy of the reactants ($G_{reactants}$) are indicated by the horizontal dashed line (blue in the video).

As the reaction progresses, we move from *left to right* on the horizontal axis. Originally molecule **A** and molecule **B** are fairly far apart from each other. As the reaction progresses, **A** and **B** must be on a collision course with each other. In order for molecule **A** to react with molecule **B**, they must eventually collide.

As **A** and **B** approach each other, **the free energy increases** because of factors such as electrostatic repulsion between the electrons on the reactants, changes in molecular geometry, and disruption of noncovalent interactions.

- This increase in energy can be seen in the free energy curve (purple in video) as the reaction progresses.

At some point, the free energy reaches a maximum value (peak) as indicated by the yellow star in the figure (below).
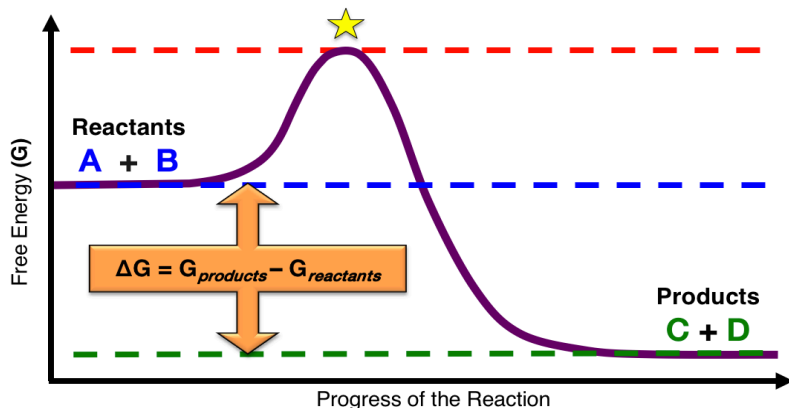
At this point, the matter no longer exists as individual reactant molecules (**A** and **B**), nor has it been converted to product molecules (**C** and **D**).

The matter exists in what we call a **transition state**, where the bonds in the reactants have not all been completely broken and/or the new bonds in the products have not been completely formed.

The **free energy** of the **transition state** is indicated by the top dashed line (red in the video).

As the reaction progresses past the transition state, new bonds are formed in the product molecules **C** and **D**, and bond angles and bond distances relax to their low energy geometries, and the product molecules move apart from each other.

All of these processes result in **lowering the free energy** as can be seen in the figure as the reaction progresses from the transition state to the products.

- The free energy of the products is indicated by the bottom dashed line (green in the video).

In this example, the free energy of the products is less than the free energy of the reactants, therefore ΔG is **negative** and the reaction is **spontaneous**.

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The amount of free energy needed to progress *from reactants to the transition state* is called the
_____ _____ (**E**ₐ).

Free Energy (G)

Reactants
A + B

Activation Energy
(E$_a$)

$\Delta G = G_{products} - G_{reactants}$

Products
C + D

Progress of the Reaction
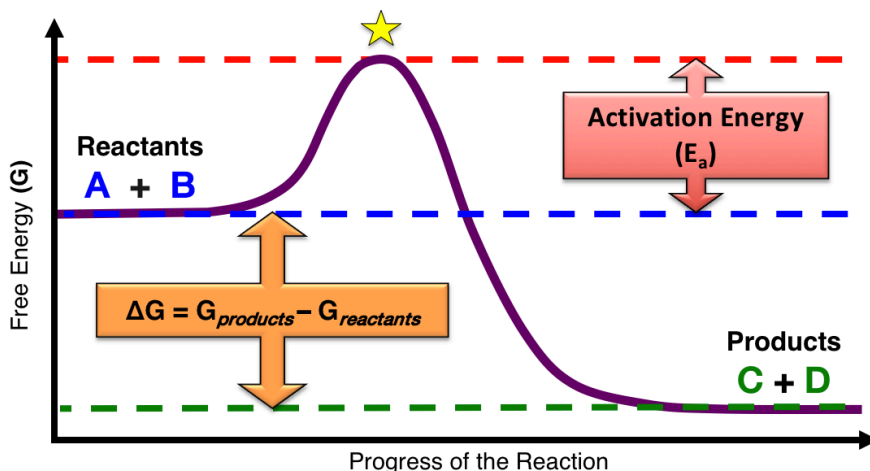
The _____ **of chemical reactions** (how quickly the reactions happen) depend on the *activation energy*.

The _____ the activation energy, the _____ the reaction rate.

Example: The energy level diagrams for two *spontaneous* reactions are shown below.
Which reaction has a *faster rate*?

Reaction 1: A + B → C

Free Energy (G)

Reactants
A + B

Product
C

Progress of the Reaction

Reaction 2: E + F → G

Free Energy (G)

Reactants
E + F

Product
G

Progress of the Reaction
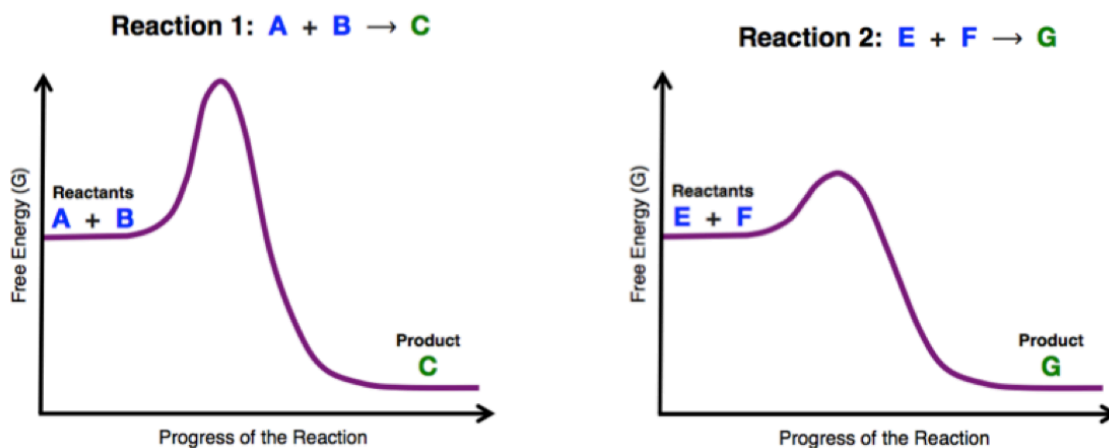
Solution: Compare the *activation energies*. The *lower* the activation energy, the *faster* the reaction rate.

Reaction 1: A + B → C

Free Energy (G)

Reactants
A + B

Activation Energy

Product
C

Progress of the Reaction

Reaction 2: E + F → G

Free Energy (G)

Reactants
E + F

Activation Energy

Product
G

Progress of the Reaction
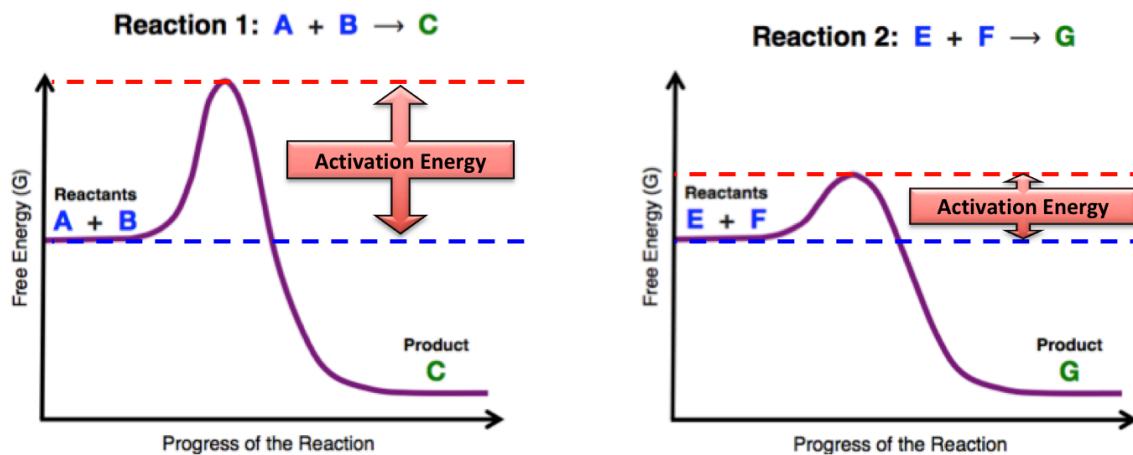
Because **Reaction 2** has a *lower* activation energy, it has the *faster reaction rate*.

The Temperature Dependence of Reaction Rates

The reaction energy level diagram shows an increase in free energy as the reaction progresses from reactants to the maximum energy peak at the *transition state*.

You just learned that this increase in energy is referred to as the ***activation energy.***

If the temperature of the reactants is increased, the reactants can more readily overcome the *activation energy* and therefore more readily be converted to products.
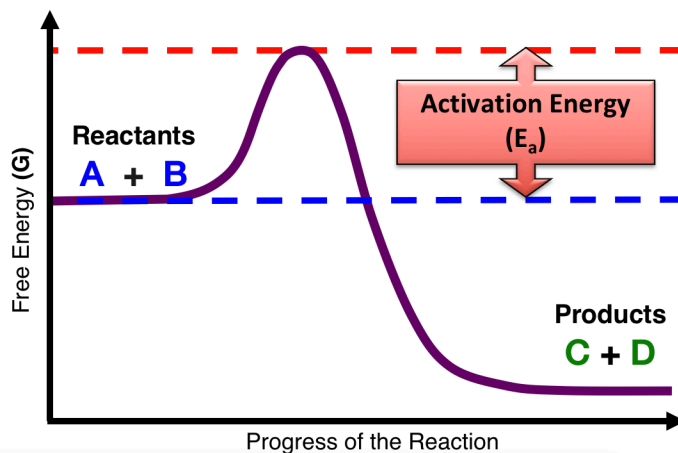
For this reason, the reaction rate depends on the _____.

- ***As the temperature increases, the reaction rate increases.***
  - In general, for every $10°C$ increase in temperature, the reaction rate doubles.
  - Conversely, for every $10 °C$ decrease in temperature, the reaction rate decreases by a factor of one-half.
    - This is one of the reasons that we keep food refrigerated; the lower temperature slows the reactions that are involved in the decomposition of food and bacterial growth.

Catalysis

Another way to change the rate of a chemical reaction is to use a _____.

A ***catalyst*** can be any *substance that increases the rate of a chemical reaction*.

Unlike reactants, catalysts are _____ _____ in a reaction.

Living organisms produce catalysts consisting of large molecules, usually proteins, that are called

_____.

- Humans have thousands of chemical reactions that must occur in order to sustain life. Many of these reactions would happen too slowly to be useful if not catalyzed by enzymes. For example, an enzyme called amylase, present in our saliva, catalyzes the digestion reaction of starch.

Industrial processes often use _____ of substances such as metals to catalyze reactions.

The Inside of a Catalytic Converter

- For example, ***catalytic converters*** use platinum or rhodium surfaces as catalysts to remove poisonous by-products (carbon monoxide, nitrogen oxides, and unreacted hydrocarbons) produced in the ***incomplete*** combustion of fossil fuels.
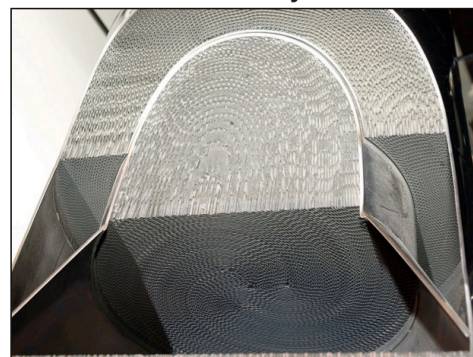
Catalysts increase the rates of reactions by _____ the _____ *energy*.

In the catalyzed reaction, the reactants require less energy to overcome the ***activation energy*** and are therefore converted to products at a ***faster*** rate.

You will learn more details of how catalysts lower the activation energy when I discuss enzymes in chapter 13.
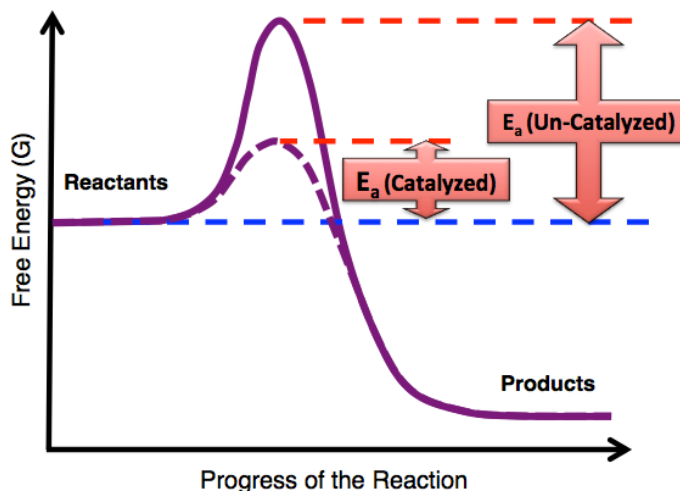
Beach Balls in a Lake Analogy for Rates of Reactions

I want to end this video by giving you an analogous model to help you understand how temperature and catalysts effect the rate of chemical reactions. The process that I will use to model chemical reactions is beach

<center>

Beach balls (in the lake) $\longrightarrow$ **Beach-balls (out of the lake)**

</center>

The Temperature Dependence of the Reaction Rate

In this model, the *height of the lake's shoreline* represents the **activation energy**.

Increasing the size of the waves in the lake is analogous to raising the temperature of a chemical reaction.

Larger waves cause the beach-balls to leave the lake ***at a faster rate*** as shown in the illustration below:

<center>Lower Temperature   Higher Temperature</center>
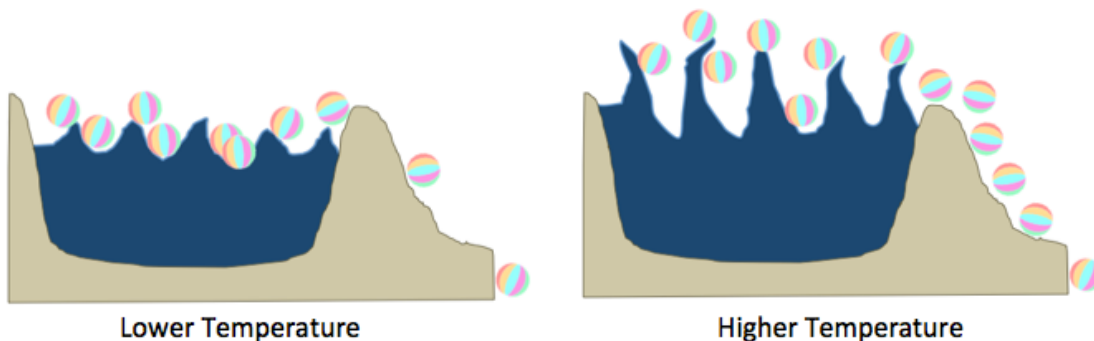
The Effect of Catalysts on the Reaction Rate

Again, the *height of the lake's shoreline* represents the **activation energy**.

The *presence of a catalyst* is analogous to ***lowering the shoreline***, and results in the beach-balls leaving the lake *at **faster** rate* as shown in the illustration below:

<center>Un-Catalyzed Reaction   Catalyzed Reaction</center>

25
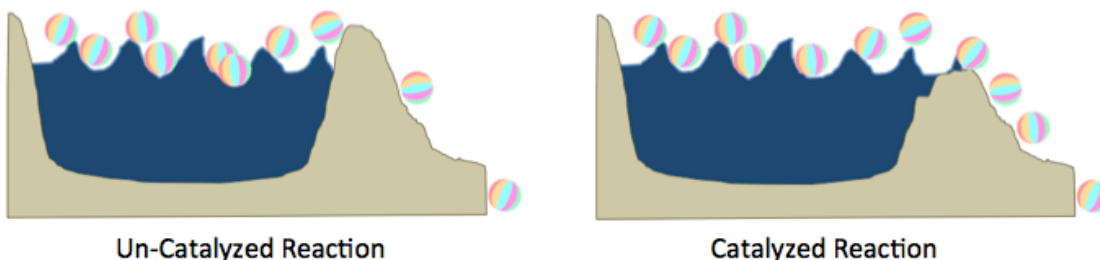
Summary of Rates of Chemical Reactions

The **reaction rate** is a measure of *how **quickly** a reaction occurs.*

The **rates** of chemical reactions depend on the ***activation energy*** and the ***temperature***.

The ***lower*** the ***activation energy***, the ***faster*** the reaction rate.

As the ***temperature increases***, the reaction rate ***increases***.

- In general, the reaction rate **doubles** with every 10 °C increase in temperature.

Catalysts increase the rate of a reaction by ***decreasing*** the **activation energy (E_a)**.

General Types of Chemical Reactions

Many reactions can be categorized into one of ***four general types*** based solely on *changes in the bonding pattern* (not the identity of the reactants or products).

The *educational goal* for this section is that, given one of these four types of reactions, you will be able to name the category in which it belongs.

1) SYNTHESIS REACTIONS

A _____ ***reaction*** is one in which a single compound is formed from two or more substances. The general form of a synthesis reaction is:

$$A + B \rightarrow AB$$

Where **A** represents an element or compound, **B** represents another element or compound, and **AB** is the compound formed from **A** and **B**. An example of a synthesis reaction is the reaction that occurs between sodium metal and oxygen gas (O_2):

$$4\,Na\,(s)\ +\ O_2\,(g)\ \rightarrow\ 2\,Na_2O\,(s)$$
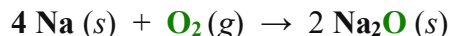
2) DECOMPOSITION REACTIONS

A _____ ***reaction*** is a reaction in which a single reactant breaks down into two or more substances. The general form of a decomposition reaction is:

$$AB \rightarrow A + B$$

- It is simply the reverse of a synthesis reaction.

An example of a ***decomposition reaction*** is the thermal (heat induced) decomposition of mercury(II) oxide:

$$2\,HgO\,(s)\ \rightarrow\ 2\,Hg\,(l)\ +\ O_2\,(g)$$

Note that the key to identifying a decomposition reaction is that one reactant species is converted to two or more product species. In our example, we start the reaction with just one reactant present, $HgO\,(s)$; after the reaction occurs, there are two different substances, $Hg\,(l)$ and $O_2\,(g)$.

3) SINGLE-REPLACEMENT REACTIONS

In a _____ *reaction*, an element *replaces* another element from a compound.

The general form of a single-replacement reaction, where **A** replaces **B**, is:

$$\textbf{A} + \textbf{BX} \rightarrow \textbf{AX} + \textbf{B}$$
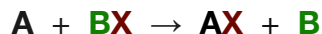
A and **B** represent different *elements*, **BX** represents a compound made from **B** and **X**, and **AX** is the compound made of **A** and **X**. *Before reacting*, element **A** is alone and element **B** is in compound **BX**. *After the reaction*, element **B** is alone and element **A** is in compound **AX**.

An example of a single-replacement reaction is:

$$\textbf{Cu}(s) + \textbf{AgNO}_3\,(aq) \rightarrow \textbf{Cu(NO}_3)_2\,(aq) + \textbf{Ag}\,(s)$$
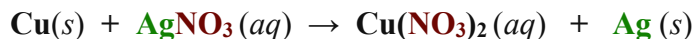
In this reaction, copper metal ($Cu\,(s)$) *replaces* the silver ion (Ag^+) in silver nitrate.

4) DOUBLE-REPLACEMENT REACTIONS

In a _____ *reaction*, two substances "***switch partners***." The general form of a single replacement reaction, where **AX** and **BY** *switch partners*, is:

$$\textbf{AX} + \textbf{BY} \rightarrow \textbf{AY} + \textbf{BX}$$
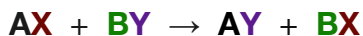
Double-replacement reactions occur in *aqueous* solutions. You will learn more about double-replacement reactions when I discuss solutions in chapter 7. An example of a double-replacement reaction is the reaction of sodium chloride and silver nitrate:

$$\textbf{NaCl}\,(aq) + \textbf{AgNO}_3\,(aq) \rightarrow \textbf{NaNO}_3\,(aq) + \textbf{AgCl}\,(s)$$
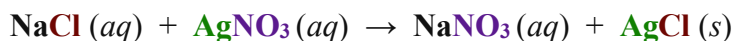
Understanding Check

Categorize each of the following reactions as either: synthesis, decomposition, single-replacement, or double-replacement.

a. $2\,H_2O\,(l) \rightarrow 2\,H_2\,(g) + O_2\,(g)$

b. $KBr\,(aq) + AgNO_3\,(aq) \rightarrow KNO_3\,(aq) + AgBr\,(s)$

c. $2\,Mg\,(s) + O_2\,(g) \rightarrow 2\,MgO\,(s)$

d. $Mg\,(s) + 2\,HCl\,(aq) \rightarrow MgCl_2\,(aq) + H_2\,(g)$
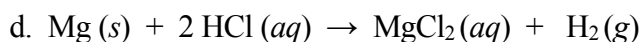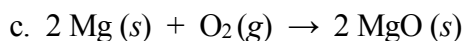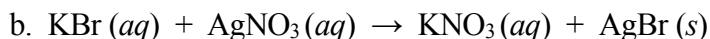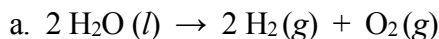
Redox Reactions

The term "*redox*" is an abbreviated combination (*portmanteau*) of the words "_____" and "_____."

In a *redox* chemical reaction, an *oxidation* and a *reduction* occur _____.

Many of the reactions that I have used as examples in previous sections are redox reactions. Redox reactions often occur in biological systems. For example, the series of chemical reactions in which we *metabolize food* and the series of chemical reactions called *photosynthesis* both contain many redox reactions.

Oxidation is the _____ *of* _____*(s)* by an atom, ion, or molecule.

Reduction is the _____ *of electron(s)* by an atom, ion, or molecule.

In a redox reaction, **electrons are _____ from one atom, ion, or molecule *to another* atom, ion, or molecule.**

- The electron(s) that are "lost" by the *oxidized species* are "gained" by the *reduced species*.

A useful mnemonic to differentiate oxidation and reduction is the term "**OILRIG**"

(**O**xidation **i**s the **L**oss of electrons; **R**eduction **i**s the **G**ain of electrons).
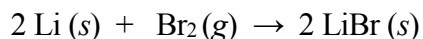
Redox Reactions of *Inorganic* Compounds

It is possible to identify redox reactions for _____ *compounds* by inspecting the chemical equation and determining if electrons are transferred from one species to another.

- One atom or ion in a reactant will **lose electron(s)** and therefore its _____ will **increase** (in the positive direction) by one charge unit for every electron that is lost.
  - The electron(s) that are lost are transferred to another reactant.

- The **charge** of the atom or ion in the reactant that **gains** the electron(s) will **decrease** (toward negative values) by one charge unit for every electron that is gained.
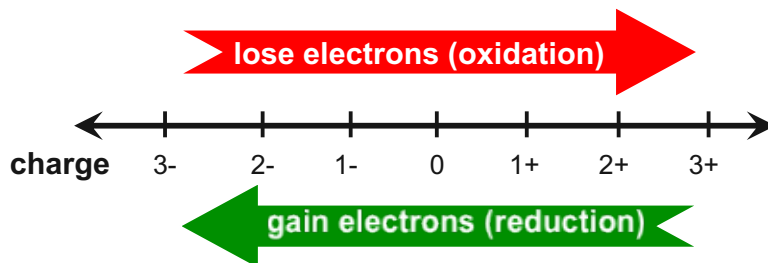
Example: Let's consider the reaction of sodium metal and oxygen:

$$4 \, Na \, (s) \; + \; O_2 \, (g) \; \rightarrow \; 2 \, Na_2O \, (s)$$
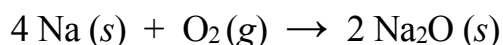
To determine if electrons are transferred from one species to another, you must understand that *the*

_____ _____ *of any pure* _____ *or* _____ *is always* _____*!*

- This fact will help you to determine the charge of each atom or ion in the reactants and products, and then to know if the charge of the species *changed* during the reaction.

- This change in the charge of an atom or ion is an indication that a redox reaction occurred.

FILL IN THE TABLE BELOW AS I DO SO IN THE VIDEO:

Oxidation *or* Reduction	Reactant	Charge in Reactant	Element	Product	Charge in Product
			sodium		
			oxygen		

Na (s) and O_2 (g) are pure elements. Because the **total charge of any pure element or compound is always ZERO**, and these two substances are each composed of *only one type of element*, the charge of each of the atoms in a piece of pure sodium metal or a sample of pure oxygen gas *is equal to ZERO*.

Now let's consider the charges on sodium and oxygen in the **Na₂O** (s) *product*.

Since sodium oxide (Na_2O) is a **compound**, it has a total charge = ZERO. We **also** must recognize that sodium oxide is an **ionic compound** (we know this because there is a metal in the compound).

Although the *total charge* of Na_2O is ZERO, the sodium cations and oxygen anions are charged particles; the charge of a sodium **ion** is always 1+, the charge of an oxide ion is always 2-.

- Note that ions combine in a ratio such that the total charge of a compound = ZERO; that is why sodium oxide has the formula Na_2O.

Now we will examine how electrons are transferred from one reactant to the other in the reaction.

We will do so by considering what happens to the charge of sodium and oxygen as they are converted from reactants to products.

- As a reactant, sodium exists as Na (s) and has a charge of ZERO.

- In the product (Na_2O), **each** sodium has a charge of **1+**.

- Since the charge of sodium _____ in the reaction, we can conclude that *each* sodium must have _____ *one electron*:

$$Na^o \; \rightarrow \; Na^+ + \; e^-$$

When a species loses electron(s), we call that **oxidation**. **Sodium was oxidized in this reaction**.

An oxidation cannot occur without a reduction; the electron(s) will be transferred to another atom or ion.

Where did the electron that sodium lost go?

Since oxygen is the only other reactant, it must have been transferred to the oxygen! Let's verify this by looking for a change in the charge of oxygen in the reaction process.

- In the reactant, oxygen exists as O_2 and has a charge of ZERO.

- In the product (Na_2O), oxygen has a charge of 2-.

Because the charge of oxygen _____ (*by two*) in the reaction, we can conclude that *each* oxygen (in O_2) must have _____ *(two) electrons*:

$$O^o + 2\ e^- \rightarrow O^{2-}$$

When a species *gains* electron(s), we call that *reduction*. **Oxygen was reduced in this reaction**.

The fact that *each* oxygen gains *two* electrons and *each* sodium only loses *one* electron is accounted for in the balanced chemical equation.

- *Four sodium atoms* react with *two oxygen atoms* (in O_2). The ratio of sodium atoms to oxygen atoms is 2:1. Two sodium atoms are required to reduce *each* oxygen atom.

Example Problem

Answer the questions for the reaction of magnesium metal and chlorine gas.

$$Mg\ (s)\ +\ Cl_2\ (g)\ \rightarrow\ MgCl_2\ (s)$$
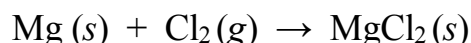
a) What is the charge of each of the magnesium atoms in the reactant [$Mg\ (s)$]? **0 (ZERO)**

b) What is the charge of each of the magnesium ions in the product? **2+**

c) Did each magnesium atom *gain* or *lose* electron(s) in this reaction? If so, how many? **lost 2e^-**

$$Mg^o\ \rightarrow\ Mg^{2+}$$
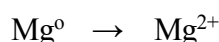
d) Was magnesium oxidized or reduced? **oxidized**

e) What is the charge of each of the chlorine atoms in the *reactant* [$Cl_2\ (g)$]? **0 (ZERO)**

f) What is the charge of the *each* of the chloride ions in the product? **1-**

g) Did each chlorine atom gain or lose electron(s) in this reaction? If so, how many? **gained 1e^-**

$$Cl^o + e^- \rightarrow\ Cl^-$$
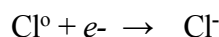
h) Was chlorine oxidized or reduced? **reduced**

Summary of Redox Reactions of *Inorganic* Compounds

It is possible to identify redox reactions for inorganic compounds by inspecting the chemical equation and determining if electrons are *transferred from one species to another*.

- If the **charge** of an atom or ion in a reactant was *increased* (toward positive) in the conversion of reactants to products, *an oxidation occurred*.

- If the **charge** of an atom or ion in a reactant was *decreased* (toward negative) in the conversion of reactants to products, *a reduction occurred*.

Redox Reactions of *Covalent* Compounds

We identified redox reactions for *inorganic compounds* by inspecting the chemical equation and determining if there was a change in the charge of atoms or ions. The transfer of electrons to or from covalent compounds is *not as easily recognized* as was the case for elements and ionic compounds in inorganic redox reactions.

For *covalent compounds*, such as organic and biological compounds, the gaining and losing of electrons is the result of a gain or loss of bond(s) to _____ *atoms* or _____ *atoms*.

For our purposes, oxidation and reduction for covalent compounds can be identified as follows:

- An atom in a covalent compound is **oxidized** if it *gains* bond(s) to *oxygen* and/or *loses* bond(s) to *hydrogen*.

- An atom in a covalent compound is **reduced** if it *loses* bond(s) to *oxygen* and/or *gains* bond(s) to *hydrogen.*

An example of a redox reaction for *covalent compounds* is the **combustion of hydrocarbons**.

- In the "complete combustion" of hydrocarbons, the hydrocarbon molecules react with oxygen gas (O_2) to form carbon dioxide and H_2O vapor. When there is an insufficient supply of O_2, "incomplete combustion" occurs and other products, such as carbon monoxide, are formed. In this course, when the term "combustion" is used, we will consider that to mean "complete combustion."

A specific example of the combustion of a hydrocarbon is the reaction of methane and oxygen gas:

$$CH_4 (g) \ + \ \mathbf{2} \, O_2 (g) \ \rightarrow \ CO_2 (g) \ + \ \mathbf{2} \, H_2O (g)$$

$$CH_4 (g) + 2 O_2 (g) \rightarrow CO_2 (g) + 2 H_2O (g)$$
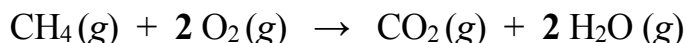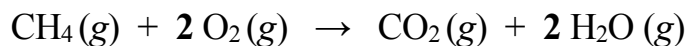
Let's use our criteria for oxidation and reduction of covalent compounds to determine which species was oxidized and which was reduced in this reaction.

- Carbon is bonded to four hydrogen atoms and to zero oxygen atoms as a reactant (in CH_4).

- After reacting, carbon is bonded to zero hydrogens and two oxygens.
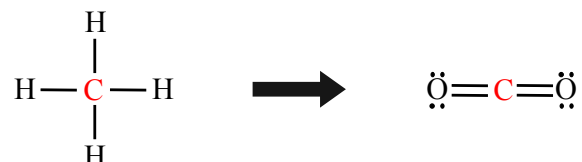
This change in carbon's bonding matches our criteria for the **oxidation** of a covalent compound.

An atom in an covalent compound is **oxidized** if it *gains bond(s)* to *oxygen* and/or *loses bond(s)* to *hydrogen*.

The carbon in methane was **oxidized** in this reaction.

Let's consider *oxygen* next. *Each* oxygen atom in O_2 is bonded to *one* other *oxygen atom* and **zero** *hydrogen atoms* before reacting.

After the reaction, oxygen appears in *both* products.
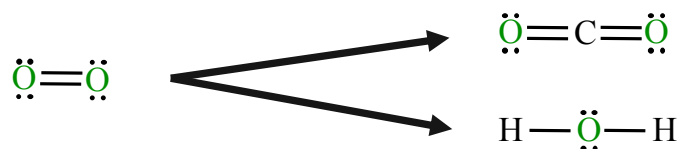
- The oxygen in CO_2 is bonded to zero *other* oxygen atoms (it *lost* a bond to oxygen in the reaction).

- The oxygen in H_2O is bonded to zero *other* oxygen atoms and to two hydrogen atoms (it *lost* a bond to oxygen **and** *gained* two bonds to hydrogen).

All of these changes in oxygen's bonding match our criteria for the *reduction* of a covalent compound.

An atom in a covalent compound is **reduced** if it *loses bond(s)* to *oxygen* and/or *gains bond(s)* to *hydrogen.*

The oxygens in **O_2 (g)** were **reduced** in this reaction.

An example of a redox reaction that is involved in biological systems is the reduction of NAD^+/oxidation of lactate.

- This is an important reaction that's involved in the metabolism of food.

$$NAD^+ \quad + \quad lactate \longrightarrow pyruvate \quad + \quad NADH \quad + \quad H^+$$
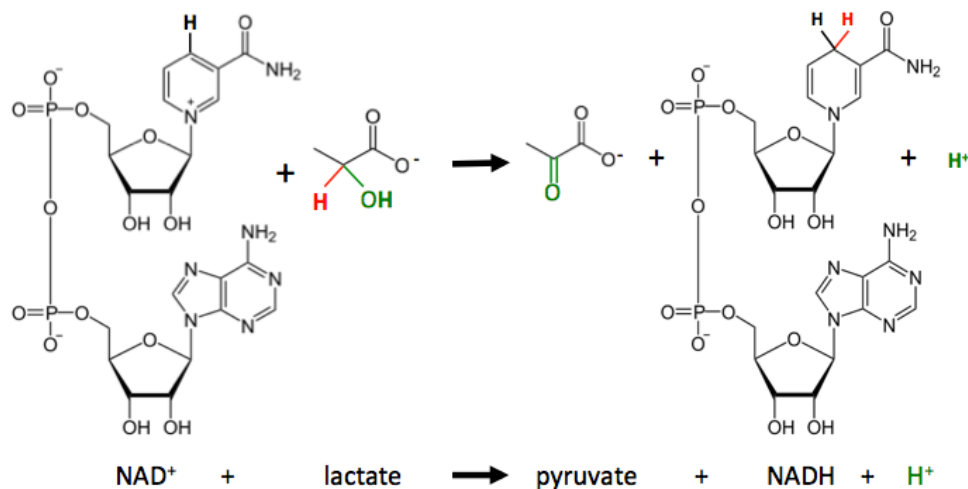
We can use our criteria for oxidation and reduction of organic compounds to determine which species was oxidized and which was reduced in this reaction.

Let's consider the change that occurred for **NAD^+**.
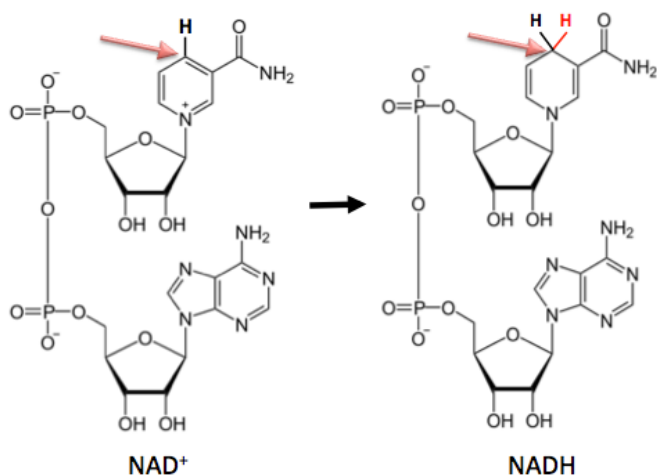
Look at the carbon *indicated by the arrow* at the very top of the six membered ring of the NAD^+. This carbon is bonded to **one** hydrogen atom as a reactant (in NAD^+). After reacting, this same carbon is bonded to **two** hydrogens.

This change in that carbon's bonding matches our criteria for the **reduction** of an organic compound.

An atom in a covalent compound is **reduced** if it *loses bond(s)* to *oxygen* and/or *gains bond(s)* to *hydrogen.*

This carbon in NAD^+ was *reduced* in this reaction. We often alternatively state this as, "NAD^+ was *reduced.*"

Now, let's consider the change that occurred for *lactate*.
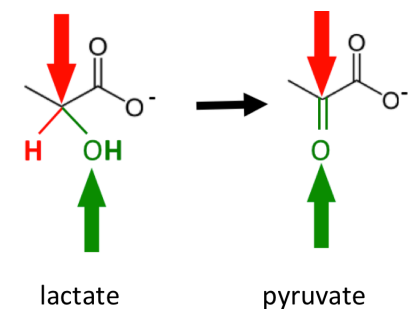
Both a carbon *and* an oxygen in lactate *lost bonds* to hydrogen.

Both of these changes match our criteria for the *oxidation* of an organic compound.

An atom in a covalent compound is **oxidized** if it *gains bond(s)* to *oxygen* and/or *loses bond(s)* to *hydrogen*.

A carbon and an oxygen in lactate were *oxidized* in this reaction. We often alternatively state this as, "lactate was *oxidized.*"

<div style="border:1px solid black; padding:10px">

Understanding Check

Indicate which atoms in the reactants in each of the following reactions were *oxidized* <u>and</u> which were *reduced*.

   a. $2\,H_2\,(g)\;+\;O_2\,(g)\;\rightarrow\;2\,H_2O\,(g)$

   b. ethene $+\;H_2\,(g)\;\rightarrow\;$ ethane

</div>
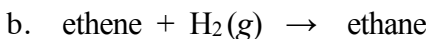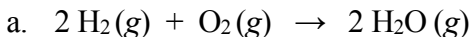
Some Industrial Uses of Redox Reactions

It is estimated that 50% of the world's population eat food that is grown using ***nitrogen fertilizers*** [1].

- The fertilizer industry employs the *reduction* of N_2 (from air) and the *oxidation* of H_2 in order to make ammonia (NH_3) in a process called **nitrogen fixation**.

$$N_2 +\; 3\,H_2 \rightarrow\; 2\,NH_3$$
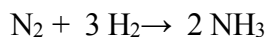
- Ammonia is either used directly or as a starting material for the synthesis of other nitrogenous fertilizers.

Many metals are mined as cations in ionic compounds (metal oxides, metal sulfides, metal carbonates, or metals combined with other anions) and then the metal cations are ***reduced*** to pure metals in an industrial process called **smelting**.

- For example, iron(II) oxide, copper nitrate, and lead sulfide, are converted to pure iron, copper, and lead, respectively. The reducing agent is usually carbon monoxide.

Electroplating processes use redox reactions to apply a thin coat of metal on another metal or conductive material.

- You may have heard the term "gold plated."

- In *gold plating*, silver or copper is often used as the *base metal*. The base metal is submerged in water containing dissolved gold cyanide (AuCN). As electrons are supplied to the base metal from the power source, they are transferred to the gold ions (reduction) and pure gold metal is deposited/plated on the base metal's surface.

- This process is used in the jewelry business and is also an important step in the manufacture of electronic devices such the electrical connectors on microchips.

[1]*Erisman, Jan Willem; MA Sutton, J Galloway, Z Klimont, W Winiwarter (October 2008). "How a century of ammonia synthesis changed the world", Nature Geoscience 1 (10): 636.*

Cathodic corrosion protection is a process that combines a small quantity of a more easily oxidized metal (called the sacrificial metal) with the metal that is to be *protected* from oxidation.

- Metal oxidation is also called **corrosion**.

- In cathodic protection, the sacrificial metal corrodes before the protected metal.

- An example of cathodic protection is *galvanized* steel.

- In the galvanization process, a thin layer of zinc is applied to steel (iron) as a sacrificial metal.

The process called "**bleaching**" uses fairly strong oxidizing agents.

- Oxidizing agents accept electrons from the species that is being oxidized.

- The substance that is commonly referred to as liquid bleach uses the hypochlorite ion (ClO^-) as an oxidizing agent.

- Bleach removes electrons from the molecules that make up "stains" or infectious agents.
    - In the case of stains, when oxidized by bleach, they no longer absorb visible light and therefore can no longer be seen.

- Other bleaching methods use oxidizing agents such as hydrogen peroxide (H_2O_2) instead of hypochlorite.

Biochemical Redox Reactions

You will learn about the chemistry of biological systems (biochemistry) in the later chapters. *You will see many redox reactions occurring in biology.*

Biological systems employ a series of chemical reactions in order to get energy from food molecules in the *cellular respiration* process.

- Many of these reactions are *redox reactions*.

The energy in food molecules originates from the sun. Sunlight is converted to chemical energy (in the form of carbohydrate molecules) in a series of chemical reactions called *photosynthesis*.

- Many of the reactions of *photosynthesis* are *redox reactions*.

Summary of Redox Reactions

Oxidation is the *loss of electron(s)* by an atom, ion, or molecule in a chemical reaction.

Reduction is the *gain of electrons* by an atom, ion, or molecule in a chemical reaction.

It is possible to identify *redox reactions* for **inorganic compounds** by inspecting the chemical equation and determining if electrons are transferred from one species to another.

- One atom or ion in a **reactant** will **lose electrons** and therefore its *charge* will **increase** (in the positive direction) by one charge unit for every electron that is lost.

- The *charge* of the atom or ion in the **reactant** that **gains** the electron(s) will **decrease** (toward negative values) by one charge unit for every electron that is gained.

For **covalent compounds** such as organic molecules:

- An atom in a covalent compound is **oxidized** if it *gains* bond(s) to *oxygen* and/or *loses* bond(s) to *hydrogen*.

- An atom in a covalent compound is **reduced** if it *loses* bond(s) to *oxygen* and/or *gains* bond(s) to *hydrogen.*

Identification of the Reduced and Oxidized Species in Redox Reactions

Inorganic Reactions
Reactants and products are ions or pure elements.

Inspect the *charges* of reactants and products in chemical equation to determine if *electrons are transferred from one reactant species to another*.

Oxidation

Reduction

loss of electron(s) by an ion or an atom in a pure element

gain of electron(s) by an ion or an atom in a pure element

Organic/Covalent Reactions
Reactants and products are covalent compounds.

Inspect the chemical equation to determine if an atom in a reactant *gained or lost bond(s) to oxygen or hydrogen atoms.*

Oxidation

Reduction

An atom in a reactant *gains* bond(s) to oxygen and/or loses bond(s) to hydrogen.

An atom in a reactant *loses* bond(s) to oxygen and/or gains bond(s) to hydrogen.

Redox Reaction Terminology

The *reactant that was oxidized* is sometimes referred to as the "**reducing agent**" because it *transferred its electron(s)* to the reactant that was reduced.

Conversely, the *reactant that was reduced* is sometimes referred to as the "**oxidizing agent**" because it *accepted electron(s)* from the reactant that was *oxidized*.

Reactions of Organic Molecules

In this remainder of this chapter, I will discuss *four classes of organic reactions* that involve the *families* of organic molecules that you were introduced to in chapter 4: hydrocarbons, alcohols, carboxylic acids, and esters.

Before we begin, let's review the structure of alcohols, carboxylic acids, and esters.

Review of *families* of Organic Molecules

The Alcohol Family

Alcohols contains one or more _____ **(-OH)** functional groups attached to a *hydrocarbon*.

The general form of an alcohol is shown below with the hydroxyl group highlighted in yellow.

Hydrocarbon —Ö–H

The Carboxylic Acid Family

Carboxylic acids contain a _____ *functional* group attached to a hydrocarbon.

Carboxyl groups contain both a *carbonyl group*, which is a carbon double bonded to an oxygen (**C=O**), *and* a *hydroxyl group* **(-OH)** that are connected to each other and the hydrocarbon (alkyl group) part.

:O:
||
Hydrocarbon —C–Ö–H
carboxyl group

The Ester Family

Esters contain a _____ *functional* group that is bonded *between two* hydrocarbon parts.

Carboxylate groups contain both a *carbonyl group* (**C=O**), *and* an *oxygen atom.*

:O:
||
Hydrocarbon —C–Ö— Hydrocarbon
carboxylate group

The boxes that represent hydrocarbons (alkyl groups) are shaded with different colors because the two hydrocarbon parts *are not always identical*.

Reactions of Organic Molecules

The *four classes of organic reactions* to be studied in this section are:

1. **Hydrogenation: Reduction of Alkenes**
2. **Hydrolysis of Esters**
3. **Hydration of Alkenes**
4. **Dehydration of Alcohols**

The **educational goal** for this section is, *if you are given the specific reactant(s) for any of these four classes of reactions, you should be able to predict (draw) the product(s).*

A good way to do this is to know the "**general form**" of the organic reaction.

I will elaborate on what is meant by the "*general form"* of an organic reaction when I discuss the hydrogenation (the reduction of alkenes).

1) Hydrogenation: Reduction of Alkenes

Alkenes and other unsaturated hydrocarbons react with hydrogen gas (H_2) in a reaction called

_____.

In the presence of a *catalyst*, such as platinum, a hydrogen atom from H_2 is added to each of the double bonded carbon atoms in the *alkene* to produce the corresponding _____.

- Hydrogen gas acts as a *reducing agent*; the carbon atoms in an alkene are *reduced* (*they gain hydrogen atoms)*.

The *general form* for the hydrogenation of alkenes reaction is shown below.

Alkene　　　　　　　　　　　**Alkane**
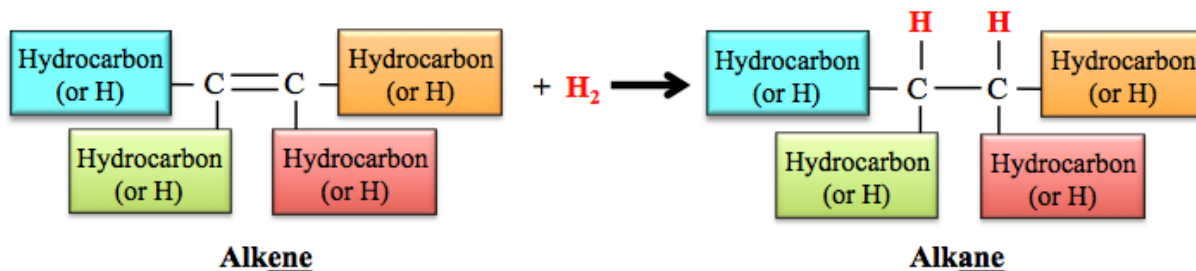
The *general form* of an equation contains the generic structures of products and reactants.

- For example, in the general form for the hydrogenation equation above, a *generic structure* representing *any alk***ene** is drawn as the *reactant* and a *generic structure* representing *any* alkane is drawn for the *product*.
- The boxes represent any hydrocarbon (alkyl group) or a hydrogen atom, and are shaded with different colors (in the video) to indicate that *the hydrocarbon parts may or may not be identical.*

Specific Example of Hydrogenation: Hydrogenation of 3-methyl-3-heptene

3-methyl-3-heptene　　　　　　　　**3-methylheptane**
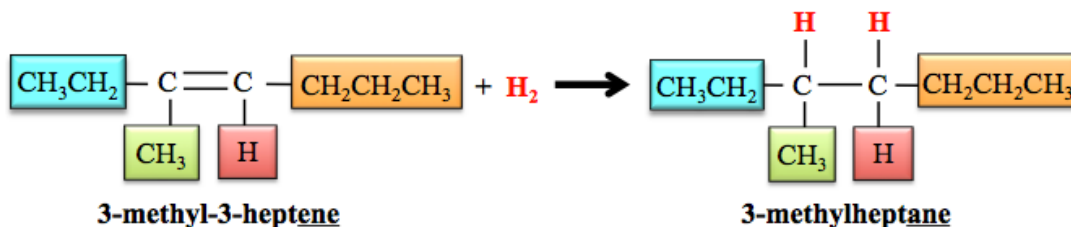
Specific Example of Hydrogenation: Hydrogenation of propene

propene + H₂ → propane
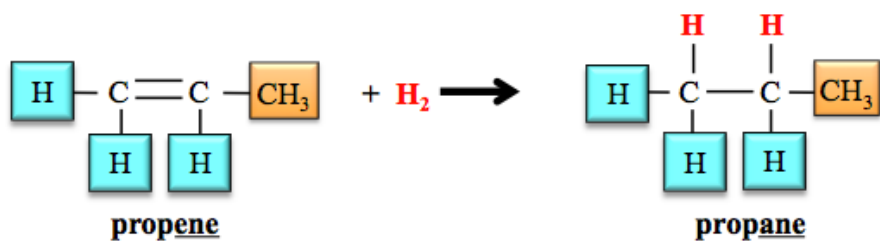
Knowing the "***general form***" of an organic reaction allows you to predict and draw the product(s) when given specific reactant(s).

Alkene + H₂ → Alkane
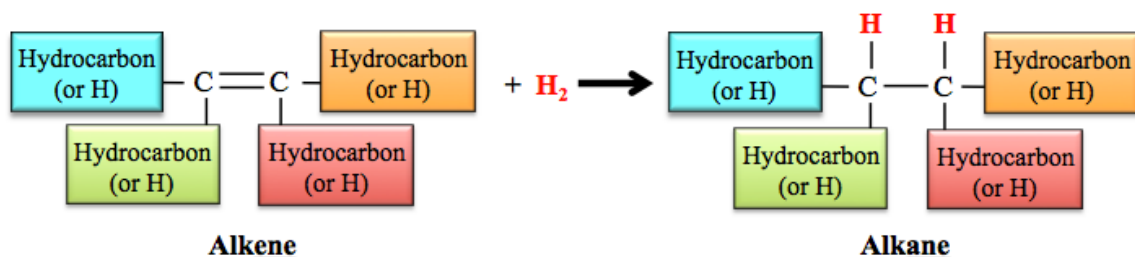
Example: Draw and name the ***product*** of the following reaction:

$$CH_2 = CHCH_2CH_2CH_3 \quad + H_2 \longrightarrow$$

$$CH_2 = CH CH_2CH_2CH_3 \quad + H_2 \longrightarrow CH_3CH_2CH_2CH_2CH_3$$
1-pent**ene** pent**ane**
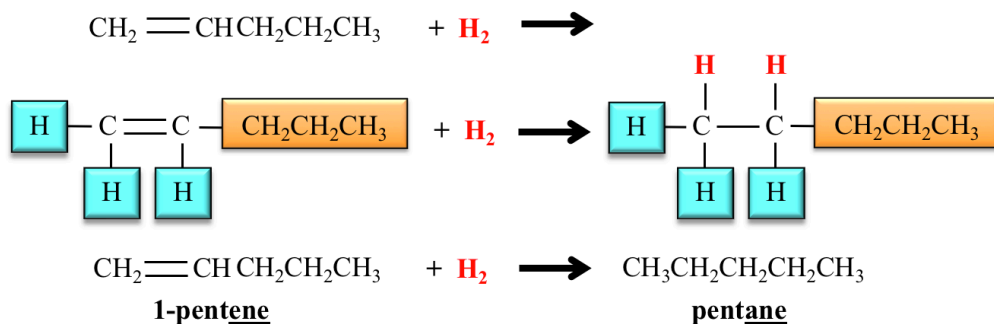
Before I ask you to try a couple of problems on your own, I want to show you another way to predict the product for hydrogenation of alkene reactions. This method will be useful in several other types of reactions that you will learn.

In the hydrogenation reaction, we made *new bonds* to **both of the atoms (carbons)** that were connected to each other with a double bond.

Chemical reactions where new bonds are formed to atoms at each end of a double bond occur so frequently that organic chemist have a special name for it: "***addition across a double bond***."

Products for reactions where *addition across a double bond* occurs can be easily predicted by learning the following method of "*flipping*" bonds.

Addition Across a Double Bond

Step #1: Draw the **H-H** directly above the double bond.
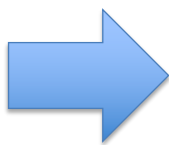
Step #2: Flip *one* of the bonds from the double bond **up** to the **H**

H—H

Hydrocarbon — C＝C — Hydrocarbon

H   H

H—H

Hydrocarbon — C＝C — Hydrocarbon

H   H
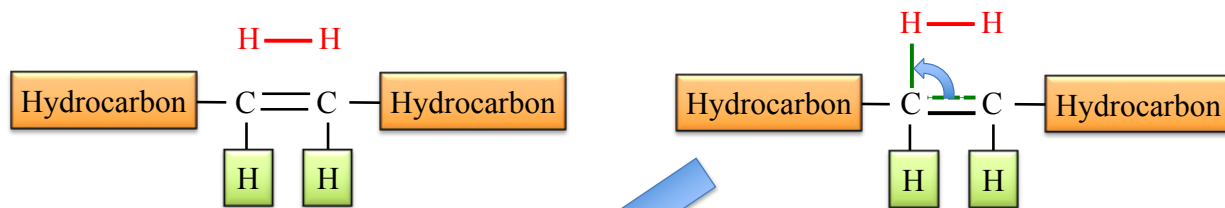
Step #3: Flip the **H-H** single bond **down** to the **C**

The product is an alk<u>ane</u>

H---H

Hydrocarbon — C — C — Hydrocarbon

H   H

H   H

Hydrocarbon — C — C — Hydrocarbon

H   H
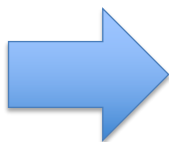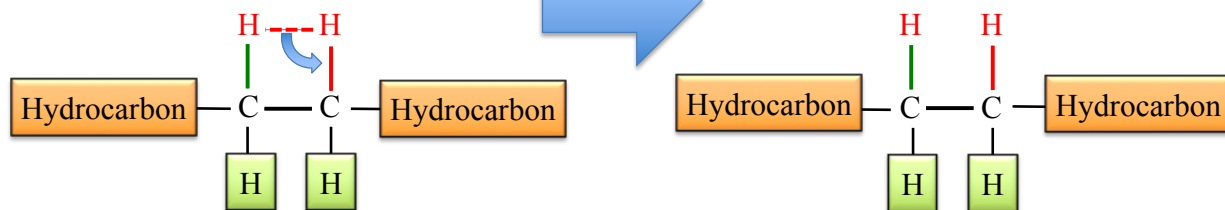
Understanding Check

Draw and name the product formed when each of the alkenes listed below react with H_2.

a. 1-butene

b. *cis*-2-butene

c. *trans*-2-pentene

Water is a reactant or product in a number of reactions important to organic and biochemistry.

The next three classes of organic reactions involve a water molecule as either a reactant or product.

2) Hydrolysis of Esters

In a _____ reaction, water (hydro) is used to break (lyse) a bond in a molecule.

The **hydrolysis of esters** reaction occurs in nature and has industrial uses.

- Example: Triglycerides (fats) are esters and undergo hydrolysis reactions in the digestion process.

In the hydrolysis of an ester, a water molecule breaks a bond in the ester to form a _____ _____ and an _____.

- The general form of the hydrolysis of esters reaction is shown below:
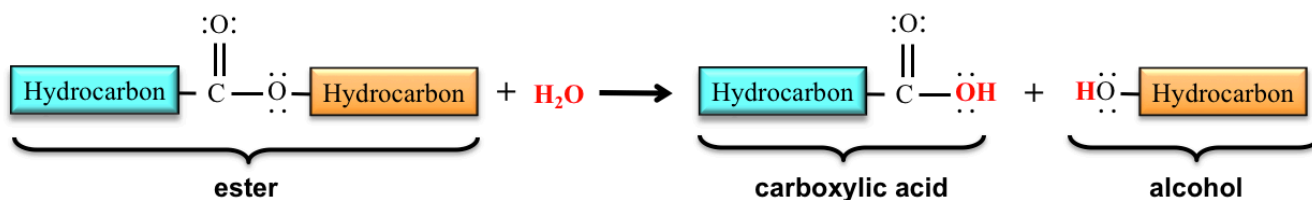
Knowing the "*general form*" of the hydrolysis of esters, and then identifying the hydrocarbon parts will allow you to predict and draw the carboxylic acid and alcohol products when given a specific *ester* reactant.

I want to show you *another way* to predict the products for hydrolysis of ester reactions.

Step 1: Draw the structural formula of the ester and identify the hydrocarbon parts.

Step 2: Break (lyse) the carbon-oxygen *single bond* between the *carbonyl* carbon and the oxygen. The *carbonyl* carbon is the carbon that is double bonded to an oxygen.

Step 3: Add the **–OH** from the water to the *carbonyl* carbon and then add the **H** from the water to the oxygen on the *other fragment*.
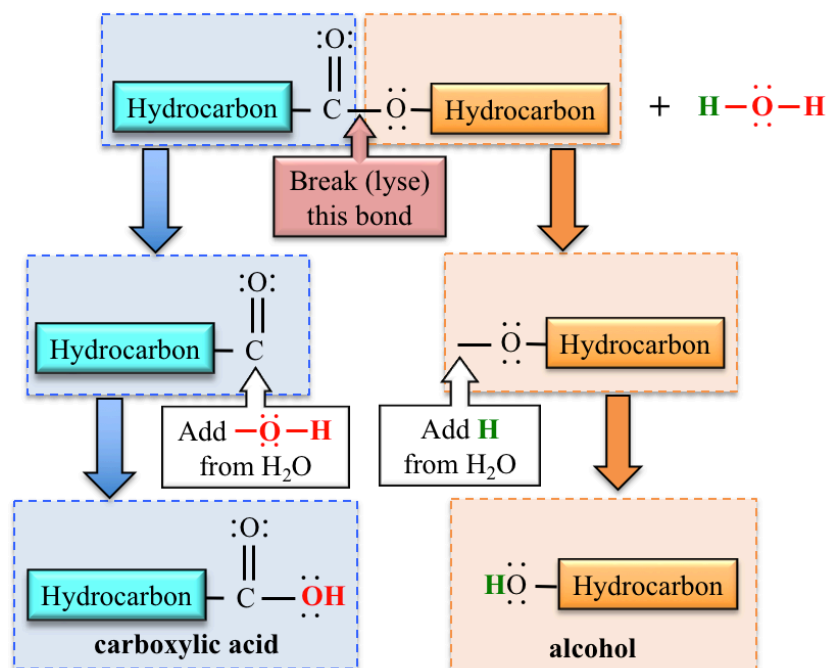
When you use these three steps, it will result in the correct *carboxylic acid* and *alcohol.*

41

Example: Predict the products of the hydrolysis of the ester shown here.

$$CH_3CH_2 \overset{\overset{\displaystyle :O:}{\|}}{—C} —\ddot{\underset{..}{O}}—CH_3 \quad + \quad H_2O$$
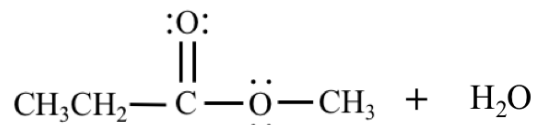
Solution:

Step 1: Draw the structural formula of the ester and identify the hydrocarbon parts.

Step 2: Break (lyse) the carbon-oxygen *single bond* <u>between</u> the *carbonyl* carbon and the oxygen. The *carbonyl* carbon is the carbon that is double bonded to an oxygen.

Step 3: Add the **–OH** from the water to the *carbonyl* carbon and then add the **H** from the water to the oxygen on the *other fragment*.

CH₃CH₂ — C ⎯ Ö ⎯ CH₃   +   H—Ö—H

Break (lyse) this bond

CH₃CH₂ — C

— Ö — CH₃

Add —Ö—H from H₂O

Add **H** from H₂O

:O:
‖
CH₃CH₂ — C — **OH**
carboxylic acid

HÖ — CH₃
alcohol
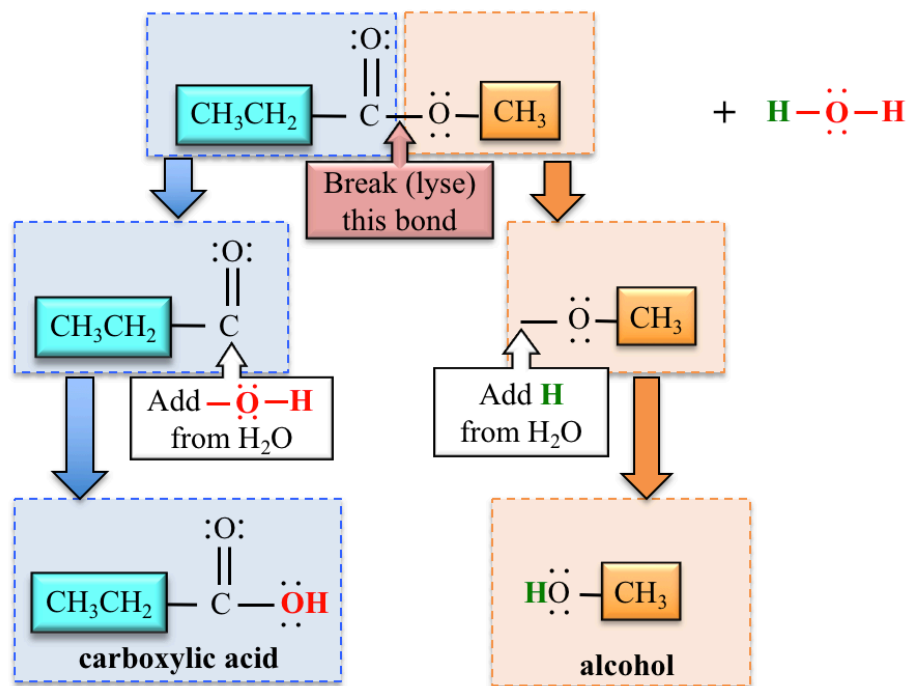
Understanding Check

Draw the structural formulas of **both products** in the hydrolysis of ethyl butanoate:

$$CH_3CH_2CH_2 \overset{\overset{\displaystyle :O:}{\|}}{—C} —\ddot{\underset{..}{O}}—CH_2CH_3 \quad + \quad H_2O \longrightarrow$$
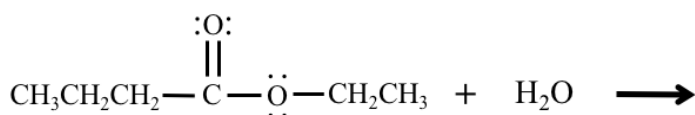
ethyl butanoate

3) Hydration of Alkenes

In _____ of alkene reactions, alkenes react with water molecules to produce alcohols.

The **general form** for the hydration of an alkene reaction is shown below:
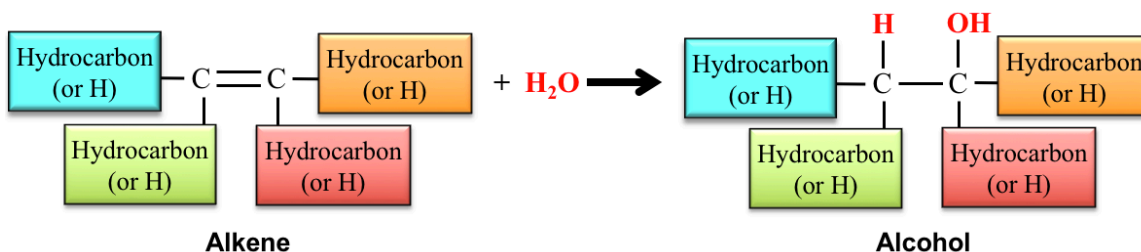
- A hydrogen atom from H_2O is added to one of the double bonded carbon atoms and the **–OH** from the H_2O is added to the **_other_** double bonded carbon atom in the **_alkene_** to produce the corresponding **_alcohol_**.

- The **double bond** in the _alkene_ is converted to a **single bond** in the _alcohol_.

A specific example of the hydration of alkenes reaction is the reaction of **_ethene_** and H_2O:
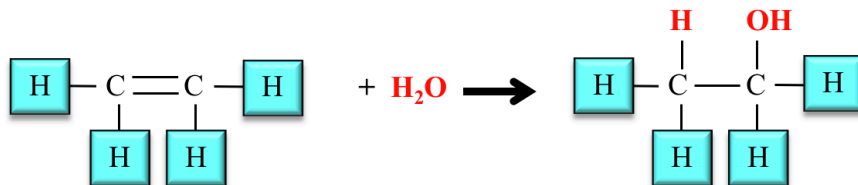
You may have noticed the similarity of this _hydration reaction_ to the _hydrogenation of alkenes_.

Hydration reactions are another example of reactions in which a molecule is **_added across a double bond_**.

In the _hydration of alkenes reaction_, water is added **_across the double bond of an alkene_**, therefore we can use the _bond flipping method_ to predict the structure of the alcohol that is produced.

EXAMPLE: **_Addition of H_2O across a double bond_**. Add H_2O across the double bond of **ethene** (hydration of ethene).

Step 1: Draw the molecule to be added across the double bond and the molecule with the double bond as shown here:
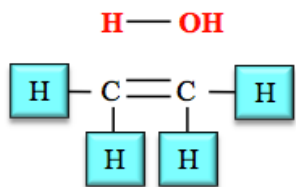
Step #1:
Draw the **H - OH** directly above the double bond.

Steps 2 and 3: **_Flip_** the bonds as shown below to get the product of the reaction.

Step #2: Flip one of the double bonds **up** to the **H**

Step #3: Flip the **H-OH** single bond **down** to the **C**

Alcohol Product

43
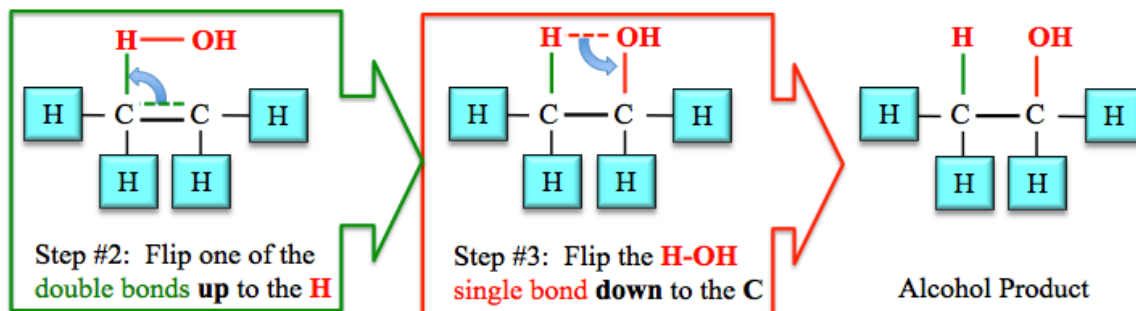
Predict the product formed by the hydration of this alkene:

$$CH_3CH_2\underset{H}{C}=\underset{H}{C}CH_2CH_3$$
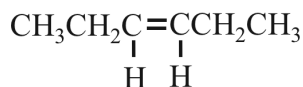
4) Dehydration of Alcohols

Dehydration of alcohols is the *reverse* of hydration of alkenes.

H₂O is _____ from an alcohol to form an alkene.

- A hydroxyl group (**-OH**) is removed from a carbon atom and an **H** is removed from a carbon that is _____ to the carbon that was bonded to the hydroxyl group. A double bond forms between these two carbons.

The **general form** for the *dehydration of an alcohol reaction* is shown below:

Alcohol   **Alkene**
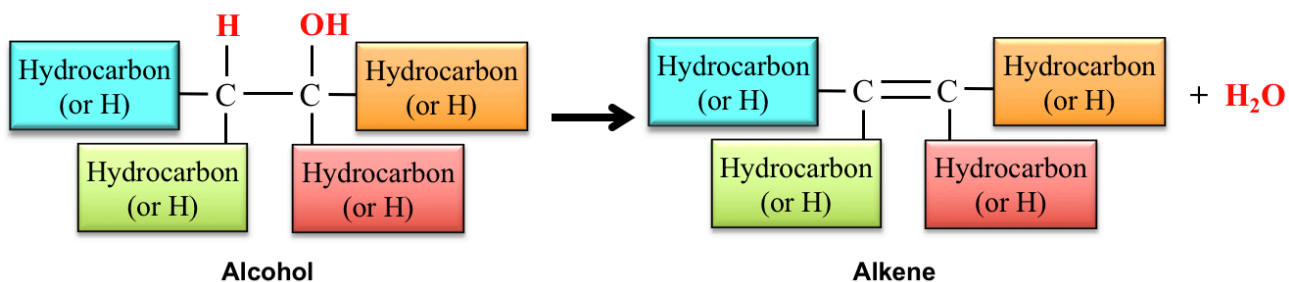
Since this reaction is the *reverse of the hydration of alkenes* reaction, we can *flip* the bonds in the *opposite order* to that which we used when we added water *across the alkene double bond*.

Doing so can be very helpful in determining the alkene product in a dehydration of alcohol reaction.

I will use the dehydration of *propyl alcohol* as an example. Beginning with the structure of the alcohol, perform the following two steps:

Step #1: Flip the bond between the C and **OH** **up** to an **H** on *an adjacent* carbon.

Step #2: Flip the **C--H** bond from the *adjacent* carbon **down** to make a double bond to the C that originally carried the OH

Alkene and H₂O Products

propyl alcohol

44
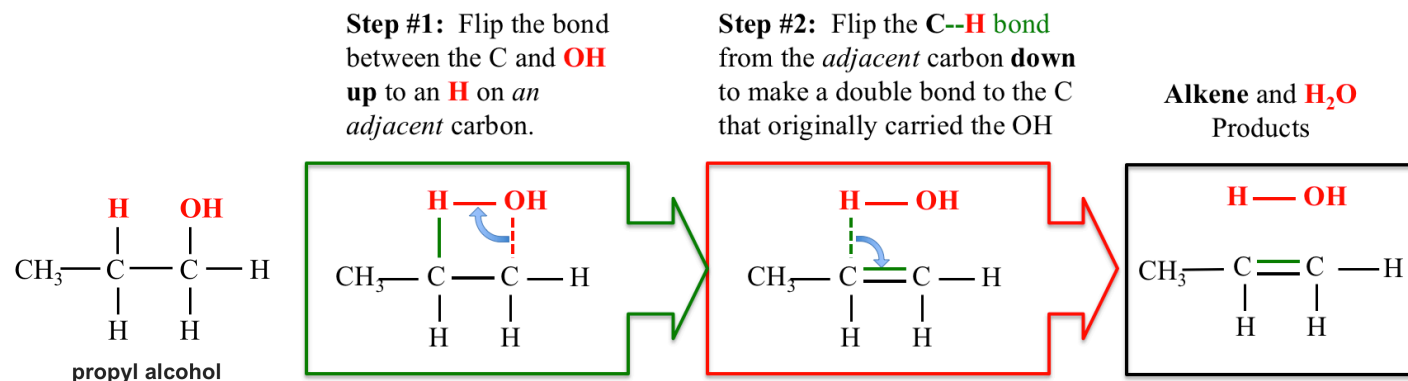
Understanding Check

Name and draw the *condensed structural formula* for the alkene that is produced when ethyl alcohol undergoes a dehydration reaction:

$$CH_3CH_2 \overset{\displaystyle OH}{|} \longrightarrow H_2O + \textcolor{red}{\textbf{?}}$$
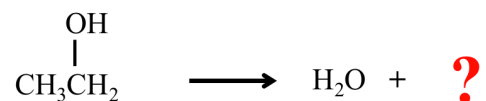
Summary of Classes of Organic Reactions

Organic Reaction Class	Reactant(s)	Product(s)
Hydrogenation of Alkenes	Alkene + H_2	Alkane
Hydrolysis of Esters	Ester + H_2O	Carboxylate ion + Alcohol
Dehydration of Alcohols	Alcohol	Alkene + H_2O
Hydration of Alkenes	Alkene + H_2O	Alcohol

Recommendation: Work on the "Chapter 6 Reactions Worksheet" as soon as you can.
- You can find this worksheet in the lecture notes package or on the website.

Balancing Equations Worksheet and Key

1. Answer the following questions about the chemical equation shown below:

$$2 H_2 + O_2 \rightarrow 2 H_2O$$
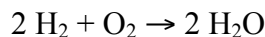
    a) What are the reactants?
    b) What is the product?
    c) What do we call the number "2" in front of the H_2 (and H_2O)?
    d) Is the reaction balanced?
    e) Why is there not a coefficient for O_2?   .
    f) How many hydrogen **atoms** are needed to produce **two** H_2O molecules?
    g) How many oxygen **atoms** are needed to produce **two** H_2O molecules?
    h) How many hydrogen **molecules** are needed to produce **two** H_2O molecules?
    i) How many oxygen **molecules** are needed to produce **two** H_2O molecules?
    j) Write the "word equation" that you would use to describe this reaction.
       • Use words in a sentence, not formulas or an arrow. ***Ignore the coefficients***.

2. Balance the following chemical equations:

a) $Fe + O_2 \rightarrow Fe_2O_3$

b) $H_2 + Cl_2 \rightarrow HCl$

c) $Ag + H_2S \rightarrow Ag_2S + H_2$

d) $CH_4 + O_2 \rightarrow CO_2 + H_2O$

e) $HgO \rightarrow Hg + O_2$

f) $Co + H_2O \rightarrow Co_2O_3 + H_2$

3. Write **balanced chemical equations** for each of the following descriptions of a chemical reaction.
       • You ***do not need to include the phases*** of the reactants or products.
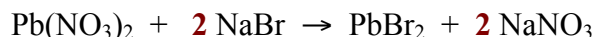   **IMPORTANT NOTE:** Before attempting to balance the equations, you must first convert the compound ***names*** into the correct chemical ***formulas***. If you begin to struggle with that, you may wish to go back to Chapter 3 and re-work the naming problems.

a) Aluminum metal ***reacts with*** copper(II) chloride ***to produce*** aluminum chloride <u>and</u> copper metal.
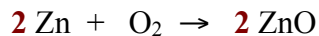
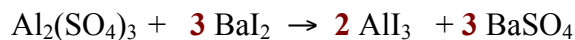b) Lead(II) nitrate reacts with sodium bromide to produce lead(II) bromide and sodium nitrate.
       • HINT: Since you have *the same polyatomic ion* (nitrate) on **both sides** of the equation you can use the shortcut that was listed in Step #1 of our balancing method.

c) Zinc metal reacts with oxygen gas to produce zinc oxide
(Recall that oxygen is one of the diatomic molecules that are referred to by their element's name).

d) Aluminum sulfate reacts with barium iodide to produce aluminum iodide and barium sulfate.
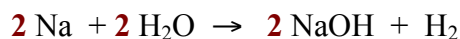
e) At temperatures reached during baking, sodium bicarbonate (baking soda) decomposes (reacts) to produce sodium carbonate, carbon dioxide, and dihydrogen monoxide.
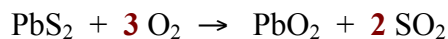 • Recall that *bicarbonate* is a polyatomic ion (<u>not</u> the same as the *carbonate* polyatomic ion).
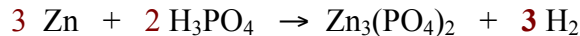
f) Sodium metal reacts with water to produce sodium hydroxide and hydrogen gas.

g) Lead(IV) sulfide reacts with oxygen gas to produce lead(IV) oxide and sulfur dioxide.

h) Zinc metal reacts with phosphoric acid to produce zinc phosphate and hydrogen gas.
  (NOTE: ***the formula of phosphoric acid is*** H_3PO_4)

SEE NEXT PAGE FOR THE ANSWER KEY

ANSWER KEY
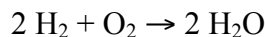
1. Answer the following questions about the chemical equation shown below:
$$2 H_2 + O_2 \rightarrow 2 H_2O$$
   a) What are the reactants? H_2 and O_2
   b) What is the product? H_2O
   c) What is the number "2" in front of the H_2 (and H_2O) called? Coefficient
   d) Is the reaction balanced? Yes
   e) Why is there not a coefficient in for O_2? When the coefficient would be "**1**", it is omitted.
   f) How many hydrogen **atoms** are needed to produce **two** H_2O molecules? **4**
   g) How many oxygen **atoms** are needed to produce **two** H_2O molecules? **2**
   h) How many hydrogen **molecules** are needed to produce **two** H_2O molecules? **2**
   i) How many oxygen **molecules** are needed to produce **two** H_2O molecules? **1**
   j) Write the "word equation" that you would use to describe this reaction.
   - Use words in a sentence, not formulas or an arrow. ***Ignore the coefficients***.
   Hydrogen ***reacts with*** oxygen to ***produce*** dihydrogen monoxide (or water). ***or***
   Hydrogen ***plus*** oxygen ***produces*** dihydrogen monoxide (or water).
   - o You can write "***forms***" instead of "***produces***"

2. Balance the following chemical equations:

a) **4** Fe + **3** O_2 → **2** Fe_2O_3

b) H_2 + Cl_2 → **2** HCl

c) **2** Ag + H_2S → Ag_2S + H_2

d) CH_4 + **2** O_2 → CO_2 + **2** H_2O

e) **2** HgO → **2** Hg + O_2

f) **2** Co + **3** H_2O → Co_2O_3 + **3** H_2

3. Write **balanced chemical equations** for each of the following descriptions of a chemical reaction.
   - You ***do not need to include the phases*** of the reactants or products.
   IMPORTANT NOTE: Before attempting to balance the equations, you must first convert the compound ***names*** into the correct chemical ***formulas***. If you begin to struggle with that, you may wish to go back to Chapter 3 and re-work the naming problems.

a) Aluminum metal ***reacts with*** copper(II) chloride ***to produce*** aluminum chloride <u>and</u> copper metal.

$$\textbf{2} Al + \textbf{3} CuCl_2 \rightarrow \textbf{2} AlCl_3 + \textbf{3} Cu$$

b) Lead(II) nitrate reacts with sodium bromide to produce lead(II) bromide and sodium nitrate.
   - HINT: Since you have *the same polyatomic ion* (nitrate) on **both sides** of the equation you can use the shortcut that was listed in Step #1 of our balancing method.

$$Pb(NO_3)_2 + \textbf{2} NaBr \rightarrow PbBr_2 + \textbf{2} NaNO_3$$

c) Zinc metal reacts with oxygen gas to produce zinc oxide
(Recall that oxygen is one of the diatomic molecules that are referred to by their element's name).

$$\textbf{2}\ Zn\ +\ O_2\ \rightarrow\ \textbf{2}\ ZnO$$

d) Aluminum sulfate reacts with barium iodide to produce aluminum iodide and barium sulfate.

$$Al_2(SO_4)_3\ +\ \textbf{3}\ BaI_2\ \rightarrow\ \textbf{2}\ AlI_3\ +\ \textbf{3}\ BaSO_4$$

e) At temperatures reached during baking, sodium bicarbonate (baking soda) decomposes (reacts) to produce sodium carbonate, carbon dioxide, and dihydrogen monoxide.
   • Recall that *bicarbonate* is a polyatomic ion (<u>not</u> the same as the *carbonate* polyatomic ion).

$$\textbf{2}\ NaHCO_3\ \rightarrow\ Na_2CO_3\ +\ CO_2\ +\ H_2O$$

f) Sodium metal reacts with water to produce sodium hydroxide and hydrogen gas.

$$\textbf{2}\ Na\ +\ \textbf{2}\ H_2O\ \rightarrow\ \textbf{2}\ NaOH\ +\ H_2$$

g) Lead(IV) sulfide reacts with oxygen gas to produce lead(IV) oxide and sulfur dioxide.

$$PbS_2\ +\ \textbf{3}\ O_2\ \rightarrow\ PbO_2\ +\ \textbf{2}\ SO_2$$

h) Zinc metal reacts with phosphoric acid to produce zinc phosphate and hydrogen gas.
   (NOTE: the formula of phosphoric acid is H_3PO_4)

$$\textbf{3}\ Zn\ +\ \textbf{2}\ H_3PO_4\ \rightarrow\ Zn_3(PO_4)_2\ +\ \textbf{3}\ H_2$$

Stoichiometry Worksheet and Key

$$2\ KClO_3 \rightarrow 2\ KCl\ +\ 3\ O_2$$

1. How many moles of O_2 will be formed from 1.65 moles of $KClO_3$?

$$\frac{1.65\ mol\ KClO_3}{} \left|\ \frac{\underline{\quad}\ mol\ O_2}{\underline{\quad}mol\ KClO_3}\ \right| = \underline{\quad}\ mol\ O_2$$

2. How many moles of $KClO_3$ are needed to make 3.50 moles of KCl?

$$\frac{3.50\ mol\ KCl}{} \left|\ \frac{}{}\ \right| = \underline{\quad}\ mol\ KClO_3$$

3. How many moles of KCl will be formed from 2.73 moles of $KClO_3$?

$$\frac{}{} \left|\ \frac{}{}\ \right| = \underline{\quad}$$

$$4\ Fe\ +\ 3\ O_2 \rightarrow 2\ Fe_2O_3$$
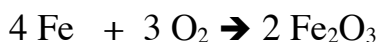
4. How many moles of Fe_2O_3 are produced when 0.275 moles of Fe is reacted?

$$\frac{0.275\ mol\ Fe}{} \left|\ \frac{}{}\ \right| = \underline{\quad}\ mol\ Fe_2O_3$$

5. How many moles of Fe_2O_3 are produced when 31.0 moles of O_2 is reacted?

$$\frac{}{} \left|\ \frac{}{}\ \right| = \underline{\quad}$$

6. How many moles of O_2 are needed to react with 8.9 moles of Fe?

$$\frac{}{} \left|\ \frac{}{}\ \right| = \underline{\quad}$$

$$2\ H_2O \rightarrow 2\ H_2\ +\ O_2$$
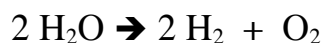
7. How many moles of O_2 are produced when 1.26 moles of H_2O is reacted?

8. How many moles of H_2O are needed to produce 55.7 moles of H_2?

9. If enough H_2O is reacted to produce 3.40 moles of H_2, then how may moles of O_2 must have been made? (a bit challenging, but just think about it and you can probably figure it out)

$$2 \text{ KClO}_3 \rightarrow 2 \text{ KCl} + 3 \text{ O}_2$$
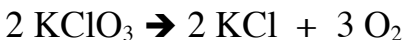
10. How many **grams** of O_2 will be formed from 3.76 grams of $KClO_3$?

3.76g $KClO_3$	1 mol $KClO_3$	__ mol O_2	__ g O_2	
	122.55 g $KClO_3$	__ mol $KClO_3$	__ mol O_2	= _____ g O_2

11. How many **grams** of $KClO_3$ are needed to make 30.0 grams of KCl?

30.0 g KCl	____ mol KCl	__ mol $KClO_3$	__ g $KClO_3$	
	____ g KCl	__ mol KCl	__ mol $KClO_3$	= _____ g $KClO_3$

12. How many grams of KCl will be formed from 2.73 g of $KClO_3$?

2.73 g $KClO_3$				
				= _____ g KCl

$$4 \text{ Fe} + 3 \text{ O}_2 \rightarrow 2 \text{ Fe}_2\text{O}_3$$
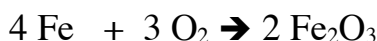
13. How many **grams** of Fe_2O_3 are produced when 42.7 **grams** of Fe is reacted?

42.7 g Fe	____ mol Fe	__ mol Fe_2O_3	__ g Fe_2O_3	
	____ g Fe	__ mol Fe	__ mol Fe_2O_3	= _____ g Fe_2O_3

14. How many **grams** of Fe_2O_3 are produced when 17.0 grams of O_2 is reacted?

17.0 g O_2				
				= _____ g Fe_2O_3

15. How many grams of O_2 are needed to react with 125 grams of Fe?

				= _____

Some cars can use butane (C_4H_{10}) as fuel:

$$2 \text{ C}_4\text{H}_{10} + 13 \text{ O}_2 \rightarrow 8 \text{ CO}_2 + 10 \text{ H}_2\text{O}$$

16. How many grams of CO_2 are produced from the combustion of 100. grams of butane?

100. g C_4H_{10}				
				= _____ g CO_2

17. How many grams of O_2 are needed to react with of 100. grams of butane?

100. g C_4H_{10}				
				= _____ g O_2

18 How many grams of H_2O are produced when 5.38g of O_2 is reacted?

KEY
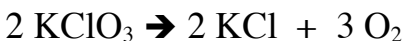
$$2\ KClO_3 \rightarrow 2\ KCl\ +\ 3\ O_2$$

1. How many moles of O_2 will be formed from 1.65 moles of $KClO_3$?

$$\dfrac{1.65\ mol\ KClO_3 \left| \dfrac{3\ mol\ O_2}{2\ mol\ KClO_3} \right.}{} = \underline{2.48}\ mol\ O_2$$

2. How many moles of $KClO_3$ are needed to make 3.50 moles of KCl?

$$\dfrac{3.50\ mol\ KCl \left| \dfrac{2\ mol\ KClO_3}{2\ mol\ KCl} \right.}{} = \underline{3.50}\ mol\ KClO_3$$

3. How many moles of KCl will be formed from 2.73 moles of $KClO_3$?

$$\dfrac{2.73\ moles\ KClO_3 \left| \dfrac{2\ mol\ KCl}{2\ mol\ KClO_3} \right.}{} = \underline{2.73}\ mol\ KCl$$

$$4\ Fe\ +\ 3\ O_2 \rightarrow 2\ Fe_2O_3$$
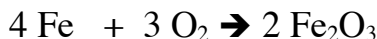
4. How many moles of Fe_2O_3 are produced when 0.275 moles of Fe are reacted?

$$\dfrac{0.275\ mol\ Fe \left| \dfrac{2\ mol\ Fe_2O_3}{4\ mol\ Fe} \right.}{} = \underline{0.138}\ mol\ Fe_2O_3$$

5. How many moles of Fe_2O_3 are produced when 31.0 moles of O_2 are reacted?

$$\dfrac{31.0\ mol\ O_2 \left| \dfrac{2\ mol\ Fe_2O_3}{3\ mol\ O_2} \right.}{} = \underline{20.7}\ mol\ Fe_2O_3$$

6. How many moles of O_2 are needed to react with 8.9 moles of Fe?

$$\dfrac{8.9\ mol\ Fe \left| \dfrac{3\ mol\ O_2}{4\ mol\ Fe} \right.}{} = \underline{6.7}\ mol\ O_2$$

$$2\ H_2O \rightarrow 2\ H_2\ +\ O_2$$
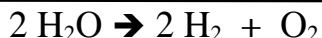
7. How many moles of O_2 are produced when 1.26 moles of H_2O is reacted?

$$\dfrac{1.26\ mol\ H_2O \left| \dfrac{1\ mol\ O_2}{2\ mol\ H_2O} \right.}{} = \underline{.630}\ mol\ O_2$$

8. How many moles of H_2O are needed to produce 55.7 moles of H_2?

$$\dfrac{55.7\ mol\ H_2 \left| \dfrac{2\ mol\ H_2O}{2\ mol\ H_2} \right.}{} = \underline{55.7}\ mol\ H_2O$$

9. If enough H_2O is reacted to produce 3.40 moles of H_2, then how may moles of O_2 must have been made?
(a bit challenging, but just think about it and you can probably figure it out)

$$\dfrac{3.40\ mol\ H_2 \left| \dfrac{1\ mol\ O_2}{2\ mol\ H_2} \right.}{} = \underline{1.70}\ mol\ O_2$$

$$2\ KClO_3 \rightarrow 2\ KCl\ +\ 3\ O_2$$
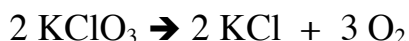
10. How many **grams** of O_2 will be formed from 3.76 grams of $KClO_3$?

3.76g $KClO_3$	1 mol $KClO_3$	3 mol O_2	32.00 g O_2	= 1.47 g O_2
	122.55 g $KClO_3$	2 mol $KClO_3$	1 mol O_2	

11. How many **grams** of $KClO_3$ are needed to make 30.0 grams of KCl?

30.0 g KCl	1 mol KCl	2 mol $KClO_3$	122.55 g $KClO_3$	= 49.3 g $KClO_3$
	74.55 g KCl	2 mol KCl	1 mol $KClO_3$	

12. How many grams of KCl will be formed from 2.73 g of $KClO_3$?

2.73 g $KClO_3$	1 mol KCl O_3	2 mol KCl	74.55 g	= 1.66 g KCl
	122.55 g $KClO_3$	2 mol KCl O_3	1 mol KCl	

$$4\ Fe\ +\ 3\ O_2 \rightarrow 2\ Fe_2O_3$$
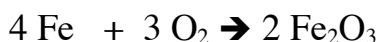
13. How many **grams** of Fe_2O_3 are produced when 42.7 **grams** of Fe is reacted?

42.7 g Fe	1 mole Fe	2 mol Fe_2O_3	159.70 g Fe_2O_3	= 61.0 g Fe_2O_3
	55.85 g Fe	4 mol Fe	1 mol Fe_2O_3	

14. How many **grams** of Fe_2O_3 are produced when 17.0 grams of O_2 is reacted?

17.0 g O_2	1 mol O_2	2 mol Fe_2O_3	159.70 g Fe_2O_3	= 56.6 g Fe_2O_3
	32.00 g O_2	3 mol O_2	1 mol Fe_2O_3	

15. How many grams of O_2 are needed to react with 125 grams of Fe?

125 g Fe	1 mol Fe	3 mol O_2	32.00 g O_2	= 53.7 g O_2
	55.85 g Fe	4 mol Fe	1 mol O_2	

Some cars can use butane (C_4H_{10}) as fuel:

$$2\ C_4H_{10}\ +\ 13\ O_2 \rightarrow 8\ CO_2\ +\ 10\ H_2O$$

16. How many grams of CO_2 are produced from the combustion of 100. grams of butane?

100. g C_4H_{10}	1 mol C_4H_{10}	8 mol CO_2	44.01 g CO_2	= 303 g CO_2
	58.14 g C_4H_{10}	2 mol C_4H_{10}	1 mol CO_2	

17. How many grams of O_2 are needed to react with of 100. grams of butane?

100. g C_4H_{10}	1 mol C_4H_{10}	13 mol O_2	32.00 g O_2	= 358 g O_2
	58.14 g C_4H_{10}	2 mol C_4H_{10}	1 mol O_2	

18 How many grams of H_2O are produced when 5.38g of O_2 is reacted?

5.38g O_2	1 mol O_2	10 mol H_2O	18.02 g H_2O	= 2.33 g H_2O
	32.00 g O_2	13 mol O_2	1 mol H_2O	

Chapter 6 Balancing and Stoichiometry Worksheet and Key

Topics:
- Balancing Equations
- Writing a chemical equation
- Stoichiometry

Practice:

1. **In the reaction: 4Li (s) + O_2 (g) → 2Li_2O (s)**

    a. what is the product?

    b. what are the reactants?

    c. what does the "(s)" after the formula of lithium oxide signify?

    d. what is the coefficient of the lithium metal?

    e. in what phase is the lithium oxide?

2. Define "chemical reaction".

3. List the observations that are evidence of a chemical reaction:

4. *Write and balance the chemical equation that relates to each of the following word equations:*
Remember that some elements exist as diatomic molecules (oxygen, nitrogen, hydrogen, halogens).
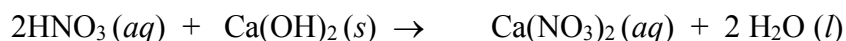a. solid zinc metal + oxygen gas → solid zinc oxide

b. HCl (*aq*) + magnesium hydroxide (*aq*) → magnesium chloride (*aq*) + water
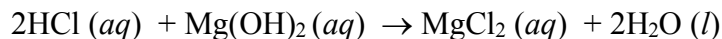
c. HNO_3 (*aq*) + calcium hydroxide (s) → calcium nitrate (*aq*) + water

5. *Balancing and Stoichiometry:*

a. $H_2 + Cl_2 \rightarrow HCl$ (needs balanced)

How many grams of HCl can be produced if 7.25 g of Cl_2 is reacted with an unlimited supply of H_2?

b. $Al + Fe_2O_3 \rightarrow Al_2O_3 + Fe$ (needs balanced)

How many grams of Fe can be produced when 10.0g of Al is reacted with an excess (unlimited) supply of Fe_2O_3?

c. $Pb(CH_3COO)_2 + H_2S \rightarrow PbS + CH_3COOH$ (needs balanced)

How many grams of PbS is produced when 5.00g of H_2S is reacted with an excess (unlimited) supply of $Pb(CH_3COO)_2$?

SEE NEXT PAGE FOR KEY

Chapter 6 Balancing and Stoichiometry Worksheet

Topics:
- Balancing Equations
- Writing a chemical equation
- Stoichiometry

Practice:

1. **In the reaction: 4Li (s) + O_2 (g) → 2 Li_2O(s)**
   a. what is the product?
   Li_2O (s)
   b. what are the reactants?
   Li (s) O_2 (g)
   c. what does the "(s)" after the formula of lithium oxide signify?
   phase = solid
   d. what is the coefficient of the lithium metal?
   4
   e. in what phase is the lithium oxide?
```` ``` ````   **solid**

2. Define "chemical reaction".

   Ionic or covalent bonds are made and/or broken, and a new substance is made.

3. List the observations that are evidence of a chemical reaction:

   A color change, the formation of a new phase, a new odor, a temperature change, the emission light, or the appearance of a flame.

4. Write and balance the chemical equation that relates to each of the following word equations:
Remember that some elements exist as diatomic molecules (oxygen, nitrogen, hydrogen, halogens).
a. solid zinc metal + oxygen gas → solid zinc oxide

   2Zn *(s)* + O_2 *(g)* → 2 ZnO *(s)*

b. HCl *(aq)* + magnesium hydroxide *(aq)* → magnesium chloride *(aq)* + water

   2HCl *(aq)* + $Mg(OH)_2$ *(aq)* → $MgCl_2$ *(aq)* + 2H_2O *(l)*

c. HNO_3 *(aq)* + calcium hydroxide (s) → calcium nitrate *(aq)* + water

   2HNO_3 *(aq)* + $Ca(OH)_2$ *(s)* → $Ca(NO_3)_2$ *(aq)* + 2 H_2O *(l)*

5. Balancing and Stoichiometry:
a. $H_2 + Cl_2 \rightarrow$ **2** HCl (needs balanced)

How many grams of HCl can be produced if 7.25 g of Cl_2 is reacted with an unlimited supply of H_2?

$$\frac{7.25 \text{ g } Cl_2}{} \; \bigg| \; \frac{1 \text{ mol } Cl_2}{70.90 \text{ g } Cl_2} \; \bigg| \; \frac{2 \text{ mol HCl}}{1 \text{ mol } Cl_2} \; \bigg| \; \frac{36.46 \text{ g HCl}}{1 \text{ mol HCl}} = \underline{7.46} \text{ g HCl}$$
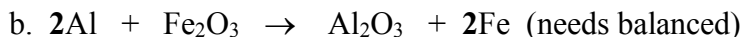
b. **2**Al + $Fe_2O_3 \rightarrow Al_2O_3$ + **2**Fe (needs balanced)

How many grams of Fe can be produced when 10.0g of Al is reacted with an excess (unlimited) supply of Fe_2O_3?

$$\frac{10.0 \text{ g Al}}{} \; \bigg| \; \frac{1 \text{ mol Al}}{26.98 \text{ g Al}} \; \bigg| \; \frac{2 \text{ mol Fe}}{2 \text{ mol Al}} \; \bigg| \; \frac{55.85 \text{g Fe}}{1 \text{ mol Fe}} = \underline{20.7} \text{ g Fe}$$

c. $Pb(CH_3COO)_2 + H_2S \rightarrow PbS$ + **2**CH_3COOH (needs balanced)

How many grams of PbS is produced when 5.00 g of H_2S is reacted with an excess (unlimited) supply of $Pb(CH_3COO)_2$?

$$\frac{5.00 \text{ g}}{} \; \bigg| \; \frac{1 \text{ mol } H_2S}{34.09 \text{ g } H_2S} \; \bigg| \; \frac{1 \text{ mol PbS}}{1 \text{ mol } H_2S} \; \bigg| \; \frac{239.27 \text{ g}}{1 \text{ mol PbS}} = \underline{35.1} \text{ g PbS}$$

Classes of Organic Reactions

1) Hydrogenation: Reduction of Alkenes

- Alkenes and other unsaturated hydrocarbons undergo a reduction reaction hydrogenation, in which hydrogen gas (H_2) in the presence of a catalyst, acts as a reducing agent.

Alkene → **Alkane**

- Example:
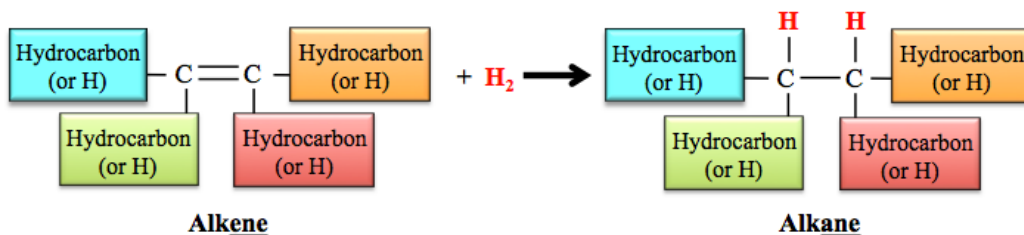
3-methyl-3-heptene → **3-methylheptane**
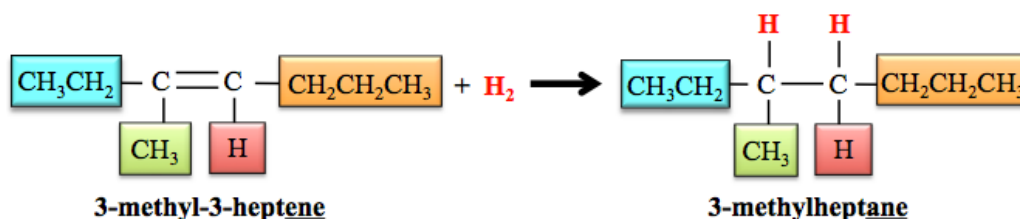
2) Hydrolysis of Esters

- The hydrolysis of an ester produces a *carboxylic acid* and an *alcohol* molecule.

ester + **H_2O** → **carboxylic acid** + **alcohol**
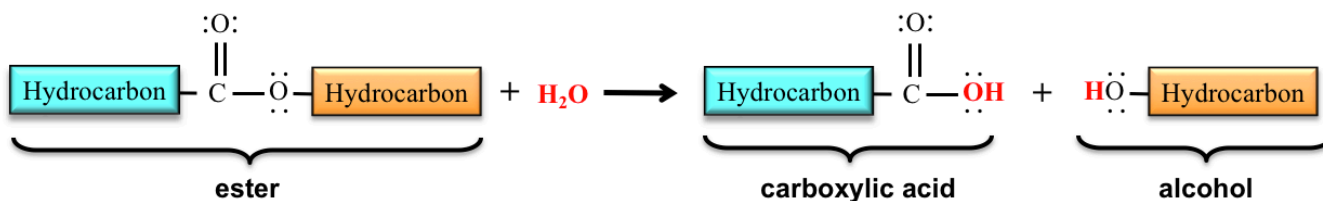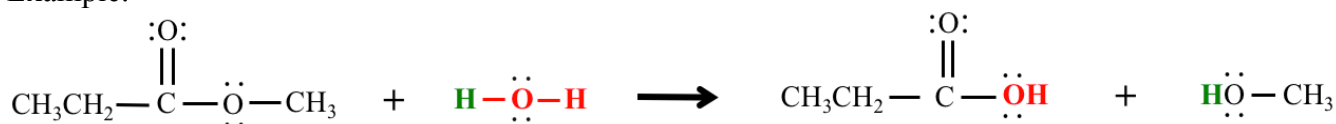
Example:

3) Hydration of Alkenes

In a hydration reaction, H_2O is added "across" a double bond in an alkene to produce an alcohol.
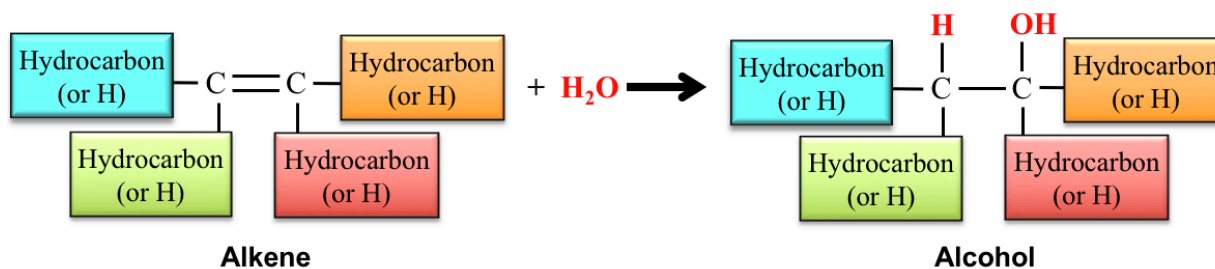
Example:
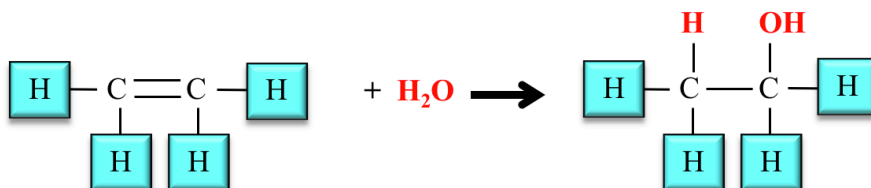
4) Dehydration of Alcohols

Dehydration is the reverse of hydration.

- Water (H_2O) is removed from an alcohol to form an alkene.

Example:

$$CH_3 - CH = CH - CH_2CH_3 + \text{ H-O-H}$$
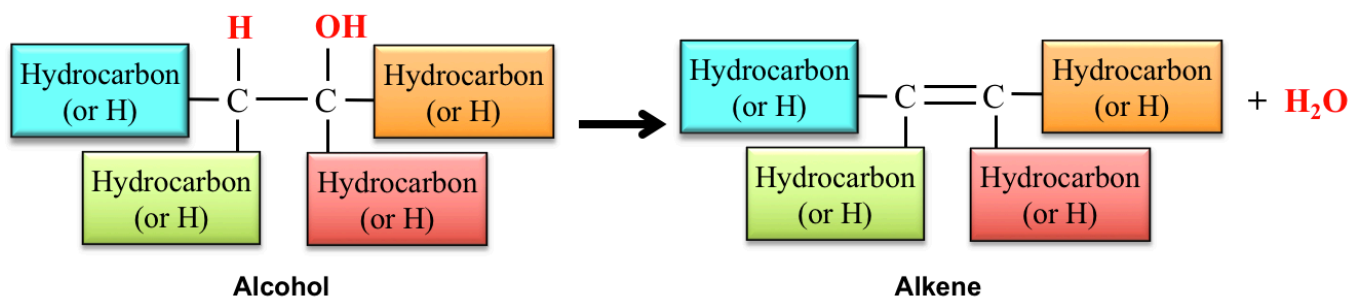
Combustion Reactions

- Hydrocarbons undergo combustion (react with oxygen O_2) to produce CO_2 (g) $+ H_2O$ (g)

$$C_xH_y + O_2 (g) \rightarrow CO_2 (g) + H_2O (g)$$
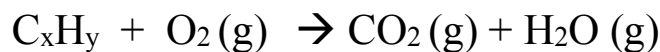
- Example: combustion of methane

$$CH_4 + 2\ O_2 (g) \rightarrow CO_2 (g) + 2\ H_2O (g)$$

Problems

Complete the following reactions:
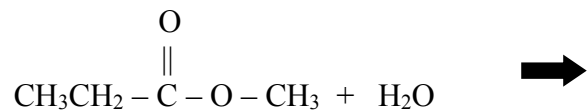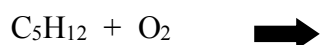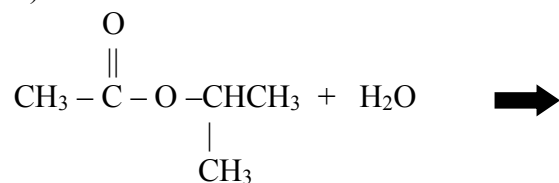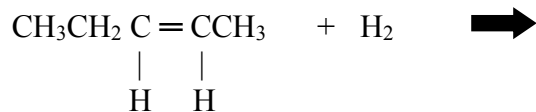
1)

$$
\begin{array}{c}
O \\
\| \\
CH_3CH_2 - C - O - CH_3 \ + \ H_2O
\end{array}
$$
➡

2) Complete and balance

$C_5H_{12} \ + \ O_2$ ➡

3)

$$
\begin{array}{c}
O \\
\| \\
CH_3 - C - O - CHCH_3 \ + \ H_2O \\
\qquad\qquad | \\
\qquad\qquad CH_3
\end{array}
$$
➡

4)

$$
CH_3CH_2 \ \underset{\substack{| \\ H}}{C} = \underset{\substack{| \\ H}}{C} CH_3 \quad + \ H_2
$$
➡

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

5)

 + H₂ ➡

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

6)

$$
\begin{array}{c}
OH \\
| \\
CH_3CH \ CH_3
\end{array}
$$
➡ $\qquad$ + $\qquad$ H_2O

7)

$$CH_3CH_2 \ C = C \ CH_2CH_3 \quad + \quad H_2O$$
$$\qquad\quad | \quad | $$
$$\qquad\quad H \quad H$$

8) Dehydration:

$$OH$$
$$|$$
$$CH_3 \ CH_2CH \ CH_2CH_3$$

9) Dehydration:

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

10)

 $\quad + \quad H_2O$
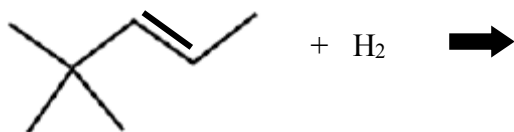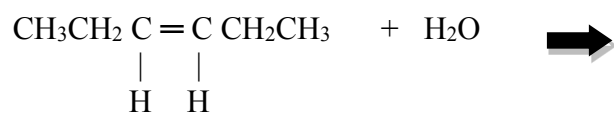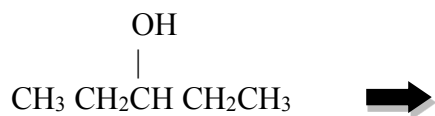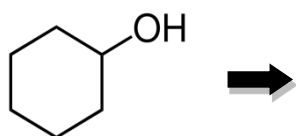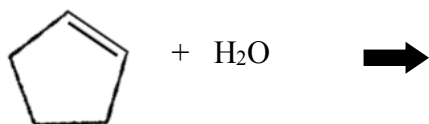
SEE NEXT PAGE FOR KEY

Chapter 6 Reactions Worksheet and Key

KEY

Complete the following reactions:
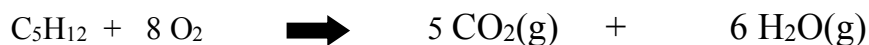
1)

$$
\begin{array}{c}
\quad\quad\quad O \\
\quad\quad\quad \parallel \\
CH_3CH_2 - C - O - CH_3 + H_2O
\end{array}
\quad\longrightarrow\quad
\begin{array}{c}
\quad\quad\quad O \\
\quad\quad\quad \parallel \\
CH_3CH_2 - C - OH + CH_3OH
\end{array}
$$

2) Complete and balance

$$C_5H_{12} + 8\,O_2 \quad\longrightarrow\quad 5\,CO_2(g) + 6\,H_2O(g)$$

3)

$$
\begin{array}{c}
\quad\quad O \\
\quad\quad \parallel \\
CH_3 - C - O - CHCH_3 + H_2O \\
\quad\quad\quad\quad\quad | \\
\quad\quad\quad\quad\quad CH_3
\end{array}
\quad\longrightarrow\quad
\begin{array}{c}
\quad\quad O \\
\quad\quad \parallel \\
CH_3 - C - OH \quad + \quad HO - CHCH_3 \\
\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad | \\
\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad CH_3
\end{array}
$$

4)

$$
\begin{array}{c}
CH_3CH_2\, C = CCH_3 \quad + \quad H_2 \\
\quad\quad\quad\quad | \quad | \\
\quad\quad\quad\quad H \quad H
\end{array}
\quad\longrightarrow\quad
CH_3CH_2CH_2CH_2CH_3
$$

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

5)

$$+ \; H_2 \quad\longrightarrow$$

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

6)

$$
\begin{array}{c}
\quad\quad OH \\
\quad\quad | \\
CH_3CH\, CH_3
\end{array}
\quad\longrightarrow\quad
CH_2 = CH\, CH_3 + \quad H_2O
$$
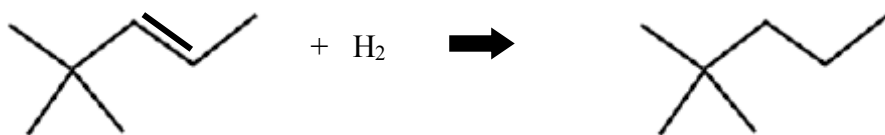
Note $CH_2 = CHCH_3$ is the exact same molecule as $CH_3CH = CH_2$ so either one is correct here!
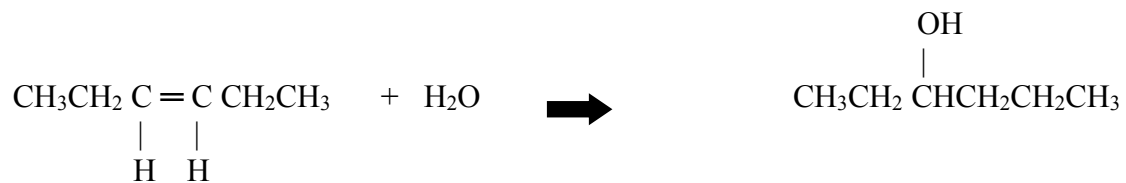
7)

$$CH_3CH_2\ C=C\ CH_2CH_3\quad+\quad H_2O\qquad\longrightarrow$$

with H and H below the double bond carbons.

$$\overset{\displaystyle OH}{\underset{\displaystyle |}{}}$$
$$CH_3CH_2\ \overset{|}{C}HCH_2CH_2CH_3$$

8) Dehydration:

$$\overset{\displaystyle OH}{\underset{\displaystyle |}{}}$$
$$CH_3\ CH_2\overset{|}{C}HCH_2CH_3\qquad\longrightarrow\qquad CH_3CH=CHCH_2CH_3\quad+\quad H_2O$$

9) Dehydration:

Hint: If you are struggling with this one, draw the line bond structure of the reactant first!

10)
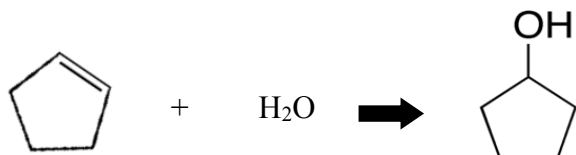
Chapter 7 Lecture Notes: Solutions, Colloids, and Suspensions

Educational Goals

1. Compare and contrast **mixtures** and **pure substances**.

2. Understand, compare, and contrast the terms **homogeneous mixture** and **heterogeneous mixture**. For a homogeneous mixture, explain the difference between **solute(s)** and **solvent**.

3. Predict the effect of temperature and pressure on the **solubility** of gases in water and the effect of temperature on the solubility of solids in water.

4. Be able to use the **Solubility Rules Table** to determine if an ionic compound will significantly dissolve in water.

5. Predict whether a **precipitation reaction** will occur when two specified aqueous solutions of ionic compounds are mixed; if a precipitation reaction will occur, write a balanced chemical equation for the reaction.

6. Compare the relative solubilities of organic molecules based on the functional groups or the relative sizes of the hydrocarbon (nonpolar) regions.

7. Explain, compare, and contrast the terms **hydrophilic**, **hydrophobic**, and **amphipathic**, and give examples of compounds that belong to each category.

8. Be able to calculate the **concentration** of a solution using various concentration units of measurements (%, parts per thousand, ppm, ppb, molarity, molality, osmolality, osmolarity, and Eq/L).

9. Given the concentration, be able to convert from the volume of solution to the amount of solute (and vice versa).

10. Given a solution's initial concentration, be able to use the **dilution equation** to determine the concentration of the solution after dilution.

11. Compare and contrast **solutions**, **suspensions**, and **colloids**.

12. Describe the processes of **diffusion** and **osmosis**. Define **osmotic pressure** and predict the effect of solute concentration on the osmotic pressure.
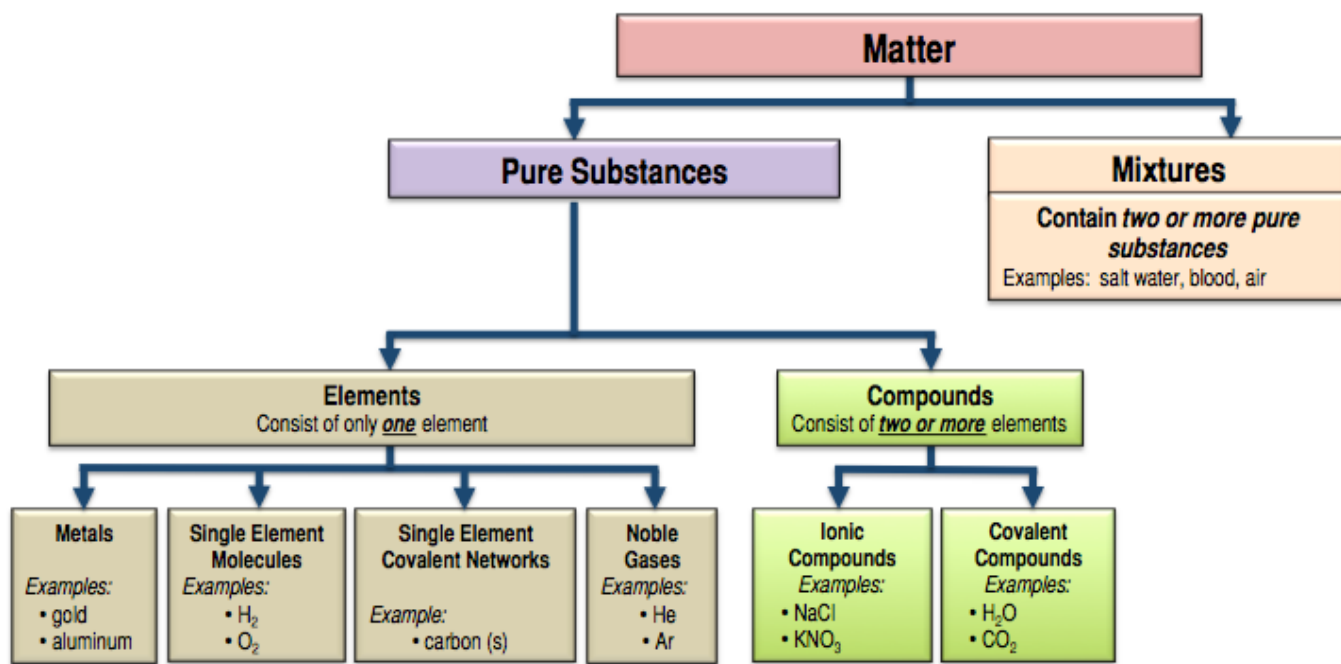
Most matter on earth is **not** composed of just one pure substance.

When *two or more pure substances* are combined, we refer to the combination as a _____.

In this chapter, you will learn about **three** types of *mixtures*:

1) **solutions**
2) **colloids**
3) **suspensions**

Macro-Scale Classification of Mixtures: Homogeneity

One way in which mixtures are classified is by their macro-scale, *visually* observed **homogeneity**.

A _____ *mixture* appears to be the same throughout the entire sample/object.

  o   Example: Sugar dissolved in water

A _____ *mixture* has visible regions of varying composition.

  a. Example: A chocolate chip cookie

Introduction to Solutions

_____ are **mixtures of pure substances** in which the pure substance particles (molecules, ions, or noble gas atoms) are _____ distributed throughout the entire volume of the mixture.

The pure substance that is in the **greatest abundance** is referred to as the _____.

- Typically, especially in biological systems, *the solvent is water*.

The other pure substance components of a solution are called _____.

With very few exceptions, the solution takes the same *physical phase* (gas, liquid, or solid) as the *solvent*.

The *solutes* are said to be "_____" in the *solvent*.

2

Solutions can be **gas-phase**, **liquid-phase**, or **solid-phase**.

An example of a **gas-phase solution** is air.

- Air is a mixture of several gases, mostly nitrogen, oxygen, and carbon dioxide.

An example of a **solid-phase solution** is brass.

- Brass is a mixture of copper and zinc. When one solid (such as zinc) is evenly dispersed in another solid (such as copper), the solid solution is called an _____.

We will focus on **liquid-phase solutions** for the remainder of this course.

- There are 3 types of *liquid-phase solutions:*

  - ***Gas*** *dissolved in a **liquid*** solvent

    - An example of a ***gas dissolved in a liquid solvent*** is CO_2 dissolved in water; this is how beverages are carbonated. Another example of a gaseous solute dissolved in liquid is O_2 dissolved in water; fish extract the O_2 from water using their gills. Whenever a gas is present above a liquid, some of the gas will dissolve in the liquid.

  - ***Liquid*** *dissolved in a **liquid*** solvent

    - An example of a ***liquid dissolved in a liquid solvent*** is ethyl alcohol dissolved in water; this is the basis of adult beverages.

  - ***Solid*** *dissolved in a **liquid*** solvent

    - An example of a ***solid dissolved in a liquid solvent*** is table salt (NaCl) or table sugar (sucrose molecules) in water.

Almost all of the solutions used in biological applications, such as in biomedical analytical labs and research labs, are *liquid-phase solutions*.

For the remainder of this course, I will use the term **solution** to mean **liquid-phase solution.**

Understanding Check

If the following pairs of pure substances are mixed in the ratios given to form solutions, identify each substance as either **solvent** *or* **solute**:

a) 5 grams of sodium chloride and 100 grams of water

b) 10 mL of ethyl alcohol and 250 mL of water

c) 100 mL of acetone and 10 mL of water

The Dissolution Process: Solvation

Another term for "*dissolving*" is _____.

In liquid and solid phase solutions, the solute and solvent particles are _____ to each other by one or more of the five types of *noncovalent interactions*.

The stronger the **solute-solvent** interactions, the more *solute* that can be dissolved.

The Dissolution of Ionic Compounds

Example: The dissolution of sodium chloride in water.

When ionic compounds dissolve, the ions _____ (become separated from each other) and enter the liquid phase solution.

● = H₂O molecule
● = Na⁺ ion
● = Cl⁻ ion

Dissolution

Sodium Chloride Crystal   **Dissolved Sodium Chloride, NaCl (aq)**
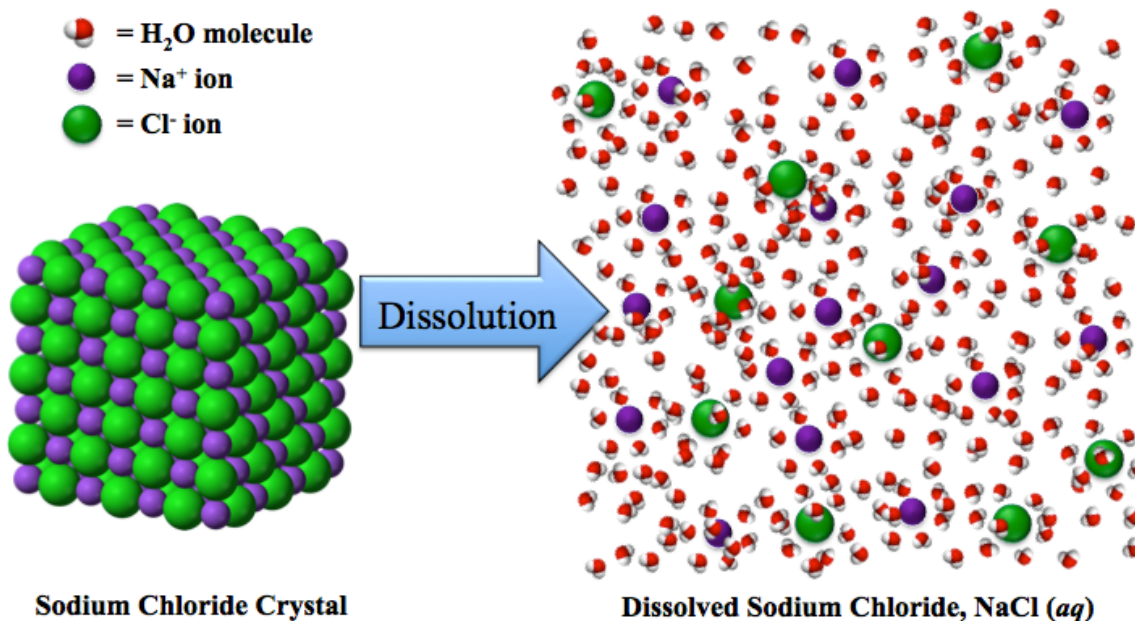
The water molecules and ions are attracted to each other through *ion-dipole forces*.

The *partially negatively-charged ends* of several water molecule dipoles are attracted to the *positive charge* of each sodium.
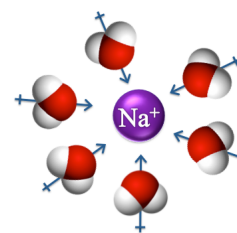
Likewise, the *partially positively-charged ends* of several water molecule dipoles are attracted to the *negative charge* of each chloride ion.
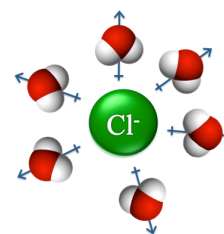
We use the term _____ to describe a *solute* particle becoming surrounded by *solvent* molecules.

Solvation causes dissolution of the solute.

The Dissolution of Molecules

Molecules will dissolve in a particular solvent when the **solute-solvent** noncovalent interactions are strong enough to overcome the solute-solute interactions.

Unlike ionic compounds that ***dissociate***, when molecules dissolve, the _____ _____ become ***solvated***.

Example: The dissolution of ethyl alcohol in water.

Ethyl alcohol dissolves in water because it has significantly strong noncovalent interactions with water.

These **solute-solvent** intermolecular forces enable the solvation of ethyl alcohol molecules by water molecules as illustrated in below.
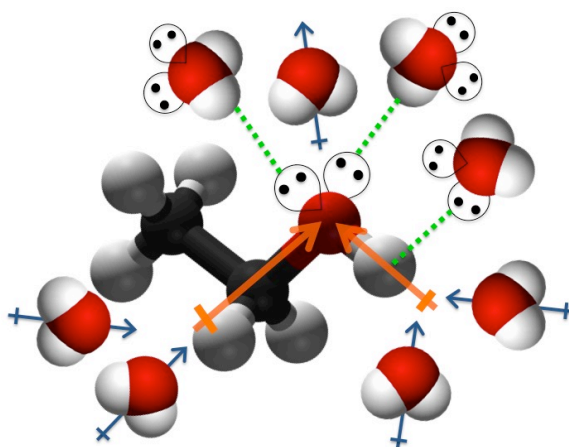
All *three* of the intermolecular forces (hydrogen bonding, dipole-dipole forces, and London forces) occur between ethyl alcohol and water.

Since water molecules are relatively small, the London forces between water and ethyl alcohol are not very strong; if they were the only intermolecular forces present, ethyl alcohol would not dissolve in water.

Since ethyl alcohol *and* water are *polar molecules*, they can also interact through dipole-dipole forces.

- The dipoles of ethyl alcohol's **highly-polar bonds** are indicated by arrows on top of the ethanol structure, and water's molecular dipoles are indicated by dipole arrows behind the water molecules.

Because of the relatively small size of solvated molecules and ions, the forces imparted upon them from *collisions* with solvent molecules are much greater than the force of gravity.

It is for this reason that solvated ions and molecules do not settle to the bottom of a mixture, but instead, move in random directions in-between collisions.

This type of random, chaotic movement is called **Brownian motion** and results in the solute being ***evenly dispersed*** within the solvent.

Since ions and molecules are **evenly dispersed** within the solvent, ***solutions are*** _____.

S*olutes* that are polar are capable of dissolving in polar *solvents*.

S*olutes* that are nonpolar are capable of dissolving in nonpolar *solvents*.

This phenomenon is summarized in the easily-remembered phrase,
"*like dissolves like.*"

Understanding Check

If you dissolved ***one mole*** of the following substances in water, how many moles of solvated ions would be present (include both cations and anions in the number of moles of solvated ions)?

     a. NaCl

     b. $BaCl_2$

Understanding Check

List ***all*** of the **noncovalent interactions** that can occur *between solute and solvent* for each of the following solutions:

     a. oxygen gas dissolved in water

     b. carbon dioxide gas dissolved in water

     c. potassium iodide dissolved in water

     d. pentane dissolved in octane

Solubility

Solubility is a term that refers to th*e* _____ *of solute* that can be dissolved.

Some *liquid-in-liquid* solutions can be made at _____ ratio of the liquids.
- For example, water and ethyl alcohol will mix no matter what the ratio is of water to ethyl alcohol.

When two liquids mix with each other in *any* ratio, we say that the substances are "_____."

Some pairs of liquids *will not* mix with each other at all.
- For example, oil will not significantly dissolve in water.
- This is why we see oil floating on the top of water when oil spills occur.

When two liquids *will not mix* with each other we say that the substances are "_____."

For most solute/solvent pairs, there is a limit on how much solute can dissolve in a particular solvent.
a) For example, you can only dissolve so much salt or sugar in water.

At some point, the solution becomes _____ and the amount of dissolved solute cannot increase.

If you continue to add a solid solute to a **saturated solution**, *the excess solute will exist as a solid* in the container.

The Solubility of *Gases* in Water

The solubility of a ***dissolved gas*** depends on *both* _____ and _____.

Whenever a gas is present above a liquid, some of the gas will dissolve in the liquid.

The higher the partial pressure of a particular gas above a liquid, the more of that gas will dissolve in the liquid.

William Henry was first to report that the amount of gas dissolved in a liquid is directly proportional to the *partial pressure* of the gas.

This relationship between the amount of gas dissolved and pressure is known as "Henry's Law."

William Henry

The **lower** the _____ of the aqueous solutions, the **greater** the *solubility of gases*.
- For example, cold water can dissolve more oxygen than warm water.

The Solubility of *Solids* in Water

The solubility of a _____ *solute* depends on _____.
- As the temperature of water increases to its normal boiling point (100°C), the solubility of most *solid* solutes _____.

Notice that this is the _____ of the behavior of ***gaseous*** solutes.

The Solubility of *Ionic Compounds* in Water

Some ionic compounds dissolve to a significant extent in water; some do not.

Ionic compounds that **do not** significantly dissolve are categorized as "*water* _____."

• *Water insoluble* compounds exist in their crystal/solid form when placed in water.

Ionic compounds that dissolve to a significant extent are classified as "*water* _____."

It is convenient to use "**solubility rules**" in order to know which ionic compounds are *water soluble* and which ones are *water insoluble*.

In this table, ionic compounds are first classified as *water soluble* or *water insoluble* based on their _____, and then exceptions are listed.

Solubility Rules Table			
Water Soluble			
Compound	**Example**	**Exceptions**	**Exception Example**
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	$NaCl$	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	$AgCl$
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	**Example**	**Exceptions**	**Exception Example(s)**
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals _or_ Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	$NaOH$
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals _or_ NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Example: Is KNO_3 water soluble?

Solution:

STEP 1: Find the solubility classification in the table based on *the identity of the anion*.

- We see that *nitrates* are in the **water soluble class**.

STEP 2: Check to see if the compound's *cation* causes the compound to be an **exception** for the solubility class.

- There are *no exceptions* for *nitrates*.

This means that *all nitrates are water soluble*, therefore KNO_3 is *water soluble*.

Solubility Rules Table			
Water Soluble			
Compound	Example	Exceptions	Exception Example
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	$NaCl$	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	$AgCl$
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	Example	Exceptions	Exception Example(s)
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals *or* Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	$NaOH$
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals *or* NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Example: Is $Cu(OH)_2$ water soluble?

Solution:

STEP 1: Find the solubility classification in the based on *the identity of the anion*.

- We see that *hydroxides* are in the **water insoluble class**.

STEP 2: Check to see if the *cation* causes the compound to be an **exception** for the solubility class.

- There are exceptions for hydroxides, however Cu^{2+} *is not* **one of them**.

Therefore $Cu(OH)_2$ is **not** *water soluble*.

- If $Cu(OH)_2$ were mixed with water, it would exist as solid crystals submerged in water.

Solubility Rules Table			
Water Soluble			
Compound	Example	Exceptions	Exception Example
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	$NaCl$	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	$AgCl$
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	Example	Exceptions	Exception Example(s)
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals *or* Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	$NaOH$
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals *or* NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Example: Is $BaSO_4$ water soluble?

Solution:

STEP 1: Find the solubility classification in the table based on *the identity of the anion*.

- We see that *sulfates* are in the **water soluble class**.

STEP 2: Check to see if the *cation* causes the compound to be an **exception** for the solubility class.

- There are some exceptions for sulfates and Ba^{2+} *is one of them*.

Therefore $BaSO_4$ is **not** *water soluble*.

Solubility Rules Table			
Water Soluble			
Compound	Example	Exceptions	Exception Example
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	$NaCl$	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	$AgCl$
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	Example	Exceptions	Exception Example(s)
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals *or* Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	$NaOH$
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals *or* NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Example: Is KOH water soluble?

Solution:

STEP 1: Find the solubility classification in the table based on *the identity of the anion*.

- We see that *hydroxides* are in the **water insoluble class**.

STEP 2: Check to see if the *cation* causes the compound to be an **exception** for the solubility class.

- There are exceptions for hydroxides, and K^+ *is one of them*; it's an alkali (Group I) metal.

Therefore KOH is *water soluble*.

Solubility Rules Table			
Water Soluble			
Compound	Example	Exceptions	Exception Example
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	NaCl	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	AgCl
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	Example	Exceptions	Exception Example(s)
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals *or* Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	NaOH
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals *or* NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Understanding Check

Determine which of the following compounds is water soluble.

a. potassium iodide

b. iron(II) nitrate

c. copper(II) hydroxide

d. silver bromide

e. sodium sulfate

f. potassium hydroxide

g. lead(II) chromate

h. ammonium hydroxide

Solubility Rules Table			
Water Soluble			
Compound	Example	Exceptions	Exception Example
Nitrates	$NaNO_3$	None	None
Chlorides, Bromides, and Iodides	NaCl	Compounds containing Ag^+, Pb^{2+}, or Hg^+, and HgI_2	AgCl
Sulfates	K_2SO_4	Compounds containing Pb^{2+}, Sr^{2+}, Ba^{2+}, or Hg^+	$PbSO_4$
Water Insoluble			
Compound	Example	Exceptions	Exception Example(s)
Hydroxides	$Mg(OH)_2$	Compounds containing alkali (Group I) metals *or* Ca^{2+}, Sr^{2+}, Ba^{2+}, NH_4^+	NaOH
Phosphates, Carbonates, and Chromates	$FePO_4$	Compounds containing alkali (Group I) metals *or* NH_4^+	K_2CO_3, Li_3PO_4, Na_2CrO_4

Electrolytes

Solutions that contain dissolved *ions* are capable of conducting electricity and are sometimes referred to as _____ *solutions*.

- Dissolved ionic compounds are called *electrolytes*.

Electrolyte solutions are required in biological functions such as the transmission of nerve impulse signals and muscle actuation.

Our bodies obtain electrolytes from food and drink.

Reactions of Ions in Aqueous Solutions

In a **double replacement reaction**, two substances "_____ *partners*."

The general form of a double replacement reaction, where compounds **AX** and **BY** *switch partners*, is:

$$AX + BY \rightarrow AY + BX$$
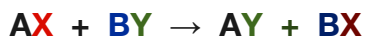
There are two types of double replacement reactions:

1) **Precipitation Reactions**
2) **Gas Producing Reactions**

1) Precipitation Reactions

Precipitation reactions may occur when **_two_** solutions that contain _____ *ions* are mixed.

In a precipitation reaction, two compounds in aqueous solution appear to exchange _____.

If one of the new pairs formed is_____ a new substance (solid/precipitate) is formed.

For a precipitation reaction to occur, at least one of the _____ formed is insoluble in water.

- Therefore, a **solid** is *always* formed in a precipitation reaction.
  - Often, many *tiny* crystals are formed and this gives the mixture a cloudy appearance. The cloudy appearance may be white, black, or some other color, depending on the identity of the particular solid that is formed.
  - We say the solid "***precipitated***" from the solution.
  - The appearance of the solid precipitate indicates the formation of **new ionic bonds** and that a _____ has occurred.

The *educational goals* for **precipitation reactions** are:

Predict if a precipitation reaction will occur when two aqueous ionic compounds are combined.

Write the balanced chemical equation for the reaction.

Method for Predicting if a Precipitation Reaction will Occur and Writing the Balanced Chemical Equation for Precipitation Reactions.

Example: The reaction that was just demonstrated; the reaction of lead(II) nitrate and potassium chromate.

Step 1: Write **_reactants' names_** and arrow for the chemical equation using **_word form_** (not formulas):

    lead(II) nitrate + potassium chromate →

Step 2: Add the "*possible*" **products** to the word equation by switching **_anions_**:

    lead(II) nitrate + potassium chromate → lead(II) chromate + potassium nitrate
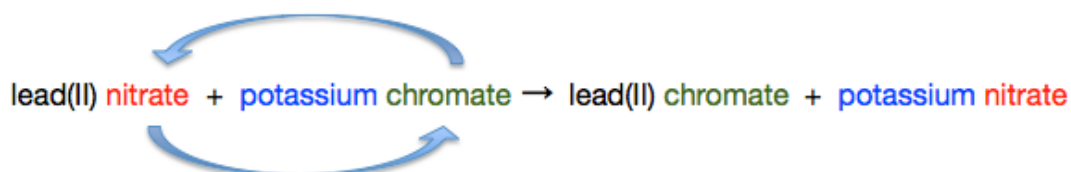
Step 3: Convert the **word** equation to a **_formula_** equation:

<p align="center">**lead(II) nitrate + potassium chromate → lead(II) chromate + potassium nitrate**</p>

$$Pb(NO_3)_2 + K_2CrO_4 \rightarrow PbCrO_4 + KNO_3$$

- **Note:** Students often need to review the section in chapter 3 that discusses naming ionic compounds in order to perform Step 3.

Step 4: ***Balance*** the equation:
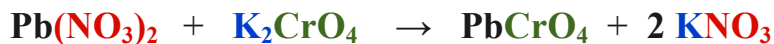
$$Pb(NO_3)_2 + K_2CrO_4 \rightarrow PbCrO_4 + 2\ KNO_3$$

Step 5: Add the ***phase*** of each of the reactants and "possible" products to the chemical equation.

- In all *precipitation reactions*, **the reactants are always aqueous**.
- Use the Solubility Rules Table to determine the phase of the "possible" products.
  - If a compound is water ***soluble***, it remains dissolved and we write "(*aq*)."
  - If a compound is water ***insoluble***, it precipitates as a solid and we write "(*s*)."

$$Pb(NO_3)_2\,(aq) + K_2CrO_4\,(aq) \rightarrow PbCrO_4\,(s) + 2\ KNO_3\,(aq)$$
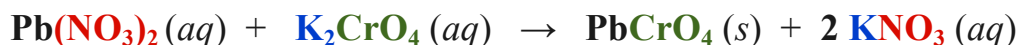
Example: The reaction of sodium chloride and silver nitrate.

Step 1: Write ***reactants' names*** and arrow for the chemical equation using ***word form*** (not the chemical formula).

<p align="center">sodium chloride + silver nitrate →</p>

Step 2: Add the "*possible*" **products** to the word equation by switching ***anions***.
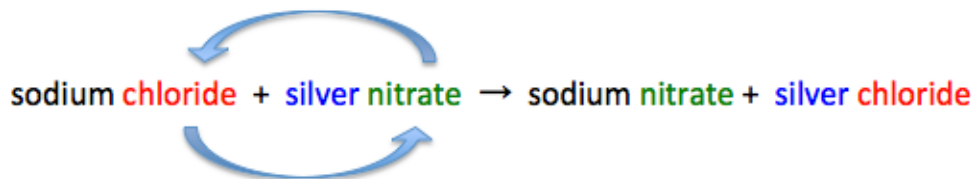
<p align="center">sodium chloride + silver nitrate → sodium nitrate + silver chloride</p>

Step 3: Convert the ***word*** equation to a ***formula*** equation.

$$NaCl + AgNO_3 \rightarrow NaNO_3 + AgCl$$

Step 4: ***Balance*** the equation:

- In this example, the equation is already balanced; each of the coefficients is "1."

$$NaCl + AgNO_3 \rightarrow NaNO_3 + AgCl$$

Step 5: Add the ***phase*** of each of the reactants and "possible" products to the chemical equation.

$$NaCl\,(aq) + AgNO_3\,(aq) \rightarrow NaNO_3\,(aq) + AgCl\,(s)$$
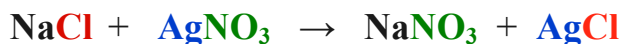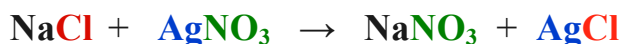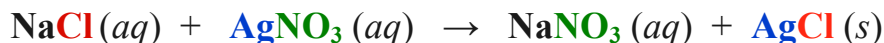
Example: Determine if a precipitation reaction would occur when a *sodium chloride solution* is mixed with a *potassium nitrate solution*.

Step 1: Write ***reactants' names*** and arrow for the chemical equation using ***word form*** (not formula):

<p align="center">sodium chloride + potassium nitrate →</p>

Step 2: Add the "*possible*" **products** to the word equation by switching *anions*:
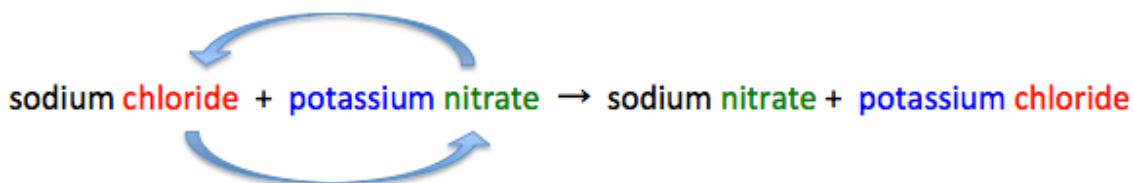
sodium chloride + potassium nitrate → sodium nitrate + potassium chloride

Step 3: Convert the *word* equation to a *formula* equation:

$$NaCl + KNO_3 \rightarrow NaNO_3 + KCl$$

Step 4: *Balance* the equation:
- In this example, the equation is already balanced; each of the coefficients is "1".

$$NaCl + KNO_3 \rightarrow NaNO_3 + KCl$$

Step 5: Add the *phase* of each of the reactants and "possible" products to the chemical equation.

$$NaCl\,(aq) + KNO_3\,(aq) \rightarrow NaNO_3\,(aq) + KCl\,(aq)$$
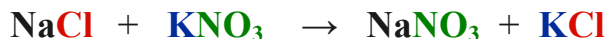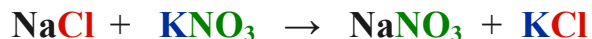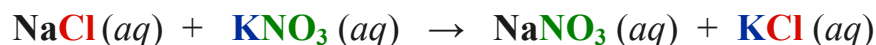
IMPORTANT: If **both** of the "possible" products *are water soluble*, then **no reaction occurred**.
- There were solvated cations and anions in each the two solutions before mixing, then the solutions were mixed and the cations and anions remained solvated in the mixture.
- No new chemical bonds were made, therefore no chemical reaction occurred.
- When no reaction occurs in precipitation reaction problems such as this example, you can write "No Reaction" instead of the "possible" products:

$$NaCl\,(aq) + KNO_3\,(aq) \rightarrow \textbf{No Reaction}$$

You try one: Determine if a precipitation reaction would occur when a silver nitrate solution is mixed with a barium chloride solution ___and___, if a reaction does occur, write the balanced chemical equation.

---

2) Gas Producing Double Replacement Reactions

A **gas producing double replacement reaction** is a special type of double replacement in which a gas is produced.

The gas producing double replacement reaction that is typically encountered in the health sciences field and, therefore the only gas producing reaction which I would like you to be familiar, is the reaction of aqueous hydrogen monochloride (**HCl**, also know as hydrochloric acid) and aqueous sodium bicarbonate (**NaHCO₃**).

$$HCl \; + \; NaHCO_3 \rightarrow HHCO_3 + NaCl$$
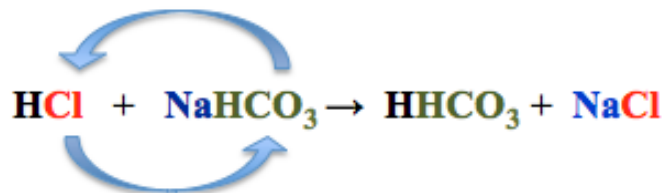
In this reaction, the ***bicarbonate*** and **chloride** anions switch partners to form aqueous ***carbonic acid*** (**HHCO₃**) and ***sodium chloride***.

- In the chemical equation ***above***, I wrote the formula of carbonic acid as **HHCO₃** in order to help you see how **Cl⁻** and **HCO₃⁻** "*switched partners*"; however the correct way to write the formula for carbonic acid is **H₂CO₃,** as described below.

$$HCl\,(aq) + NaHCO_3\,(aq) \rightarrow \boxed{HHCO_3}\,(aq) + NaCl\,(aq)$$

carbonic acid

$$HCl\,(aq) + NaHCO_3\,(aq) \rightarrow \boxed{H_2CO_3}\,(aq) + NaCl\,(aq)$$

Carbonic acid _____ to **H₂O** (*l*) and **CO₂**(*g*)

$$HCl\,(aq) + NaHCO_3\,(aq) \rightarrow \boxed{H_2O\,(l) + CO_2\,(g)} + NaCl\,(aq)$$

Gas Producing Double Replacement Reaction
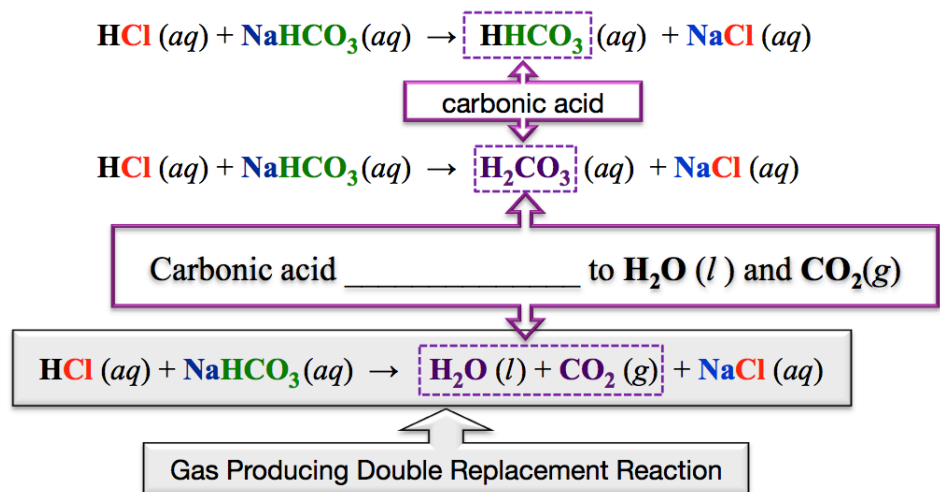
The overall gas producing double replacement reaction equation is written in the grey box on the right.

This particular gas producing reaction is important in medicine because sodium bicarbonate is used as an over-the-counter therapeutic agent to treat acid indigestion (heartburn).

- Sodium bicarbonate is the primary active ingredient in many antacids, such as alka-seltzer.
- Sodium bicarbonate "neutralizes" acid in the stomach to produce water, carbon dioxide gas, and salt.

You will learn much more about acids in later chapters.

14

The Solubility of Organic Molecules

Molecules will dissolve in a particular solvent when the **solute-solvent** noncovalent interactions are strong enough to _____ the solute-solute interactions.

The *more* **solute-solvent** noncovalent attractive interactions that can occur, the more solute that can be dissolved.

It is for this reason that *polar solutes* are capable of dissolving in *polar solvents*, and *nonpolar* solutes are capable of dissolving in *nonpolar solvents*, as summarized by the phrase "*like dissolves like*."

For an organic molecule to have significant **water solubility**, it must be _____ and/or capable of _____ _____ with water.

Dipole-Dipole

Electrostatic attractive force between *two polar molecules*.
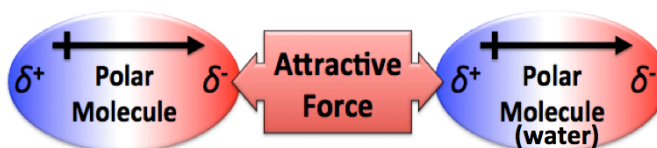
Hydrogen Bonding

Electrostatic attractive force between the partially positive charged hydrogen end of an O-H, N-H, or F-H bond and the negative charge of a lone pair on an O, F, or N.
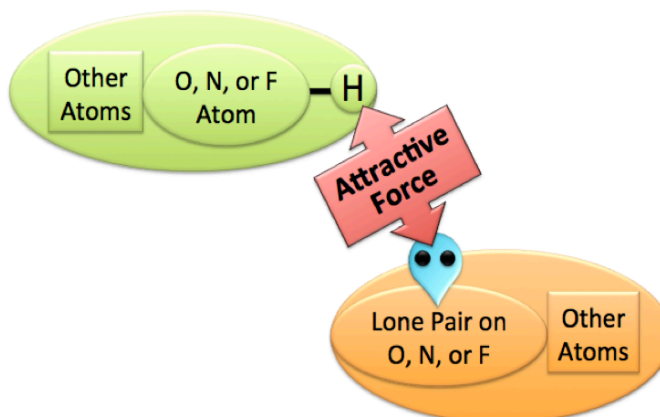
We can use the general rule of "**like dissolves like**" to predict the *relative water solubilities* of various organic solute molecules.

Let's consider the water solubility of the *organic molecule families* that I introduced you to in chapter 4: **hydrocarbons**, **alcohols**, **carboxylic acids**, and **esters**.

Water Solubility of Hydrocarbons

Hydrocarbons are _____ molecules.

They are **not** capable of *hydrogen bonding* or *dipole-dipole interactions*, therefore they are _____ significantly soluble in water.

Water Solubility of Alcohols, Carboxylic Acids, and Esters

Alcohols and many other families of organic molecules are attracted to water through hydrogen bonding and/or dipole-dipole interactions.

The *general form* of an **alcohol** molecule is: | Hydrocarbon |—$\ddot{\text{O}}$−H

As the _____ _____ of various alcohol molecules gets *larger, the water solubility* _____.

This trend of decreasing solubility as the hydrocarbon part of organic molecules gets larger is also seen in **carboxylic acids**, **esters**, and all of the other types of organic molecules that you will be introduced to in later chapters.

| Hydrocarbon |—$\overset{\displaystyle :\text{O}:}{\underset{\displaystyle ||}{\text{C}}}$−$\ddot{\text{O}}$−H

general form of a **carboxylic acid**
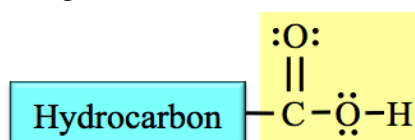
| Hydrocarbon |—$\overset{\displaystyle :\text{O}:}{\underset{\displaystyle ||}{\text{C}}}$−$\ddot{\text{O}}$—| Hydrocarbon |
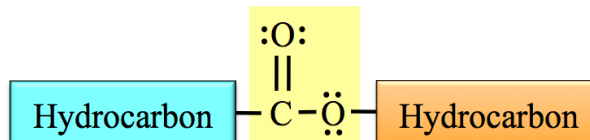
general form of an **ester**

As the hydrocarbon part of a molecule gets _____, London forces become more important (stronger), the molecule becomes _____ polar, and the organic molecules are *more attracted to each other* than they are to water molecules.

- When this occurs, it is *lower in energy* for the organic molecules to be surrounded by other organic molecules and therefore the water solubility drastically decreases.

The table below shows the trend in decreasing water solubility for some alcohol molecules as their hydrocarbon part gets larger.

Molecule Name	Condensed Structure	Solubility in Water
methanol	CH_3OH	miscible in any ratio with water
ethanol	CH_3CH_2OH	miscible in any ratio with water
1-propanol	$CH_3CH_2CH_2OH$	miscible in any ratio with water
1-butanol	$CH_3CH_2CH_2CH_2OH$	slightly soluble
1-pentanol	$CH_3CH_2CH_2CH_2CH_2OH$	insoluble

The Solubility of Organic Molecules in *Non Aqueous* Solutions

Not all solutions involve water as the solvent.

Non water *polar solvents* behave quite like water in regard to their ability to dissolve polar solutes better than nonpolar solutes.

On the other hand, *nonpolar solvents* dissolve *nonpolar* _____ more readily than polar solutes; *like dissolves like*.

- For example, *pentane* **cannot** be significantly dissolved in water, however it **can** be dissolved in *hexane*.

pentane

$$CH_3-CH_2-CH_2-CH_2-CH_3$$

hexane

$$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$$

16
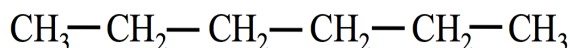
a. List the following carboxylic acids in order of *increasing solubility in water* (least soluble to most soluble).

$$CH_3CH_2CH_2CH_2CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OH$$

hexanoic acid

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OH$$

ethanoic acid

$$CH_3CH_2CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OH$$
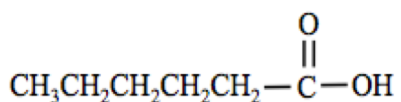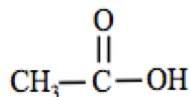
butanoic acid

- List the following esters in order of *increasing solubility in water*.

$$CH_3CH_2CH_2CH_2CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_2CH_3$$

ethyl hexanoate

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_2CH_3$$

ethyl ethanoate

$$CH_3CH_2CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_2CH_3$$
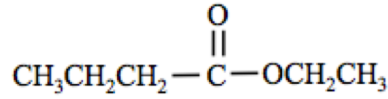
ethyl butanoate

Concentration of Solutions

The term "_____" refers to the *amount of a solute in a solution*.

Other *qualitative* (non numeric) descriptions of the amount of solute are sometimes used:
- A solution with a relatively large amount of solute is said to be "_____."
- A solution with a relatively small amount of solute is said to be "_____."

In this video you will see how to *quantitatively* (with numeric values) describe the *amount of solute that is present in a solution*.

The *concentration* of a solution is the _____ _____ of solute that is dissolved in a particular quantity of solution (or solvent).

Various Units Used for Concentration

Percent (%) Concentration

There are three different percent (%) concentration units that are commonly used:

> **percent weight to weight: % (w/w)**
> **percent volume to volume: % (v/v)**
> **percent weight to volume: % (w/v)**

Percent *Weight to Weight*

Percent *weight to weight* - % (w/w) - is defined as the ratio of the **mass** of the **solute** to the **mass** of the _____ _____, multiplied by **100**:

$$\% \text{ (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times 100$$

Example: A **10% (w/w)** sodium chloride solution contains *10 grams* of dissolved sodium chloride in every *100 grams of solution*.

Percent weight to weight is also referred to as "*mass percent*" or "*gram percent.*"

Percent *Volume to Volume*

Percent *volume to volume* - % (v/v) – is defined as the ratio of the volume of the *solute* to the volume of the *entire solution*, multiplied by **100**:

$$\% \text{ (v/v)} = \left(\frac{\text{volume of } solute}{\text{volume of } solution}\right) \times 100$$

Example: Percent volume to volume is commonly used to indicate the concentration of alcohol in adult beverages where % (v/v) is referred to as "*alcohol by volume* (ABV)" or "*alcohol percent by volume.*"

In this beer, there are **7.2 mL** of *alcohol* for every **100 mL** of *beer*
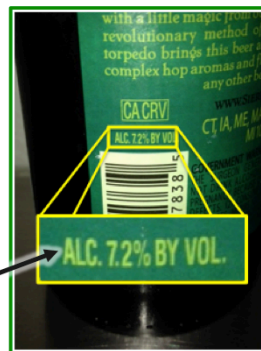
Percent *Weight to Volume*

Percent *weight to volume* - % (w/v) - is defined as the number of grams of *solute* contained in **100 mL** of *solution.*

% (w/v) is calculated by multiplying the ratio of the grams of the *solute* to the volume (mL) of the *entire solution*, by **100**.

$$\% \text{ (w/v)} = \left(\frac{\text{grams of } solute}{\text{mL of } solution}\right) \times 100$$

Example: Potassium iodide (KI) is used to treat iodine deficiencies. What is the %(w/v) of a 75 mL solution containing 2.0g of KI?

$$\% \text{ (Weight/Vol)} = \left(\frac{\text{grams of Solute}}{\text{mL of Solution}}\right) \times 100$$

$$\% \text{ (Weight/Vol)} = \left(\frac{2.0 \text{ g of KI}}{75 \text{ mL of Solution}}\right) \times 100$$

$$= \textbf{2.7 \% (w/v)}$$

Percent *Weight to Weight* Example

What is the % (w/w) concentration of a sodium chloride solution prepared by adding 5.0 grams of sodium chloride to 130.0 g of water?

Solution: Calculate the concentration using the equation/definition of % (w/w):

$$\% \text{ (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution}\right) \times 100$$

a. The mass of the *solute* (sodium chloride) was given: **5.0 g**
b. The mass of the *solution* is equal to the mass of the *solute* (NaCl, 5.0 g) *plus* the mass of the *solvent* (water, 130.0 g) = **135.0 g**

$$\% \text{ (w/w)} = \left(\frac{5.0 \text{ g}}{135.0 \text{ g}}\right) \times 100 = 3.7 \text{ \% (w/w)}$$

In a 3.7 % (w/w) solution, there are 3.7 g of *solute* contained in every 100 g of *solution*.

Note that in this % (w/w) problem, the mass units cancel, therefore we can use any mass units as long as we use the same unit for the mass of solute **and** mass of solution.

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Concentration in Parts per Thousand, Parts per Million, Parts per Billion, Parts per Trillion

Parts per thousand, parts per million (ppm), parts per billion (ppb), and parts per trillion (ppt) are defined in a similar way as percent concentration however, _____ of multiplying the ratios of solute to solution by **100**, they are multiplied by a **thousand**, **million**, **billion**, or **trillion**, respectively.

Just like percent (%) concentration, parts per thousand, ppm, ppb, and ppt units can be **(w/w)**, **(v/v)**, or **(w/v)**.

For example, the definitions or percent, parts per thousand, ppm, ppb, and ppt, **in (w/w)**, are:

$$\% \text{ (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times 100$$

$$\text{parts per thousand (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times 1000$$

$$\text{ppm (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times \left(1 \times 10^{6} \right)$$

$$\text{ppb (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times \left(1 \times 10^{9} \right)$$

$$\text{ppt (w/w)} = \left(\frac{\text{mass of } solute}{\text{mass of } solution} \right) \times \left(1 \times 10^{12} \right)$$

The ppm, ppb, and ppt units are often used for very dilute solutions.

If you were to mix **one drop** of alcohol into an Olympic-size pool such as the one shown here, the alcohol concentration would be about **20 part per trillion (ppt)**.

The volume of an Olympic-size swimming pool is about 2.5×10^{9} mL. The volume of one drop of ethyl alcohol is about 0.050 mL. What is the ppt (v/v) concentration of alcohol if 0.050 mL (~1 drop) is mixed into a pool with a volume of 2.5×10^{9} mL?

$$\text{ppt (v/v)} = \left(\frac{\text{volume of } solute}{\text{volume of } solution} \right) \times \left(1 \times 10^{12} \right)$$

- Volume of the **solute** (alcohol in this example) was given: **0.050 mL**
- The volume of the **solution** is equal to the volume of the **solute** (alcohol, 0.050 mL) **plus** the volume of the **solvent** (water, 2.5×10^{9} mL) = **2.5×10^{9} mL**

Insert the volume of the solute and the volume of the solution into the equation for ppt (v/v):

$$\text{ppt (v/v)} = \left(\frac{0.050 \text{ mL}}{2.5 \times 10^{9} \text{ mL}} \right) \times \left(1 \times 10^{12} \right) = 20. \text{ ppt (v/v)}$$

Understanding Check: The legal limit of blood alcohol concentration while driving in most states corresponds to *about* 0.080 grams of alcohol per 100.0 grams of blood (solution).

What is the **parts per thousand (w/w)** blood alcohol concentration at this legal limit?

Concentration in Molarity

Chemists often use a concentration unit of measure called _____.

Molarity is defined as the number of _____ *of solute* per _____ *of solution*.

It can be calculated by taking the ratio of moles of solute to the volume (in liters) of solution:

$$\text{Molarity} = \left(\frac{\text{moles of } solute}{\text{liters (L) of } solution} \right)$$

Calculating a solution's molarity using this equation/definition results in units of **moles/L**.

The mole/L unit is often referred to as _____ and abbreviated as "___."

Keep in mind, the "**M**" *can be interchanged with* "**mole/L**."
- For example, 0.030 **moles/L** = 0.030 **M** (molar)

Example: A solution is prepared by dissolving 0.10 moles of the amino acid alanine in enough water to give a final volume of 0.075 L. What is the *molarity* of the solution?

alanine
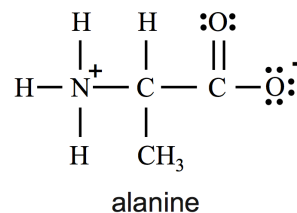
$$\text{Molarity (M)} = \left(\frac{\text{moles of solute}}{\text{liters of solution}} \right)$$

$$\text{Molarity (M)} = \left(\frac{0.10 \text{ moles}}{0.075 \text{ L}} \right)$$

$$= 1.3 \text{ M or } 1.3 \text{ moles/L}$$

Understanding Check: A solution is prepared by dissolving 0.057 moles of adrenaline in enough water to give a final volume of 1.80 L. What is the *molarity* of the solution?

adrenaline
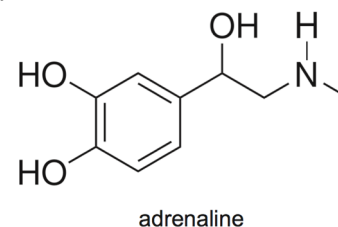
In some **molarity** calculations, since mass (grams) is the parameter that is *directly measurable*, you will begin with the *number of **grams** of solute*.

When this is the case, use the solute's molar mass to convert from grams to moles.

grams of solute $\longrightarrow$ moles of solute

$$\text{Molarity (M)} = \left(\frac{\text{moles of solute}}{\text{liters of solution}}\right)$$
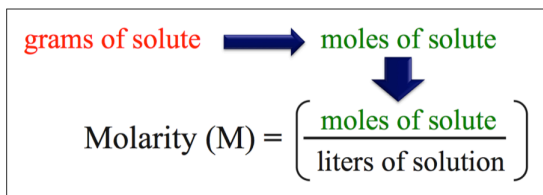
You will need to do this in the following *Understanding Check* problem.

Understanding Check: What is the molarity of a solution that is prepared by dissolving 3.83 grams of glucose ($C_6H_{12}O_6$) in enough water to make 5.00 L of solution?

Concentration in Osmolarity

The **osmole** (osmol) unit is used to indicate *the number of moles of dissolved* _____.

The concentration unit of measure called _____ is commonly defined as the number of **moles of dissolved particles (osmoles)** per **liter of solution**.

Osmolarity can be calculated by taking the ratio of osmoles of solute to the volume (in liters) of solution:

$$\text{Osmolarity} = \left(\frac{\text{osmoles of } solute}{\text{liter (L) of } solution}\right)$$

Calculating a solution's osmolarity using this equation results in units of _____.

The **osmoles/L** unit is often referred to as _____ and abbreviated as "**osM**."

What is the difference between a solution's osmolarity and molarity?

$$\text{Osmolarity} = \left(\frac{\text{osmoles of } solute}{\text{liter (L) of } solution}\right) \quad \text{Molarity} = \left(\frac{\text{moles of } solute}{\text{liters (L) of } solution}\right)$$

Sometimes it is the **same**, and *sometimes* it is **different**.

Ionic compound solutes dissociate (break apart into ions) into *individual ions* when solvated.
- For every mole of an *ionic compound* that is dissolved, the solution contains **two or more moles** of dissolved particles (osmoles), therefore the solution's molarity and osmolarity **have different values**.

Molecular compound solutes do not dissociate when solvated.
- For every mole of a dissolved *molecular compound,* the solution contains one mole of dissolved particles (one osmole), therefore the solution's molarity and osmolarity **have the same value**.

Example: Osmolarity for a Molecular Compound

If 0.50 moles of glucose (a molecular compound) is dissolved in enough water to make 2.00 L of solution, what is the *osmolarity* of the solution?

$$Osmolarity = \left(\frac{\text{osmoles of } solute}{\text{liter (L) of } solution} \right)$$

To calculate the **os*molarity***, we need to know two quantities: the number of **osmoles** of the *solute* **AND** the volume **(L)** of the *solution.*
- **osmoles** of the *solute* (glucose): since glucose is a covalent compound, it **does not dissociate** *into ions* when dissolved. For every mole of a molecular compound that is dissolved, the solution will contain one mole of dissolved particles (one osmole).
  - 0.50 moles of glucose were dissolved, therefore the solution contains **0.50 osmoles** of glucose.
- liters (L) of *solution* was given: **2.00 L**

Insert the **osmoles** of the *solute* and liters (L) of *solution* into the equation for osmolarity:

$$Osmolarity = \left(\frac{0.50 \text{ osmoles}}{2.00 \text{ L}} \right) = 0.25 \text{ osmoles/L or } 0.25 \text{ osmolar}$$

Note that in this example, since glucose is a **molecular** (non dissociation) compound, the **molarity** and the **osmolarity** have the **same** value.

Example: Osmolarity for an Ionic Compound

If 0.50 moles of sodium chloride (*an ionic compound*) are dissolved in enough water to make 2.00 L of solution, what is the *osmolarity* of the solution?

$$Osmolarity = \left(\frac{\text{osmoles of } solute}{\text{liter (L) of } solution} \right)$$

- **osmoles** of the *solute* (**NaCl**): Sodium chloride dissociates when dissolved, so for every *mole* of sodium chloride, the solution will contain *one mole* of dissolved sodium ions *plus* *one mole* of dissolved chloride ions.

$$NaCl(s) \rightarrow Na^+ (aq) + Cl^- (aq)$$

$$\boxed{\begin{array}{c} \text{one osmole} \\ \text{of } Na^+ \end{array}} + \boxed{\begin{array}{c} \text{one osmole} \\ \text{of } Cl^- \end{array}} = \textbf{2 osmoles}$$
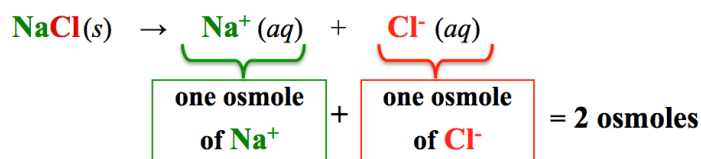
Multiply the number of moles of sodium chloride by a *factor of 2* to convert *moles* of sodium chloride to *osmoles*:

$$0.50 \text{ moles } NaCl \left(\frac{2 \text{ osmoles}}{\text{mole } NaCl} \right) = \textbf{1.0 osmoles}$$

- liters (L) of *solution* was given: **2.00 L**

Insert the **osmoles** of the *solute* and liters (L) of *solution* into the equation for osmolarity:

$$Osmolarity = \left(\frac{1.0 \text{ osmoles}}{2.00 \text{ L}} \right) = 0.50 \text{ osmoles/L or } 0.50 \text{ osmolar}$$

Even though we started with the *same number of moles of solute* and the *same volume of solution* in this example as we did in the previous example for a glucose solution, the osmolarity values are different *because of the difference in the number of particles (osmoles) that are formed upon dissolution of molecular vs. ionic solutes.*

In the *Understanding Check* problem that follows, I will ask you to calculate the osmolarity of a $BaCl_2$ solution.

Keep in mind that for every *one mole* of $BaCl_2$ that dissolves, **3 osmoles** are formed.

$$BaCl_2(s) \rightarrow Ba^{2+}(aq) + 2\,Cl^-(aq)$$

| one osmole of Ba^{2+} | + | two osmoles of Cl^- | = 3 osmoles |
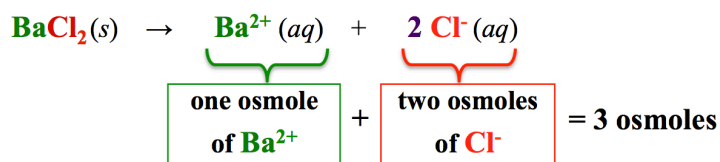
Understanding Check: If 0.50 moles of $BaCl_2$ (*an ionic compound*) is dissolved in enough water to make 2.00 L of solution, what is the *osmolarity* of the solution?

Converting between Molarity and Osmolarity

Knowing the number of _____ (osmoles) that are formed upon dissolution of a solute will enable you to easily convert between *molarity* and *osmolarity*.

The number of osmoles formed per mole of solute dissolved can be used as a _____ _____.

Example for an Ionic Compound Solute: If the *molarity* of a NaCl solution is **1.2 M**, what is the *osmolarity*?

$$\frac{1.2 \text{ moles NaCl}}{L} \cdot \frac{2 \text{ osmoles}}{1 \text{ mole NaCl}} = 2.4 \left(\frac{\text{osmoles}}{L}\right)$$

| Molarity (moles/L) | Conversion Factor (osmoles/mole NaCl) | Osmolarity (osmoles/L) |

Converting between molarity and osmolarity for **molecular solutes** is simple!

The *molarity* is _____ to *osmolarity* for **molecular solutes** because they do not dissociate.

Example for a Molecular Compound Solute:
- Glucose is a molecular compound; if the *molarity* of a glucose solution is **1.2** M, then the *osmolarity* is **1.2** osmoles/L.

Understanding Check: If the molarity of an $FeCl_3$ (an ionic compound) solution is 0.010 M, what is the osmolarity?

　　　　HINT: Think about how many osmoles are produced when one mole of $FeCl_3$ dissociates.

Concentration in Molality

_____ is defined as the number of **moles of solute** per **kg of solvent**.

Molality can be calculated by taking the ratio of **moles** of solute to the **mass** (in kilograms) of the _____:

$$Molality = \left(\frac{\text{moles of } solute}{\text{kg of } solvent} \right)$$

Calculating a solution's molality using this equation/definition results in units of **moles/kg**.

The **moles/kg** unit is often referred to as **molal** and abbreviated as "***m***."
- The "***m***" unit *can be interchanged with* "**moles/kg**."

Calculation of Molality Example

What is the molality of a solution that is prepared by dissolving 0.125 moles of sodium chloride in 1.60 kg of water?

$$Molality = \left(\frac{\text{moles of } solute}{\text{kg of } solvent} \right)$$

- The **moles** of the **solute** (NaCl) was given: **0.125 moles**
- The **mass** of the **solvent** (water) was given: **1.60 kg**

Insert the moles of the *solute* and kg of *solvent* into the equation for molality:

$$Molality = \left(\frac{0.125 \text{ moles}}{1.60 \text{ kg}} \right) = 0.0781 \text{ moles/kg} \text{ or } 0.0781 \, m$$

In a **0.0781 molal (*m*)** solution, there are **0.0781 *moles of solute*** contained in every ***kg of solvent***.

Understanding Check: What is the ***molality*** of a solution that is prepared by dissolving 1.34 moles of ethyl alcohol in 0.75 kg of water?

Concentration in Osmolality

Osmolality is defined as the number of _____ per _____ **of solvent**.

It can be calculated taking the ratio of ***osmoles*** (moles of dissolved particles) to the mass (in kilograms) of the solvent:

$$Osmolality = \left(\frac{\text{osmoles of } solute}{\text{kg of } solvent} \right)$$

Calculating a solution's osmolality using this equation/definition results in units of **osmoles/kg**.
- The os**moles/kg** unit is often referred to as **osmolal**

Concentration in Equivalents per Liter (Eq/L)

Some properties of solutions depend on the *total charge* of the _____ in solution.

- For example, the ability of a solution to conduct electricity depends on the total charge of the ions in solution. In cells, membrane potentials that generated nerve signals depend on the total charge of ions in solution.

An **equivalent** (**Eq**) is defined as a *mole of* _____.

The concentration unit of measure called **equivalents per liter (Eq/L)** is defined as the number of **equivalents *(Eq)*** of solute (*moles of charge*) per *liter of solution*:

$$Eq/L = \left(\frac{\text{Eq of } solute}{\text{liter (L) of } solution} \right)$$

At first glance, an **equivalent** (**Eq**) *may appear to be the same* as an *osmole*, however this is not always the case.

An **equivalent** is a mole of *charge*; an **osmole** is a mole of *dissolved particles*.

I will elaborate by comparing the number of osmoles vs. the number of equivalents present when one mole of $BaCl_2$ is dissolved.

When **one mole** of $BaCl_2$ is dissolved, *3 osmoles* are formed.
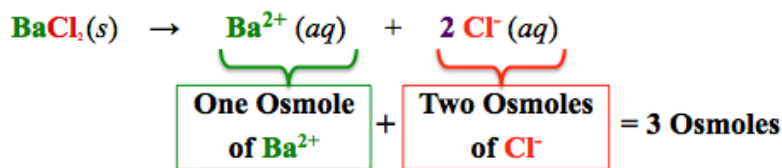
When **one mole** of $BaCl_2$ is dissolved, **4 equivalents (Eq)** are formed.
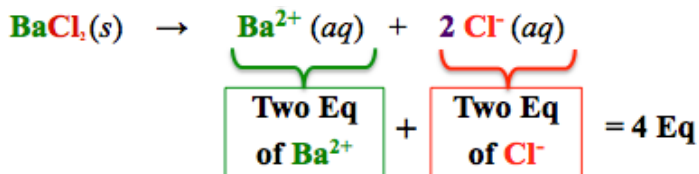
- Since barium ions have a "**2+**" **charge**, one mole of barium ions contains *two moles of charge* (*two* equivalents).
- The **two** moles of chloride ions contain a total of *two* equivalents (*two* moles of a "**1-**" charge).

Understanding Check

When **one mole** of $Fe_2(SO_4)_3$ is dissolved in water:

    a. How many **equivalents** are present?

    b. How many equivalents of **sulfate** are present (equivalents from sulfate only)?

    c. How many equivalents of **iron(III)** are present (equivalents from Fe^{3+} only)?

Example for Calculating Eq/L

If 0.50 moles of $BaCl_2$ is dissolved in enough water to make 2.00 L of solution, what is the **Eq/L** *concentration* of the solution?

$$Eq/L = \left(\frac{Eq\ of\ solute}{liter\ (L)\ of\ solution} \right)$$

Eq present:
- For every *one mole* of $BaCl_2$ dissolved, **4 Eq** are formed (two **Eq** of Ba^{2+} and two **Eq** of Cl^-).

$$BaCl_2(s) \rightarrow Ba^{2+}(aq) + 2\ Cl^-(aq)$$

$$\boxed{\begin{array}{c}\textbf{Two Eq}\\ \textbf{of }Ba^{2+}\end{array}} + \boxed{\begin{array}{c}\textbf{Two Eq}\\ \textbf{of }Cl^-\end{array}} = \textbf{4 Eq}$$
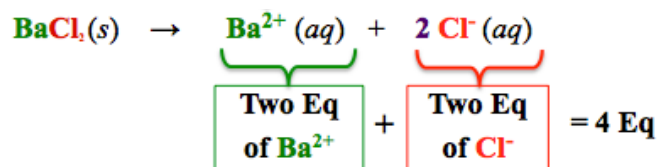
- Multiply the number of moles of $BaCl_2$ by a factor of **4** to convert *moles* of $BaCl_2$ to **Eq**:

$$0.50\ moles\ BaCl_2 \left(\frac{\textbf{4 Eq}}{mole\ BaCl_2} \right) = \textbf{2.0 Eq}$$

liters (L) of *solution* was given: **2.00 L**

Insert the **Eq** present and liters (L) of *solution* into the equation for **Eq/L** concentration:

$$Eq/L = \left(\frac{2.0\ Eq}{2.00\ L} \right) = 1.0\ Eq/L$$

Understanding Check

If 0.015 moles of $Fe_2(SO_4)_3$ is dissolved in enough water to make 2.5 L of solution, what is the **Eq/L** *concentration* of the solution?

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Calculations for Solutions

In this section, you will learn how do calculations to find how much solute is contained in a specified amount of solution *and* how much solution contains a specified amount of solute.

The key to mastering these calculations is to be aware of the following two statements:

- The _____ between the *amount of solute* and the *amount of solution* is the *concentration*.

- You can convert between the *amount of* _____ and the *amount of* _____ by *using the* _____ *as a* _____ _____.

Molarity Concentration Calculations for Solutions

The *molarity* (_____) of a solution gives us the *relationship* between the **amount (moles) of solute** and the **volume (L) of solution**.

We use the *molarity* as a *conversion factor* when converting between the moles of solute in a given volume (L) of solution, *or* the volume (L) of solution that will contain a given amount (moles) of solute.
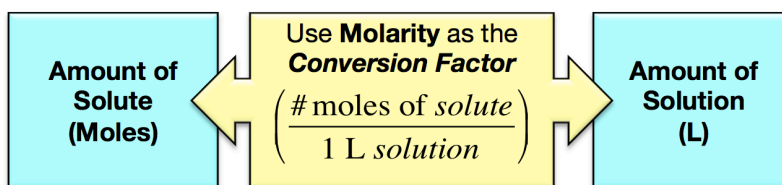
Volume of Solution to Amount of Solute Example

Suppose you know that a patient received 3.50 **L** of a 0.278 **M** glucose IV solution, how many moles of glucose were administered to the patient?

STEP 1) Set up the equation using the given quantity:

$$\frac{3.50 \text{ L solution}}{} \Bigg| = ? \text{ moles glucose}$$

STEP 2) Use the *molarity* as a **conversion factor** to find the **number of moles**:

$$\frac{3.50 \text{ L solution}}{} \Bigg| \frac{0.278 \text{ moles glucose}}{1 \text{ L solution}} = 0.973 \text{ moles glucose}$$
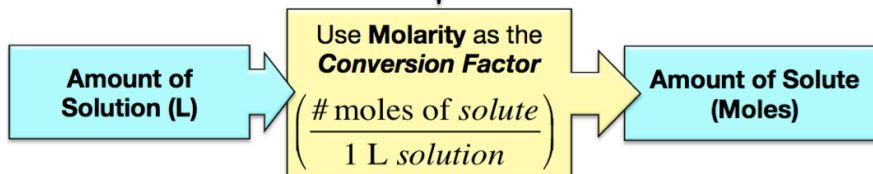
3.50 L of a **0.278 M** glucose solution will contain **0.973** moles of glucose.

Moles of Solute to Volume (L) of Solution Example

Suppose you wished to administer 0.200 moles of glucose from a 0.278 M glucose IV solution to a patient, what **volume** (in liters) of the solution would need to be dispensed?

STEP 1) Set up the equation using the given quantity:

$$\frac{0.200 \text{ moles glucose}}{} \Bigg| = \ ? \ \text{L solution}$$

STEP 2) Use the **molarity** as a **conversion factor** to find the **volume (L) of solution:**

$$\frac{0.200 \ \cancel{\text{moles glucose}}}{} \Bigg| \frac{1 \text{ L solution}}{0.278 \ \cancel{\text{moles glucose}}} = 0.719 \text{ L solution}$$

Amount of Solute (Moles)	Use **Molarity** as the **Conversion Factor** $\left(\dfrac{1 \text{ L } solution}{\# \text{ moles of } solute}\right)$	Amount of Solution (Liters)

0.719 L of a **0.278 M** glucose solution would be given to the patient in order to provide 0.200 moles of glucose.

Another Molarity Concentration Calculation Example

Next, I want to show you an example problem that combines the concepts of the **previous two videos** (calculating a solution's concentration) *and* the concepts of this section (calculations of how much solute is contained in a certain amount of solution *or* how much solution contains a certain amount of solute).

If 1.25 g of acetone (C_3H_6O) is dissolved in enough water to make 0.550 L of solution;

    a) What is the **molarity (M)** of the solution?
    b) How many **moles** of acetone are contained in 0.0679 L of this acetone **solution**?
    c) What **volume (L)** of this acetone solution would contain 0.0079 **moles** of acetone?

a) What is the **molarity (M)** of the solution?

$$\text{Molarity} = \left(\frac{\text{moles of } solute}{\text{liters (L) of } solution}\right)$$

- **moles** of the **solute** (acetone)

   We were not given the number of moles **directly**, however, we were given the *grams* of acetone (1.25 g). Use the *molar mass* of acetone (**58.09 g/mole**) to convert from grams to moles.

$$\frac{1.25 \ \cancel{\text{grams } C_3H_6O}}{} \Bigg| \frac{1 \text{ mole } C_3H_6O}{58.09 \ \cancel{\text{grams } C_3H_6O}} = 0.0215 \text{ moles } C_3H_6O$$

- **L** of **solution** was given: **0.550 L**

Insert the moles of the *solute* and liters (L) of *solution* into the equation for molarity:

$$\text{Molarity} = \left(\frac{0.0215 \text{ moles}}{0.550 \text{ L}}\right) = 0.0391 \text{ moles/L} \ \text{ or } \ 0.0391 \text{ M}$$

b) How many *moles* of acetone are contained in 0.0679 L of this acetone *solution*?

   STEP 1) Set up the equation using the given quantity:

$$\frac{0.0679 \text{ L solution}}{} \Bigg| = $$

   STEP 2) Use the *molarity* as a **conversion factor** to find the **number of moles**:

$$\frac{0.0679 \text{ L solution}}{} \Bigg| \frac{0.0391 \text{ moles acetone}}{1 \text{ L solution}} = 0.00265 \text{ moles acetone}$$

| Amount of Solution (L) | → | Use **Molarity** as the *Conversion Factor* $\left(\dfrac{\#\text{moles of } solute}{1 \text{ L } solution}\right)$ | → | Amount of Solute (Moles) |
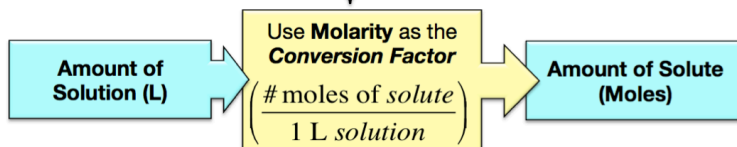
c) What **volume (L)** of this acetone solution would contain 0.0079 *moles* of acetone?

   STEP 1) Set up the equation using the given quantity:

$$\frac{0.0079 \text{ moles acetone}}{} \Bigg| = $$

   STEP 2) Use the *molarity* as a **conversion factor** to find the **volume (L) of solution:**

$$\frac{0.0079 \text{ moles acetone}}{} \Bigg| \frac{1 \text{ L solution}}{0.0391 \text{ moles acetone}} = 0.20 \text{ L solution}$$

| Amount of Solute (Moles) | → | Use **Molarity** as the *Conversion Factor* $\left(\dfrac{1 \text{ L } solution}{\#\text{moles of } solute}\right)$ | → | Amount of Solution (Liters) |
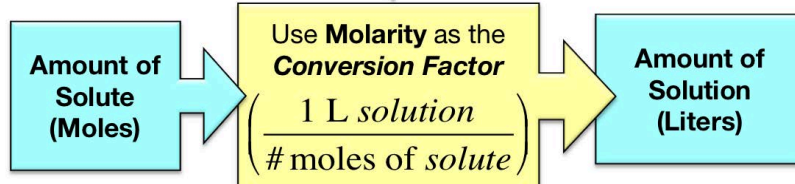
Understanding Check: If a particular wine has an ethyl alcohol molarity concentration of 2.8 M, what volume (in liters) of wine contains 10.4 moles of ethyl alcohol (the lethal dosage)?

Understanding Check: How many *grams* of silver nitrate ($AgNO_3$) are contained in 0.384 L of a 0.200 M silver nitrate solution?

Percent (%) Concentration Calculations for Solutions

Percent (%) concentration gives the relationship between the *amount of solute* and the *amount of solution*:

Amount of Solute (Grams) → Use %(w/w) as the **Conversion Factor** $\left(\dfrac{\#\text{ grams of } solute}{100 \text{ grams of } solution}\right)$ → Amount of Solution (Grams)

Amount of Solute (mL) → Use %(v/v) as the **Conversion Factor** $\left(\dfrac{\#\text{ mL of } solute}{100 \text{ mL of } solution}\right)$ → Amount of Solution (mL)

Amount of Solute (Grams) → Use %(w/v) as the **Conversion Factor** $\left(\dfrac{\#\text{ grams of } solute}{100 \text{ ml of } solution}\right)$ → Amount of Solution (mL)
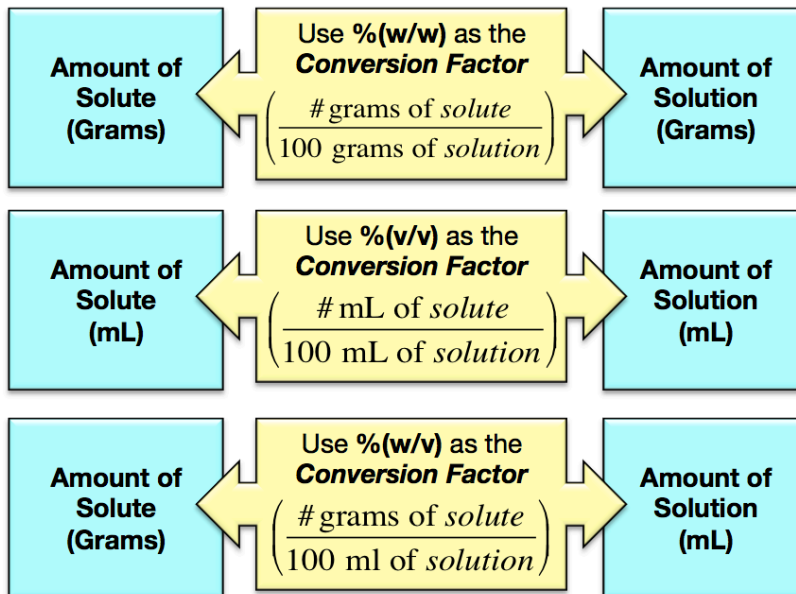
Example: Using % (w/v) to Convert From Volume (mL) of Solution to Grams of Solute

Normal saline intravenous (IV) drips are composed of sterile, 0.90 %(w/v) aqueous sodium chloride (NaCl) solutions. They are used to treat or prevent dehydration and hypovolemia.

If a patient received 2475 mL of a normal saline solution, how many grams of sodium chloride were delivered?

$$\frac{2475 \text{ mL solution}}{} \left| \frac{0.90 \text{ grams NaCl}}{100 \text{ mL solution}} \right. = 22 \text{ grams NaCl}$$

Amount of Solution (mL) → Use %(w/v) as the **Conversion Factor** $\left(\dfrac{\#\text{ grams of } solute}{100 \text{ ml of } solution}\right)$ → Amount of Solute (grams)
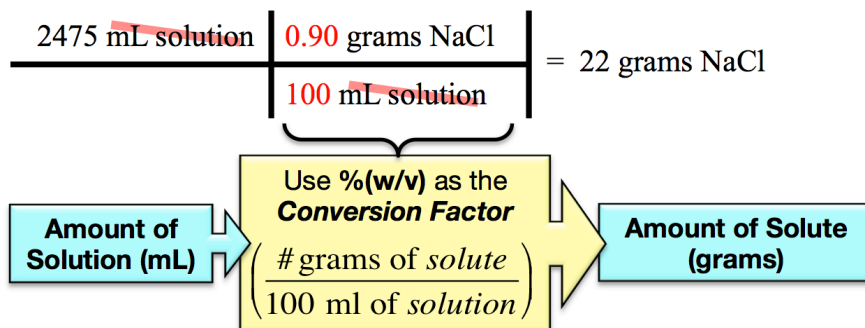
If a patient received 2475 mL of a normal saline solution, then **22 grams** of sodium chloride were delivered.

Example: Using %(w/v) to Convert From Grams of Solute to Volume (mL) of Solution

What volume (mL) of a normal saline solution (0.90% (w/v)) contains 12.5 grams of sodium chloride?

$$\frac{12.5 \text{ grams NaCl}}{} \left| \frac{100 \text{ mL solution}}{0.90 \text{ grams NaCl}} \right. = 1400 \text{ mL solution}$$

Amount of Solute (grams) → Use %(w/v) as the **Conversion Factor** $\left(\dfrac{100 \text{ ml of } solution}{\#\text{ grams of } solute}\right)$ → Amount of Solution (mL)
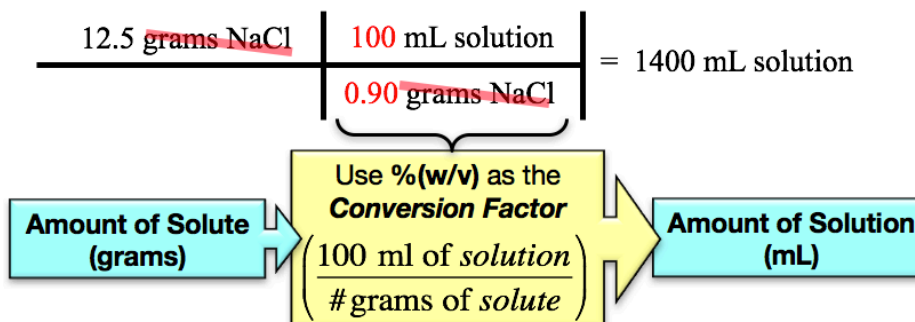
1400 mL of a normal saline solution contain 12.5 grams of sodium chloride.

The label of the medication vial tells you that the concentration of morphine sulfate for an intravenous injection is 1.0% (w/v). If you wish to administer 0.0025 grams of morphine sulfate, what volume (mL) would you inject?

The method for converting between the ***amount of solute*** and the ***amount of solution*** can also be used for **%(w/w)** and **%(v/v)**.

   %(w/w) is used to convert between the ***mass*** of solute *and* the ***mass*** of solution:
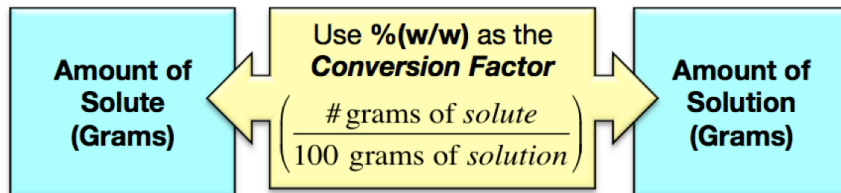
   %(v/v) is be used to convert between the **volume** of a liquid solute and the **volume** of the solution:
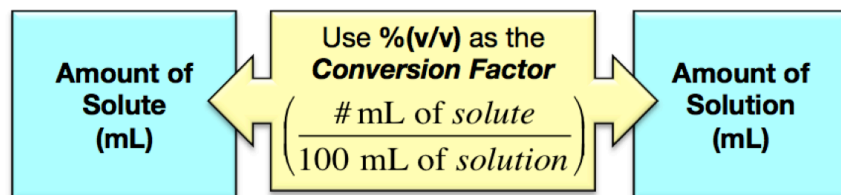
Osmolarity Concentration Calculations for Solutions

Osmolarity concentration is a relationship between the amount of solute and the amount of solution:
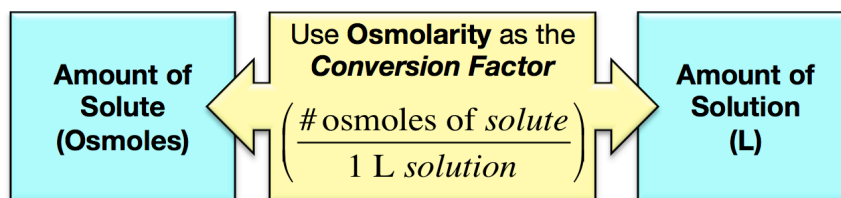
The **osmolarity (osmoles/L)** of a solution gives us the number of ***osmoles of solute*** contained in ***1 L of solution***.

   • It can therefore be used to **convert** between _____ *of solute* and _____ *of solution*.

Example: Using **Osmolarity** to convert between *L of Solution* and *Osmoles of Solute*

How many *osmoles of solute* are contained in 2.75 L of a solution that has a concentration of 0.0750 *osmole/L*?

$$\frac{2.75 \text{ L solution}}{} \quad \Bigg| \quad \frac{0.0750 \text{ osmoles}}{1 \text{ L solution}} \quad = \ 0.206 \text{ osmoles}$$

Amount of Solution (L)	Use **Osmolarity** as the *Conversion Factor* $\left(\dfrac{\#\text{osmoles of } solute}{1 \text{ L } solution}\right)$	Amount of Solute (osmoles)
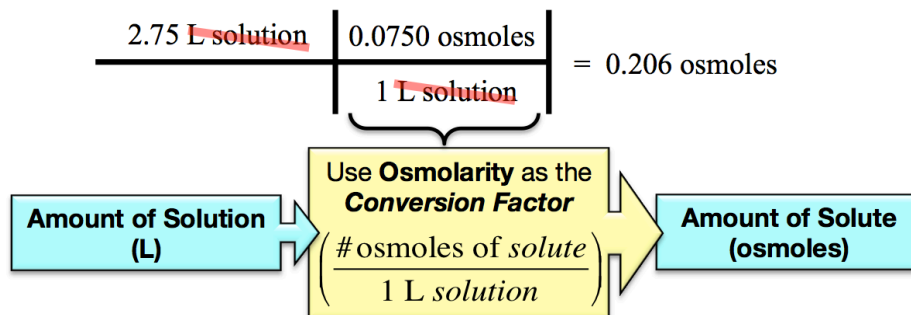
0.206 *osmoles* are contained in 2.75 L of a 0.0750 *osmole/L solution*.

Equivalents per Liter (Eq/L) Concentration Calculations for Solutions

Eq/L concentration is a relationship between the amount of solute and the amount of solution:

Amount of Solute (Eq)	Use **Eq/L** as the *Conversion Factor* $\left(\dfrac{\#\text{Eq of } solute}{1 \text{ L of } solution}\right)$	Amount of Solution (L)
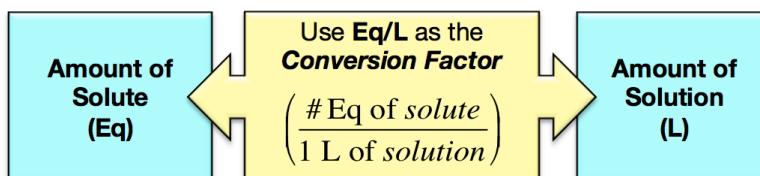
The **Eq/L** of a solution gives us the number of *equivalents of solute* contained in *1 L of solution*.
  • It can therefore be used to convert between _____ *of solute* and *L of solution*.

Example: Using **Eq/L** to convert between *L of Solution* and *Equivalents of Solute*

How many equivalents of solute are contained in 0.830 L of a 0.0100 M $Fe_2(SO_4)_3$ solution?

Solution:

Amount of Solution (L)	Use **Eq/L** as the *Conversion Factor* $\left(\dfrac{\#\text{Eq of } solute}{1 \text{ L } solution}\right)$	Amount of Solute (Eq)

We are given the solution concentration in molarity (M = mole/L), but we need to get (Eq/L) in order to solve the problem. First (Step 1) we will convert molarity (mole/L) to (Eq/L), and then (Step 2) we will use the Eq/L concentration as a conversion factor to convert from liters of solution to equivalents of solute.

Step 1

Molarity (moles/L)	→	Eq/L

Step 2

Amount of Solution (L)	Use **Eq/L** as the *Conversion Factor* $\left(\dfrac{\#\text{Eq of } solute}{1 \text{ L } solution}\right)$	Amount of Solute (Eq)

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Step 1

0.0100 M | Molarity (moles/L) | → | Eq/L

$$Fe_2(SO_4)_3\,(s) \rightarrow 2\,Fe^{3+}\,(aq) + 3\,SO_4^{2-}\,(aq)$$

6 Eq of Fe^{3+} + **6 Eq of SO$_4^{2-}$**

12 total Eq
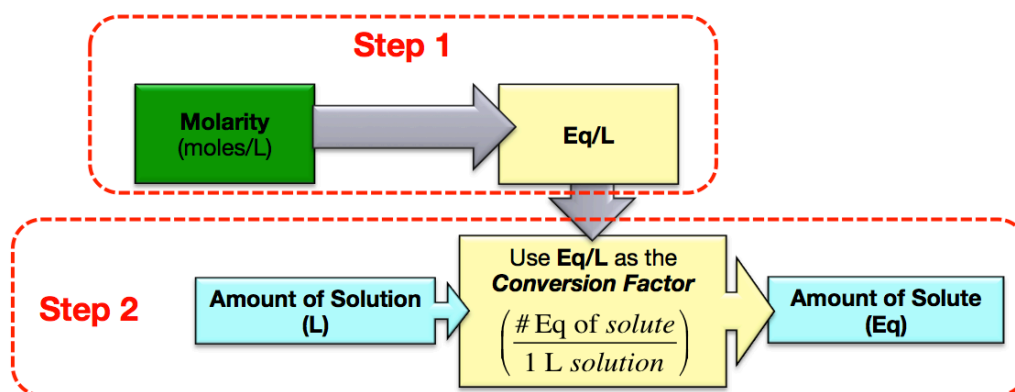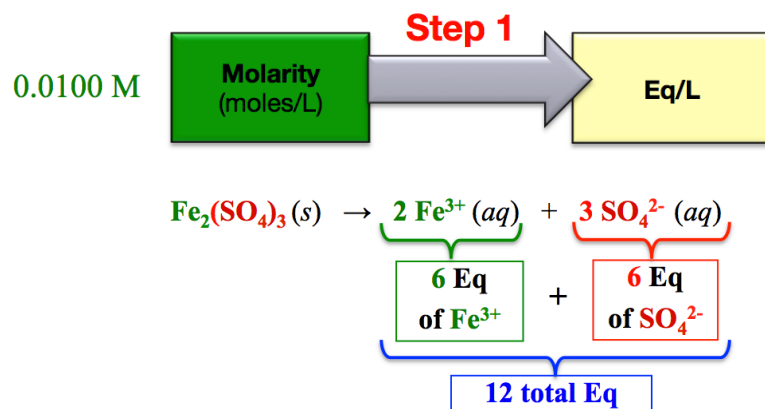
$$\frac{0.0100 \text{ moles } Fe_2(SO_4)_3}{L} \cdot \frac{12 \text{ Eq}}{1 \text{ mole } Fe_2(SO_4)_3} = 0.120 \left(\frac{\text{Eq}}{L}\right)$$

Molarity (moles/L) — Equivalents per Liter

Step 2:

$$\frac{0.830 \text{ L solution}}{} \cdot \frac{0.120 \text{ Eq}}{1 \text{ L solution}} = 0.0996 \text{ Eq}$$

Amount of Solution (L) → Use **Eq/L** as the **Conversion Factor** $\left(\dfrac{\#\,Eq \text{ of } solute}{1\,L\,solution}\right)$ → Amount of Solute (Eq)

0.0996 Eq of solute are contained in **0.830 L** of a **0.0100 M** $Fe_2(SO_4)_3$ solution.

Example: Using **Eq/L** to convert between *L of Solution* and *Equivalents of Solute*

How many equivalents of **sulfate (*not total equivalents*)** are contained in 0.830 L of a 0.0100 M $Fe_2(SO_4)_3$ solution?

Solution:

Amount of Solution (L) → Use **Eq/L** as the **Conversion Factor** $\left(\dfrac{\#\,Eq \text{ of } solute}{1\,L\,solution}\right)$ → Amount of Solute (Eq)
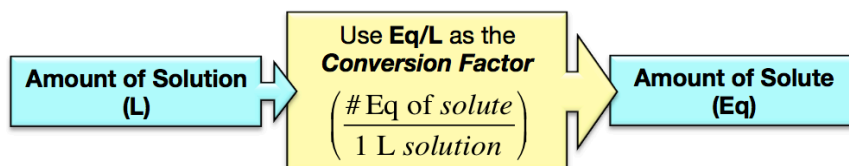
We will do this problem in the same way as we did for the previous example problem, *with one exception*: we will convert the given **molarity** (0.0100 M) to **Eq of SO$_4^{2-}$/L**.

Step 1

0.0100 M | Molarity (moles/L) | → | Eq SO_4^{2-}/L

$$Fe_2(SO_4)_3\,(s) \;\rightarrow\; 2\,Fe^{3+}\,(aq) \;+\; 3\,SO_4^{2-}\,(aq)$$
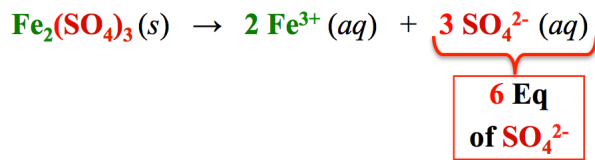
6 Eq of SO_4^{2-}

$$\frac{0.0100 \text{ moles } Fe_2(SO_4)_3}{L} \left| \frac{6 \text{ Eq } SO_4^{2-}}{1 \text{ mole } Fe_2(SO_4)_3} \right. = 0.0600 \left(\frac{\text{Eq } SO_4^{2-}}{L}\right)$$

Molarity (moles/L)

Step 2:

$$\frac{0.830 \text{ L solution}}{} \left| \frac{0.0600 \text{ Eq } SO_4^{2-}}{1 \text{ L solution}} \right. = 0.0498 \text{ Eq } SO_4^{2-}$$

Amount of Solution (L) → Use **Eq/L** as the *Conversion Factor* $\left(\dfrac{\#\,Eq \text{ of } solute}{1 \text{ L } solution}\right)$ → Amount of Solute (Eq)

Molality and Osmolality Concentration Calculations for Solutions

Molality is used to covert between ***moles of solute*** and ***kg of*** _____:

Amount of Solute (Moles) ⇄ Use **Molality** as the *Conversion Factor* $\left(\dfrac{\#\,moles \text{ of } solute}{1 \text{ kg of } solvent}\right)$ ⇄ Amount of Solvent (kg)
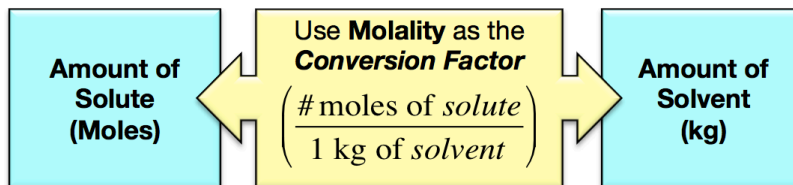
Osmolality is used to covert between ***osmoles of solute*** and ***kg of solvent***:

Amount of Solute (Osmoles) ⇄ Use **Osmolality** as the *Conversion Factor* $\left(\dfrac{\#\,osmoles \text{ of } solute}{1 \text{ kg of } solvent}\right)$ ⇄ Amount of Solvent (kg)
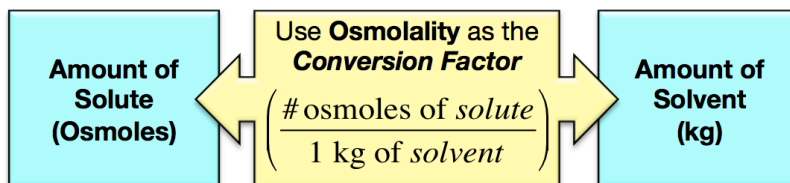
In practice, it is more useful to know how much solute is contained in a particular **amount of solution** *(not solvent)* or how much **solution (*not solvent*)** contains a particular amount of solute.

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In order to work with the *amount of solution* **instead** *of the amount of solvent,* a very useful approximation can be made *for dilute aqueous solutions*.

In the case of dilute aqueous solutions, *the solution is almost entirely solvent.*

Since 1 kg of water has a volume of 1 L, it is a reasonable approximation to equate *the amount of solution* to *the amount of solvent;* 1 kg of solvent is *assumed* to be the same as 1 L of solution.

Using this approximation, the *molality* is _____ to the *molarity*.

<div style="border:1px solid #ccc; background:#fdf6c3; padding:8px;">

For *Dilute Aqueous Solutions*:
Molality Units Can Be Replaced by Molarity Units:

$$\left(\frac{\#\,\text{moles of } solute}{1 \text{ kg of } solvent}\right) \Longrightarrow \left(\frac{\#\,\text{moles of } solute}{1 \text{ L } solution}\right)$$

      molality   **molarity**

</div>
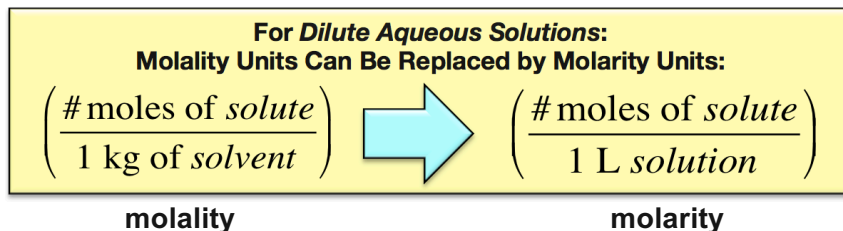
For the same reason, using this approximation, the *osmolality* is *equal* to the *osmolarity*.

<div style="border:1px solid #ccc; background:#fdf6c3; padding:8px;">

For *Dilute Aqueous Solutions*:
Osmolality Units Can Be Replaced by Osmolarity Units:

$$\left(\frac{\#\,\text{osmoles of } solute}{1 \text{ kg of } solvent}\right) \Longrightarrow \left(\frac{\#\,\text{osmoles of } solute}{1 \text{ L } solution}\right)$$

      osmolality   **osmolarity**

</div>
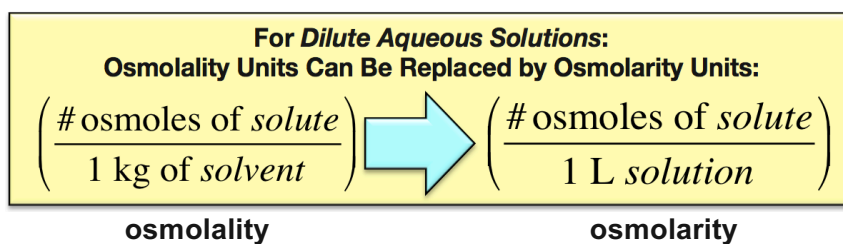
Summary of Conversion Factors for Solution Calculations

Amount of Solute	When converting Between — Use One of the Following Concentrations as the Conversion Factor:	Amount of Solution
moles of solute	molarity (moles/L)	liters (L) of solution
osmoles of solute	osmolarity (osmoles/L)	liters (L) of solution
equivalents (Eq) of solute	equivalents/L (Eq/L)	liters (L) of solution
mass of solute (typically grams)	% (w/w) typically (g solute/100 g solution)	mass of solution (typically grams)
volume of solute (typically mL)	% (v/v) typically (mL solute/100 mL solution)	volume of solution (typically mL)
grams of solute	% (w/v) (g solute/100 mL solution)	mL of solution
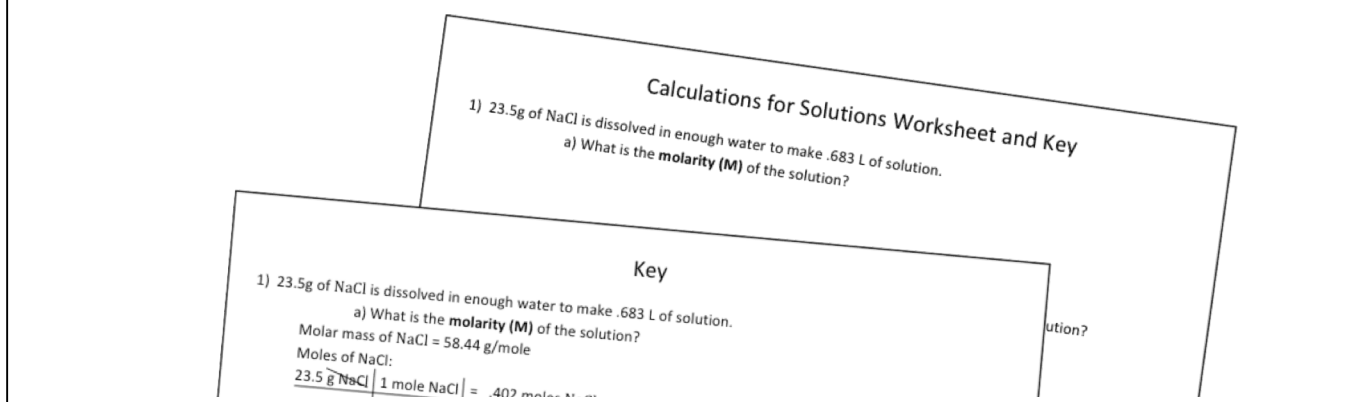
The Solubility of Biological Compounds

Biological compounds are the _____ _____ that occur in biological organisms.

Examples of biological compounds that you will learn about in this book are: steroids, fatty acids, bile salts, phospholipids, glycolipids, cholesterol, triglycerides (animal fat and vegetable oil), proteins, carbohydrates, RNA, and DNA.

Biological compounds can be put into one of three categories based on their _____ _____.

1) **Hydrophilic**
2) **Hydrophobic**
3) **Amphipathic**

1) Hydrophilic Compounds

Hydrophilic compounds _____ in water.

- The word *hydrophilic* is derived from an ancient Greek word that is translated as "*loving water*."

Compounds that are significantly _____ and/or can _____ _____ with water tend to be water soluble.

As a general rule, molecules that have at least _____ *polar functional group* for every _____ *carbon atoms* are water soluble, and therefore classified as **hydrophilic**.

- You saw *four polar functional groups* in chapter 4: the hydroxyl group (-OH), the carbonyl group (C=O), the carboxyl group (-COOH), and the carboxylate group (COO).

- There are a few other polar functional groups that you will see in later chapters.

- The presence of _____ _____will also help a biological compound to dissolve in water because of the attraction of water molecules' dipoles to the charged region of the compound (ion-dipole interactions).

Examples of Hydrophilic Compounds: Monosaccharides

The Structural Formulas of Three Monosaccharides

D-Glucose
(makes up starch and
cellulose; source of energy)

D-Ribose
(occurs in ATP, RNA,
and coenzymes)

D-Fructose
(sweeter than table sugar,
a component of corn
syrup, occurs in fruit)
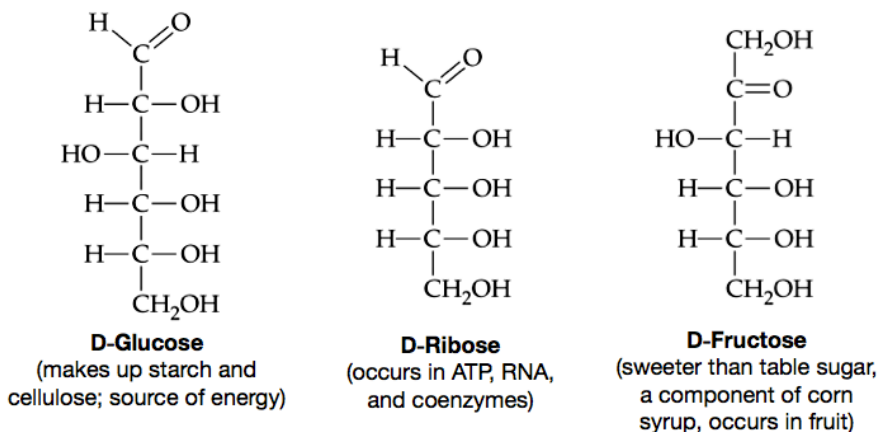
2) Hydrophobic Compounds

Hydrophobic compounds _____-_____ *dissolve* in water.

- The word *hydrophobic* is derived from an ancient Greek word that is translated as "*having a horror/fear of water.*"

As a general rule, molecules that have <u>less than</u> **one** *polar functional group* for every *five carbon atoms* do not dissolve in water and are therefore *hydrophobic*.

An Example of a Hydrophobic Compound: Cholesterol

Note that cholesterol does have *one* polar hydroxyl (-OH) functional group, however the nonpolar part of the molecule is so large that the ratio of polar functional group to total carbons is *much less* than 1:5 and therefore cholesterol does not dissolve in water.

Cholesterol
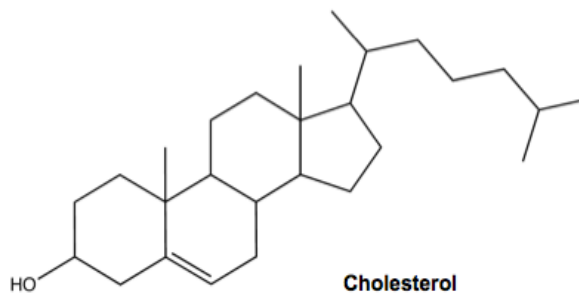
3) Amphipathic Compounds

Amphipathic compounds have _____ a large *nonpolar* region, which is *not* strongly attracted to water, *and* an *extremely polar* and/or *formally-charged* region, which is quite strongly attracted to water.

An Example of an Amphipathic Compound: A Glycolipid

The particular glycolipid shown in the structure below is one of the most prevalent of the glycolipids that make up cell membranes within the brain.
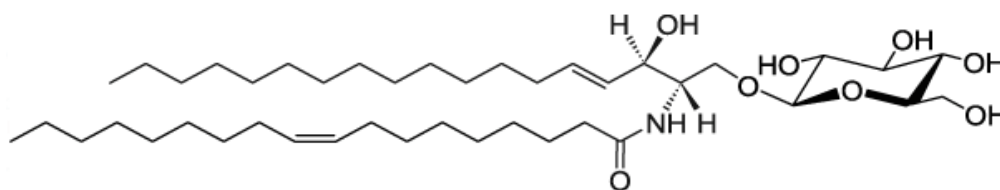
Amphipathic compounds are often illustrated using a _____ for the **polar head** that is attached to **one or more long tubular structures** that represent the carbon chains in the **nonpolar tail**.

Nonpolar "Tail"	Polar "Head"
A nonpolar region that *does not* have significant attractive interactions with water, however it is strongly attracted to large nonpolar regions of other particles.	The polar hydroxyl groups and the carbonyl group is strongly attracted to water.
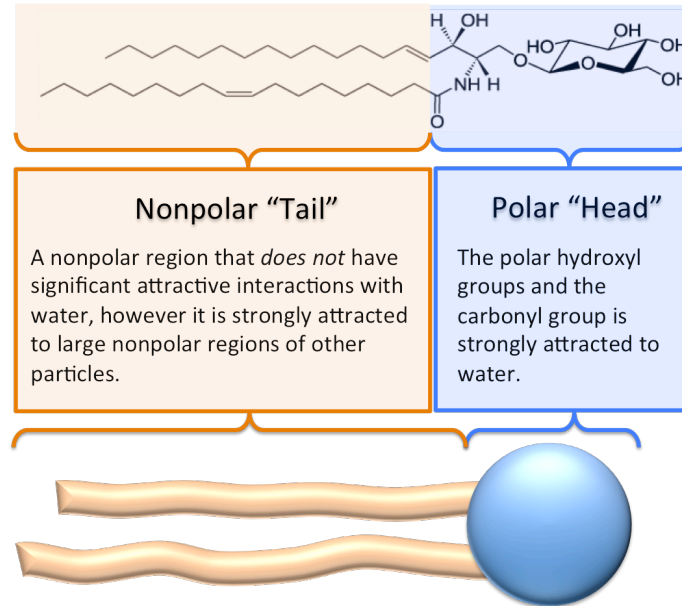
In some amphipathic compounds, such as the glycolipid shown above, there are *two* carbon chains that make up the nonpolar tail; in other amphipathic compounds, the tail is composed of *only one* carbon chain.

An example of an amphipathic compound that has a *single* carbon chain tail is *palmitate*.

Palmitate

Nonpolar "Tail"   Polar "Head"
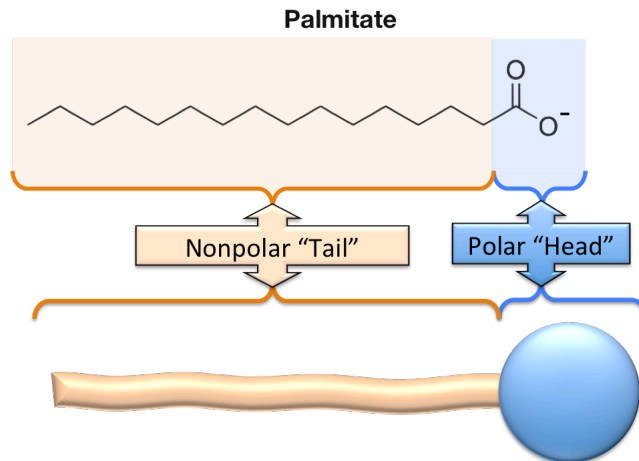
When amphipathic molecules are put into water they do not dissolve; they exist as **monolayers** and/or **micelles.**

- As _____, amphipathic compounds form a single (mono) layer of individual particles oriented with their polar heads toward the water and their nonpolar tails pointing upward.
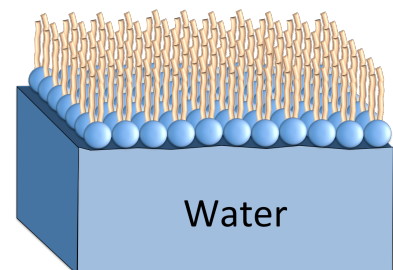
Water

Amphipathic compounds can also exist in water as
_____ arrangements called _____.

The amphipathic compounds making up micelles
are oriented with their **polar heads** outward, toward
the water, and their **nonpolar tails** inward, away
from the water.

a micelle

cross-sectional view
of a micelle
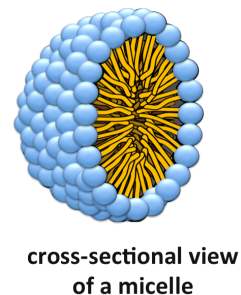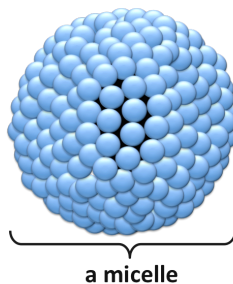
Soap consists of palmitate and/or similar *amphipathic compounds*.
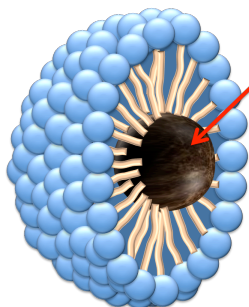
Oil
Droplet

As you know, soap *and* water are much more effective at removing oil
from skin than is just water alone. This is because there is no strong
attraction between the nonpolar oil molecules and water; however, soap
forms micelles that *encapsulate* the oil within their nonpolar tail interiors.
Micelles containing the oil can move into the rinse water and away from
the skin.

When a liquid contains compounds that are *encapsulated* by amphipathic
compounds in micelles, the mixture is called an _____.

Understanding Check

Predict whether each of the following biological compounds is **hydrophobic** or **amphipathic**?

a.
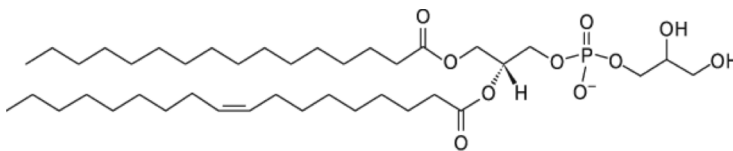
b.
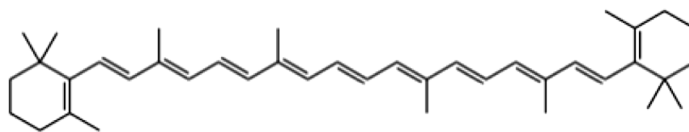
beta-carotene (a molecule in the vitamin A group)

Understanding Check

Predict whether each of the following biological compounds is **hydrophilic** or **hydrophobic**?

a.   b.
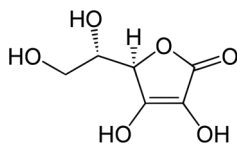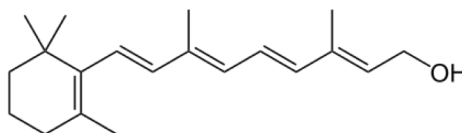
vitamin C   retinol (a molecule in the vitamin A group)

Understanding Check

The ion shown below is called *laurel sulfate*. Laurel sulfate is *amphipathic* and is often used in
shampoo. Is the **polar head** located on the **right-hand _or_ left-hand** end of the molecule as it is
illustrated below?

laurel sulfate

Dilutions

Dilution is the process of **adding** more *solvent* to a solution.

A series of dilutions (left to right) of an aqueous solution containing a colored solute.

When considering *dilutions*, the **concentration** of the solution is *inversely proportional* to the volume of the solution.

- For example, if enough solvent is added to *double* the volume, then the **concentration** is *decreased by a factor of 1/2*.

As you saw in chapter 5 with Boyle's gas law, when properties are *inversely proportional*, the **product** of the *initial* and *final* properties are **equal**.

In the case of dilution, the **product** of the initial (un-diluted) concentration (C_1) and the volume before dilution (V_1) *is equal to* the **product** of the final (diluted) concentration (C_2) and the final volume (V_2):

$$C_1 \cdot V_1 = C_2 \cdot V_2$$

This equation is called the "_____ _____" and it can be used with any of the concentration units of measure that include the *volume of solution* (molarity, osmolarity, % (w/v), % (v/v), or Eq/L).

- For example, the dilution equation can be written using **molarity (M)** concentration:

$$M_1 \cdot V_1 = M_2 \cdot V_2$$

Example: You begin with 25 mL of a 1.8 M aqueous LiCl solution and add enough water to give a final volume of 35 mL. What is the new concentration?

$$\boxed{\textbf{Strategy: } M_1 \cdot V_1 = M_2 \cdot V_2}$$

$$\frac{M_1\,V_1}{V_2} = \frac{M_2\,\cancel{V_2}}{\cancel{V_2}}$$

$M_1 = 1.8$ M	$M_2 = ?$
$V_1 = 25$ mL	$V_2 = 35$ mL

$$M_2 = \frac{M_1\,V_1}{V_2} = \frac{(1.8\text{ M})\ (25\ \cancel{\text{mL}})}{(35\ \cancel{\text{mL}})} = \textbf{1.3 M}$$

Understanding Check

If 1.70 L of a 1.50 M solution is diluted to a final volume of 3.50 L, what is the final concentration?

Colloids and Suspensions

When particles that are larger than typical molecules or ions are put into another medium, typically water, the resulting mixture is classified as either a **colloid** or a **suspension** depending on the _____ _____.

In _____, the dispersed particles (***colloidal particles***) are small enough that they ***do not*** settle *to the bottom of their container*.

Conversely, in _____, the solid particles are large enough that gravity causes them to *settle to the bottom of their container* unless the mixture is repeatedly or constantly stirred or shaken.

Colloids

Colloidal particles are typically in the size range of ***1 nanometer up to 1 micrometer***.

Because of their relatively small size, the kinetic energy from collisions with the particles making up the medium, typically water molecules, overcomes the force of gravity and the particles remain evenly dispersed in the medium.

If the particles are very small, the colloid will not "scatter" light and it will therefore appear clear or colored (but not cloudy). As the particle size gets larger, a colloid mixture will appear cloudy since the light entering the medium is scattered in many different directions by particles.

The ***micelles*** that you learned about in this chapter are examples of colloids.

Another example of a colloid is milk.

- Milk contains small agglomerations of many individual protein molecules (these particles are called "casein") as well as particles composed of emulsified fat (triglyceride) molecules. It is these fat particles that are separated from milk to make butter. Milk is classified as a *colloid* rather than a *suspension* because the colloidal particles do not settle to the bottom. Note that milk containers do not say "*shake well before using*" because the particles are small enough to remain evenly dispersed.

Other examples of colloids are mayonnaise and hand lotion.

Suspensions

The solid particles contained in **suspensions** are typically larger than 1 micrometer.

Because of their relatively large size compared to colloidal particles, the force of gravity causes the particles to settle to the bottom of the container. The settling process may take seconds or several hours. When stirred or shaken, the suspension will appear cloudy since the particles are large enough to scatter light.

An example of a suspension is muddy water.

- If muddy water is constantly stirred, the clay/dirt particles are evenly distributed throughout the container; however, if the stirring is discontinued, the particles will settle to the bottom of the container.

Another example of a suspension is orange juice.

If a liquid contains solid particles and is labeled "_____ _____ before using," then ***it is a suspension***.

Understanding Check

If sand is added to a glass of water, is the resulting mixture a colloid or suspension?

Diffusion and Osmosis

Diffusion

Just like gases, solute and solvent particles in liquid phase solutions travel in random directions until they collide with other particles or the container wall.

This type of random movement is called **Brownian motion** and results in a process called _____.

Diffusion is defined as the net transport of a substance, due to *Brownian motion,* from a region of _____ concentration of the substance to a region of _____ concentration of the substance.

It is the random movement of particles that causes them to be evenly mixed.

In the diffusion process, substances will **spontaneously** move from an area of **greater concentration** (of the particular substance) **to lesser concentration** until it is evenly distributed.

H₂O Molecule

Food Coloring Molecule

Before Diffusion of Food Coloring Molecules Occurs

After Diffusion of Food Coloring Molecules Occurs
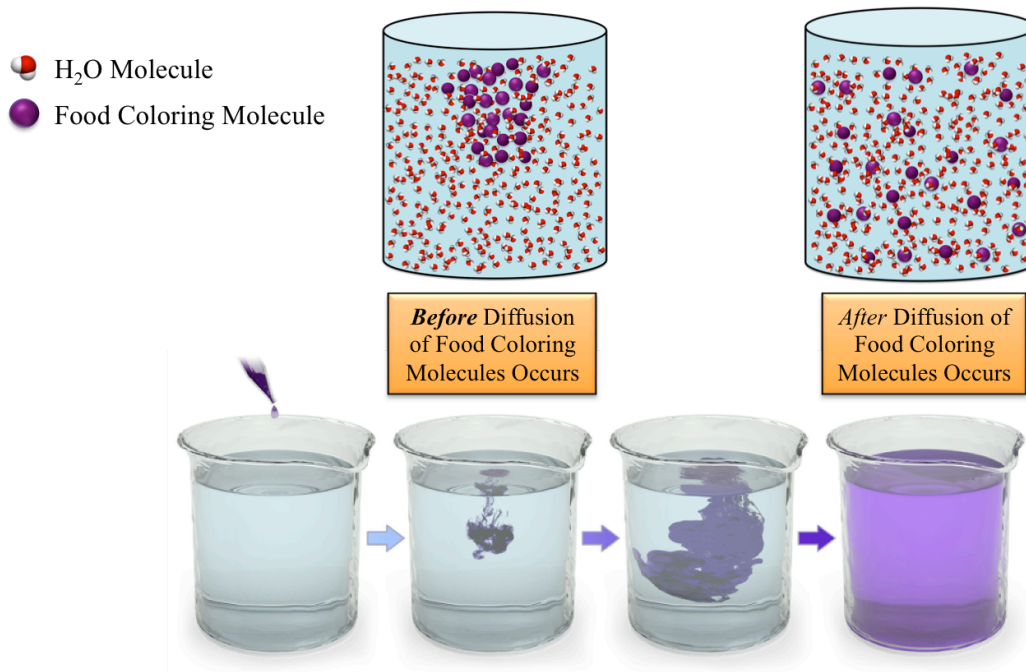
When a substance is not evenly distributed and has a **greater concentration** in one region and a **lesser concentration** in another region, we say that there is a "_____ _____."

_____ a **concentration gradient** is present, and there is not a physical barrier preventing transport, diffusion will occur.

- We say that the diffusing species move "_____ *the concentration gradient*."

There can only be a net movement of dissolved particles from areas of **lesser concentration** to areas of **greater concentration** (**against** the concentration gradient) **when external _____ is supplied**.

Osmosis

A _____ _____ is any type of physical barrier through which only certain substances can pass.

- For example, many membranes, both natural and synthetic, are **permeable** to water (allow water to pass) but are **impermeable** to ions (do not allow ions to pass).

As a general rule, *biological membranes* in cells, are **permeable** to nonpolar molecules and small polar molecules, and are **impermeable** to ions and large polar molecules.

Water molecules pass through holes (pores) in biological membranes called **aquaporins**.

Osmosis *is the net transport of* _____ *from a solution with a **lesser solute** particle concentration through a semipermeable membrane t*o a solution with a **greater solute** particle concentration.

Note that a semipermeable membrane allows **solvent** to *continuously* move *back and forth **between both sides of a membrane***; however, in **osmosis**, there is a greater amount of solvent transported in the direction from the side of the membrane with **lesser solute** particle concentration to the side of the membrane with **greater solute** particle concentration, resulting in a **net (overall) transport of solvent** in that direction.

We will only discuss osmosis for **aqueous solutions**, therefore for our purposes, **osmosis** *is the net transport of* _____ _____ *from a* solution with a **lesser solute** particle concentration *through a semipermeable membrane* to a solution with a **greater solute** particle concentration.

Osmosis is very important in biology because cell membranes are semipermeable.

The difference in solute particle concentration (osmolarity) between the _____ of the cell and the _____ solution has important implications in maintaining the viability of the cell.
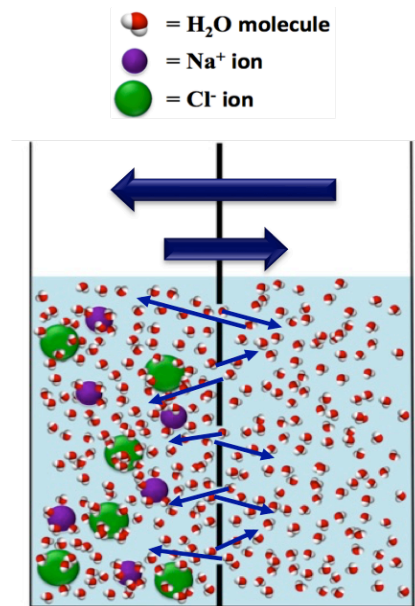
Consider the three different cases for *the solution that surrounds a cell*:

Microscope Images of Human Red Blood Cells in Hypertonic, Isotonic, and Hypotonic Solutions
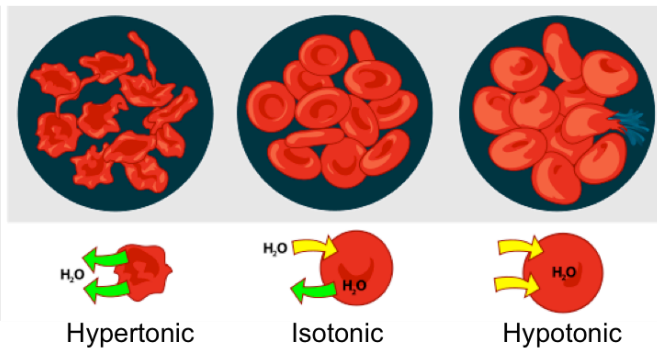
1. In a _____ **solution**, there is a greater solute particle concentration outside the cell than inside of the cell, so there is a net flow of water from the inside to the outside of the cell. This results in the shrinking of the cell.

2. In an _____ **solution**, the concentration of solute particles is the same on the inside and outside of the cell, therefore the flow of water in and out of the cell *are equal* and the cell maintains it natural and healthy (viable) shape.

3. In a _____ **solution**, there is a lesser solute particle concentration outside the cell than inside the cell, and there is a net flow of water from the outside to the inside of the cell. This results in the swelling and possible bursting of the cell.

The pressure associated with the *transport of water* in the osmosis process is called _____ _____.

Initial State:
Equal amounts of liquid are placed on opposite sides of a membrane. Saltwater on one side and pure water on the other side.

Osmosis

Final State:
Water molecules moved from the chamber with pure water (right side) to the side with greater solute concentration (left side):

The water levels change *until* the pressure caused from the difference in water column heights **is equal to the *osmotic pressure***.

The greater the difference in _____ between each side of the semipermeable membrane, the greater the ***osmotic pressure***.

For membranes that form a continuous enclosure around a solution, such as those of biological cells, the *osmotic pressure* is the pressure required to stop the net transport of water into *or* out of cells.
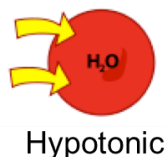
When the solution around a cell becomes ***hypotonic***, there is a lesser solute particle concentration outside the cell than inside the cell, and therefore there is a net flow of water from the outside to the inside of the cell.

As water flows into the cell, the pressure on the inside of the cell increases (imagine inflating a balloon).

The pressure in the cell will continue to increase until either (1) the ***osmotic pressure*** is reached and osmosis stops, **or** (2) the cell bursts. The bursting of red blood cells is called *hemolysis* and is evidenced by the appearance of red color in the blood *plasma*.

H₂O

Hypotonic

Understanding Check: Which of the following systems (#1 or #2) would have a ***greater* osmotic pressure**:

System #1: 1.00 M sodium chloride on one side of a semipermeable membrane and pure water on the other side.

or

System #2: 0.500 M sodium chloride on one side of a semipermeable membrane and pure water on the other side.

HINT: The greater the **difference in osmolarity** between each side of the semipermeable membrane, the **greater** the *osmotic pressure*.

Understanding Check:
Which of the following systems (#1 or #2) would have a ***greater* osmotic pressure**:

System #1: 1.00 M NaCl on one side of a semipermeable membrane and pure water on the other side.

or

System #2: 1.00 M $Fe_2(SO_4)_3$ on one side of a semipermeable membrane and pure water on the other side.

Calculations for Solutions Worksheet and Key

1) 23.5g of NaCl is dissolved in enough water to make .683 L of solution.

        a) What is the **molarity (M)** of the solution?

        b) How many **moles** of NaCl are contained in 0.0100 L of the above NaCl solution?

        c) What **volume (L)** of this NaCl solution would contain 0.200 moles of NaCl?

2) 12.5g of glucose ($C_6H_{12}O_6$) is dissolved in enough water to make 750.0 mL of solution.

        a) What is the **molarity (M)** of the solution?

        b) How many **moles** of glucose are contained in 237 mL of the above glucose solution?

        c) What **volume (L)** of this glucose solution would contain 0.079 moles of glucose?

3) 45.7 g of magnesium chloride ($MgCl_2$) is dissolved in 2.40 kg of water.

a) What is the **molality (*m*)** of the solution?

b) How many **moles** of $MgCl_2$ are contained in 1.76 kg of solvent?

c) How many kg of **solvent** would contain 0.0150 moles of $MgCl_2$?

4) 114.5 g of KCl is dissolved in enough water to make 3.6 L of solution.

a) How many **osmoles** are in **one mole** of KCl when it dissolves?

b) What is the **osmolarity** of the solution?

c) How many **osmoles** are contained in 1.00 L of the above potassium chloride solution?

d) How many liters (L) of **this potassium chloride solution** would contain 0.350 osmoles?

5) 7.58 g of 2-propanol (C_3H_8O) is added to enough water to make 1.50 L of solution.

   a) How many **osmoles** are in **one mole** of 2-propanol when it dissolves?

   b) What is the **osmolarity** of the solution?

   c) How many **osmoles** are contained in 25.00 mL of the above 2-propanol solution?

   d) How many liters (L) of **this 2-propanol solution** would contain 0.00575 osmoles?

6) 46.0 g of barium nitrate is dissolved in 2.60 kg of water.

   a) How many **osmoles** are in **one mole** of barium nitrate when it dissolves?

   b) What is the **osmolality** of the solution?

7) A glucose ($C_6H_{12}O_6$) solution is prepared by adding 5.00 grams of glucose to enough water to make 200.0 ml of solution.

   a) What is the %(w/v) of the solution?

   b) What volume (mL) of this solution would contain 0.0735 grams of glucose?

   c) How many grams of glucose would be present in 185 mL of this solution?

8) 234.5 g of KCl is dissolved in enough water to make 3.6 L of solution.

a) How many **equivalents of potassium (K^+)** are in **one mole** of KCl when it dissolves?
(note: you are concerned with the Eq from K^+ *only*, do not include Eq from Cl^-**)**

b) What is the concentration of **potassium** in **(Eq/L)**?

c) How many **equivalents (Eq) of** K^+ are contained in 0.700 L of the above potassium chloride solution?

d) How many liters (L) of this potassium chloride solution would contain **0.050 equivalents Eq of K^+**?

9) 0.250 g of aluminum sulfate is dissolved in enough water to make 150 **mL** of solution.

a) How many **equivalents of sulfate ion (SO_4^{2-})** are in **one mole** of aluminum sulfate when it dissolves?
(note: you are concerned with the Eq from SO_4^{2-} *only*, do not include Eq from Al^+**)**

b) What is the concentration of **sulfate** in **(Eq/L)**?

c) How many **equivalents (Eq) of** SO_4^{2-} are contained in **0.0280 L** of the above aluminum sulfate solution?

d) How many liters (L) of this aluminum sulfate solution would contain **0.0025 equivalents Eq of SO_4^{2-}**?

Molarity calculations (fill-in all the boxes)

solute	moles of solute	grams of solute	volume of solution	Concentration (Molarity, M=mole/L)
NaCl	3.00 moles		0.500 L	
NaCl		13.5 g	0.150 L	
NaCl	0.375 moles			1.00 M
NaCl		0.059 g		0.30 M
KNO_3	1.57 moles			0.770 M
KNO_3		1.98 g		2.00 M
KNO_3			0.288 L	0.197 M

Osmolarity calculations

solute	moles of solute	osmoles of solute	grams of solute	volume of solution	Concentration (Osmolar = **osmole/L**)
KCl	2.40 moles			0.600 L	
KCl			1.5 g	0.750 L	
KCl	0.050 moles				1.00 osmolar
KCl			0.892 g		0.150 osmolar
glucose $C_6H_{12}O_6$	1.50 moles				1.22 osmolar
glucose $C_6H_{12}O_6$			1.17 g		0.0100 osmolar
glucose $C_6H_{12}O_6$				0.375 L	0.0750 osmolar

Key

1) 23.5g of NaCl is dissolved in enough water to make .683 L of solution.

   a) What is the **molarity (M)** of the solution?

   Molar mass of NaCl = 58.44 g/mole

   Moles of NaCl:

   $$\frac{23.5 \text{ g NaCl}}{} \left| \frac{1 \text{ mole NaCl}}{58.44 \text{ g NaCl}} \right. = .402 \text{ moles NaCl}$$

   Molarity $= \left(\dfrac{\text{moles}}{\text{liter solution}} \right) = \left(\dfrac{0.402 \text{ moles NaCl}}{0.683 \text{ L of solution}} \right) = 0.589$ moles NaCl/L = **0.589 M NaCl**

   b) How many **moles** of NaCl are contained in 0.0100 L of the above NaCl solution?

   | **Concentration of the solution** |

   $$\frac{0.0100 \text{ L solution}}{} \left| \frac{0.589 \text{ moles NaCl}}{\text{L of solution}} \right. = \textbf{0.00589 mole NaCl}$$

   - Note: The concentration gives us the relationship between the **amount of solute** and **the amount of solution**....we use the *concentration* as a **conversion factor**!!!!

   c) What **volume (L)** of this NaCl solution would contain 0.200 moles of NaCl?

   | **Concentration of the solution** |

   $$\frac{0.200 \text{ moles of NaCl}}{} \left| \frac{\text{L of solution}}{0.589 \text{ moles NaCl}} \right. = \textbf{.340 L of solution}$$

2) 12.5g of glucose ($C_6H_{12}O_6$) is dissolved in enough water to make 750.0 mL of solution.

   a) What is the **molarity (M)** of the solution?

   Molar mass of glucose = 180.18 g/mole

   Moles of glucose:

   $$\frac{12.5 \text{ g glucose}}{} \left| \frac{1 \text{ mole glucose}}{180.18 \text{ g glucose}} \right. = 0.0694 \text{ moles glucose}$$

   Molarity $= \left(\dfrac{\text{moles}}{\text{liter solution}} \right) = \left(\dfrac{0.0694 \text{ moles glucose}}{0.7500 \text{ L of solution}} \right) = 0.0925$ mole glucose/L = **0.0925 M glucose**

   b) How many **moles** of glucose are contained in 237 mL of the above glucose solution?

   $$\frac{0.237 \text{ L solution}}{} \left| \frac{0.0925 \text{ moles glucose}}{\text{L of solution}} \right. = \textbf{0.0219 mole glucose}$$

c) What **volume (L)** of this glucose solution would contain 0.079 moles of glucose?

$$\frac{0.079 \text{ moles glucose}}{} \left| \frac{\text{L of solution}}{0.0925 \text{ moles glucose}} \right. = \textbf{0.85 L of solution}$$

3) 45.7 g of magnesium chloride ($MgCl_2$) is dissolved in 2.40 kg of water.

a) What is the **molality (m)** of the solution?

Molar mass of $MgCl_2$ = 95.21 g/mole

Moles of $MgCl_2$:

$$\frac{45.7 \text{ g } MgCl_2}{} \left| \frac{1 \text{ mole } MgCl_2}{95.21 \text{ g } MgCl_2} \right. = 0.480 \text{ moles } MgCl_2$$

Molality $= \left(\dfrac{\text{moles}}{\text{kg of solvent}} \right) = \left(\dfrac{0.480 \text{ moles } MgCl_2}{2.40 \text{ kg of solvent}} \right) = 0.200 \text{ moles } MgCl_2 \text{ /kg} = \textbf{0.200 } \textit{m} \textbf{ } MgCl_2$

b) How many **moles** of $MgCl_2$ are contained in 1.76 kg of solvent?

Concentration of the solution

$$\frac{1.76 \text{ kg solvent}}{} \left| \frac{0.200 \text{ moles } MgCl_2}{1 \text{ kg of solvent}} \right. = \textbf{0.352 moles } MgCl_2$$

c) How many kg of **solvent** would contain 0.0150 moles of $MgCl_2$?

Concentration of the solution

$$\frac{0.0150 \text{ moles } MgCl_2}{} \left| \frac{1 \text{ kg of solvent}}{0.200 \text{ moles } MgCl_2} \right. = \textbf{0.0750 kg of solvent}$$

4) 114.5 g of KCl is dissolved in enough water to make 3.6 L of solution.

a) How many **osmoles** are in **one mole** of KCl when it dissolves?

one mole of KCl = 2 **osmoles**

- This relationship can be used as a **conversion factor** to *convert* between **moles** and **osmoles**:

$$\left(\frac{\textbf{2 osmoles}}{\textbf{1 mole } KCl} \right) \quad \text{or} \quad \left(\frac{\textbf{1 mole } KCl}{\textbf{2 osmoles}} \right)$$

b) What is the **osmolarity** of the solution?
- First get the moles of KCl then convert to osmoles:

Molar mass of KCl = 74.55 g/mole
- Osmoles in solution:

114.5 g KCl	1 mole KCl	**2 osmoles**	= 3.072 osmoles
	74.55 g KCl	**1 mole KCl**	

$$\text{Osmolarity} = \left(\frac{\textbf{osmoles}}{\textbf{L of solution}} \right) = \left(\frac{3.072 \text{ osmoles}}{3.6 \text{ L of solution}} \right) = 0.85 \text{ osmoles /L solution} = \textbf{0.85 osmolar}$$

c) How many **osmoles** are contained in 1.00 L of the above potassium chloride solution?

Concentration of the solution		
1.00 L solution	0.85 osmoles	= **0.85 osmoles**
	L of solution	

- As in the case of molarity (M) and molality (*m*) , the concentration (os*molarity* this time) gives us the relationship between the **amount of solute** and **the amount of solution**....we use the *concentration* as a **conversion factor**!!!!

d) How many liters (L) of **this potassium chloride solution** would contain 0.350 osmoles?

0.350 osmoles	L of solution	= **0.41 L of solution**
	0.85 osmoles	

5) 7.58 g of 2-propanol (C_3H_8O) is added to enough water to make 1.50 L of solution.

a) How many **osmoles** are in **one mole** of 2-propanol when it dissolves?
one mole of 2-propanol = **one osmole** (2-propanol does not dissociate into ions)

b) What is the **osmolarity** of the solution?
Molar mass of 2-propanol = 60.11 g/mole
- Osmoles in solution:

7.58 g 2-propanol	1 mole 2-propanol	**1 osmole**	= 0.126 osmoles
	60.11 g 2-propanol	**1 mole 2-propanol**	

$$\text{Osmolarity} = \left(\frac{\textbf{osmoles}}{\textbf{L of solution}} \right) = \left(\frac{0.126 \text{ osmoles}}{1.50 \text{ L of solution}} \right) = 0.0840 \text{ osmoles /L solution}$$

$$= \textbf{0.0840 osmolar}$$

c) How many **osmoles** are contained in 25.00 mL of the above 2-propanol solution?

$$\frac{0.02500 \; \text{L solution}}{} \; \Bigg| \; \frac{0.0840 \; \text{osmoles}}{\text{L of solution}} \; = \; \textbf{0.00210 osmoles}$$

d) How many liters (L) of **this 2-propanol solution** would contain 0.00575 osmoles?

$$\frac{0.00575 \; \text{osmoles}}{} \; \Bigg| \; \frac{\text{L of solution}}{0.0840 \; \text{osmoles}} \; = \; \textbf{0.0685 L of solution}$$

6) 46.0 g of barium nitrate is dissolved in 2.60 kg of water.

a) How many **osmoles** are in **one mole** of barium nitrate when it dissolves?

one mole of $Ba(NO_3)_2 = $ 3 **osmoles**

- $Ba(NO_3)_2$ dissociates into 3 particles, one Ba^{2+} ion and 2 nitrate ions
- This relationship can be used as a **conversion factor** to *convert* between **moles** and **osmoles**:

$$\left(\frac{\textbf{3 osmoles}}{\textbf{1 mole } Ba(NO_3)_2} \right) \quad \text{or} \quad \left(\frac{\textbf{1 mole } Ba(NO_3)_2}{\textbf{3 osmoles}} \right)$$

b) What is the **osmolality** of the solution?

Molar mass of $Ba(NO_3)_2$ = 261.35 g/mole

- Osmoles in solution :

$$\frac{46.0 \; \text{g } Ba(NO_3)_2}{} \; \Bigg| \; \frac{1 \; \text{mole } Ba(NO_3)_2}{261.35 \; \text{g } Ba(NO_3)_2} \; \Bigg| \; \frac{\textbf{3 osmoles}}{1 \; \text{mole } Ba(NO_3)_2} \; = \; 0.528 \; \textbf{osmoles } Ba(NO_3)_2$$

$$\text{Osmolality} = \left(\frac{\textbf{osmoles}}{\textbf{kg of solvent}} \right) = \left(\frac{0.528 \; \text{osmoles}}{2.60 \; \text{kg of solvent}} \right) = 0.203 \; \text{osmoles/kg}$$

$$= \textbf{0.203 osmolal}$$

7) A glucose ($C_6H_{12}O_6$) solution is prepared by adding 5.00 grams of glucose to enough water to make 200.0 ml of solution.

a) What is the %(w/v) of the solution?

$$\%(w/v) = \left(\frac{\textbf{g solute}}{\textbf{mL of solution}} \right) \times 100 = \left(\frac{5.00 \; \text{g glucose}}{200.0 \; \text{mL}} \right) \times 100\% = \textbf{2.50 \% (w/v)}$$

b) What volume (mL) of this solution would contain 0.0735 grams of glucose?
- Use the concentration as a conversion factor!

$$\frac{0.0735 \text{ g glucose}}{} \quad \frac{100. \text{ mL}}{2.50 \text{ g glucose}} \quad = \textbf{2.94 mL of solution}$$

Note: 2.50 % (w/v) means there are 2.50 g in 100 mL of solution = your conversion factor.

c) How many grams of glucose would be present in 185 mL of this solution?
- Use the concentration as a conversion factor!

$$\frac{185 \text{ mL solution}}{} \quad \frac{2.50 \text{ g glucose}}{100. \text{ mL solution}} \quad = \textbf{4.63 g glucose}$$

8) 234.5 g of KCl is dissolved in enough water to make 3.6 L of solution.

a) How many **equivalents of potassium (K$^+$)** are in **one mole** of KCl when it dissolves?
one mole of KCl = 1 **Eq K$^+$** (recall that an equivalent is a mole of charge)
- This relationship can be used as a **conversion factor** to *convert* between **moles** and **equivalents**:

$$\left(\frac{\textbf{1 Eq K}^+}{\textbf{1 mole KCl}} \right) \quad \text{or} \quad \left(\frac{\textbf{1 mole KCl}}{\textbf{1 Eq K}^+} \right)$$

b) What is the concentration from **potassium** in **(Eq K$^+$/L)**?
- First get the moles of KCl then convert **equivalents (Eq)**:
Molar mass of KCl = 74.55 g/mole
- **Equivalents (Eq)** in solution :

$$\frac{234.5 \text{ g KCl}}{} \quad \frac{1 \text{ mole KCl}}{74.55 \text{ g KCl}} \quad \frac{\textbf{1 Eq K}^+}{1 \text{ mole KCl}} \quad = \textbf{3.146 Eq K}^+$$

$$\textbf{(Eq/L)} = \left(\frac{\textbf{\# Eq K}^+}{\textbf{L of solution}} \right) = \left(\frac{3.146 \text{ Eq K}^+}{3.6 \text{ L of solution}} \right) = \textbf{0.87 Eq K}^+\textbf{/L solution}$$

c) How many **equivalents Eq of K⁺** are contained in 0.700 L of the above potassium chloride solution?

- As in the case of molarity (M), the concentration (**Eq/L** this time) gives us the relationship between the **amount of solute** and **the amount of solution**....we use the *concentration* as a **conversion factor**!!!!

Concentration of potassium ions in solution		
0.700 ~~L solution~~	$\dfrac{0.87 \text{ Eq K}^+}{\text{~~L of solution~~}}$	= **0.61 Eq K⁺**

d) How many liters (L) of this potassium chloride solution would contain **0.050 equivalents Eq of K⁺** ?

0.050 ~~Eq K⁺~~	$\dfrac{1 \text{ L of solution}}{0.87 \text{ ~~Eq K⁺~~}}$	= **0.057 L of solution**

9) 0.250 g of aluminum sulfate is dissolved in enough water to make 150 mL of solution.

a) How many **equivalents of sulfate ion (SO$_4^{2-}$)** are in **one mole** of aluminum sulfate when it dissolves?
one mole of Al$_2$(SO$_4$)$_3$ = 6 **Eq SO$_4^{2-}$** (recall that an equivalent is a mole of charge/mole of compound)
  - **3 moles sulfate ions x (2 moles of charge/1 mole sulfate ions) = 6 Eq**

- This relationship can be used as a **conversion factor** to *convert* between **moles** and **equivalents**:

$$\left(\frac{6 \text{ Eq SO}_4^{2-}}{1 \text{ mole Al}_2(\text{SO}_4)_3} \right) \quad \text{or} \quad \left(\frac{1 \text{ mole Al}_2(\text{SO}_4)_3}{6 \text{ Eq SO}_4^{2-}} \right)$$

b) What is the concentration of **sulfate** in **(Eq/L)**?

- First get the moles of Al$_2$(SO$_4$)$_3$ then convert **equivalents (Eq)**:
Molar mass of Al$_2$(SO$_4$)$_3$= 342.17 g/mole
- **Equivalents (Eq)** in solution :

0.250 g ~~Al₂(SO₄)~~	$\dfrac{1 \text{ mole ~~Al₂(SO₄)₃~~}}{342.17 \text{ g ~~Al₂(SO₄)₃~~}}$	$\dfrac{6 \text{ Eq SO}_4^{2-}}{1 \text{ ~~mole Al₂(SO₄)₃~~}}$	= **0.00438 Eq SO$_4^{2-}$**

  - Note: we must convert from **mL** of solution to **L** of solution

(Eq/L) = $\left(\dfrac{\text{\# Eq SO}_4^{2-}}{\text{L of solution}} \right)$ = $\left(\dfrac{0.00438 \text{ Eq SO}_4^{2-}}{0.15 \text{ L of solution}} \right)$ = **0.029 Eq SO$_4^{2-}$/L solution**

c) How many **equivalents (Eq) of SO_4^{2-}** are contained in **0.0280 L** of the above aluminum sulfate solution?

- As in the case of molarity (M), the concentration (**Eq/L** in this case) gives us the relationship between the **amount of solute** and **the amount of solution**….we use the *concentration* as a **conversion factor**!!!!

Concentration of sulfate ions in solution	

$$\frac{0.0280 \text{ L solution}}{} \times \frac{0.029 \text{ Eq } SO_4^{2-}}{\text{L of solution}} = \textbf{0.00081 Eq } SO_4^{2-}$$

d) How many liters (L) of this aluminum sulfate solution would contain **0.0025 equivalents Eq of SO_4^{2-}**?

$$\frac{0.0025 \text{ Eq } SO_4^{2-}}{} \times \frac{1 \text{ L of solution}}{0.029 \text{ Eq } SO_4^{2-}} = \textbf{0.086 L of solution}$$

Molarity calculations (fill-in all the boxes)

solute	moles of solute	grams of solute	volume of solution	Concentration (Molarity, M=mole/L)
NaCl	3.00 moles	**175 g**	0.500 L	**6.00 M**
NaCl	.231 moles	13.5 g	.150 L	**1.54 M**
NaCl	.375 moles	**21.9 g**	**.375 L**	1.00 M
NaCl	**.0010 moles**	.059 g	**.0033 L**	0.30 M
KNO$_3$	1.57 moles	**159 g**	**2.04 L**	.770 M
KNO$_3$	**.0196 moles**	1.98 g	**.00980 L**	2.00 M
KNO$_3$	**.0567 moles**	**5.73 g**	.288 L	.197 M

Osmolarity calculations

solute	moles of solute	osmoles of solute	grams of solute	volume of solution	Concentration (Osmolar = **Osmole/L**)
KCl	2.40 moles	**4.80 osmoles**	**179 g**	0.600 L	**8.00 osmolar**
KCl	0.020 moles	**0.040 osmoles**	1.5 g	0.750 L	**0.053 osmolar**
KCl	.050 moles	**0.10 osmoles**	**3.7 g**	**0.10 L**	1.00 osmolar
KCl	**0.0120 moles**	0.0240 osmoles	0.892 g	**0.160 L**	0.150 osmolar
glucose C$_6$H$_{12}$O$_6$	1.50 moles	**1.50 osmoles**	**270. g**	**1.23 L**	1.22 osmolar
glucose C$_6$H$_{12}$O$_6$	**0.00649 moles**	**0.00649 osmoles**	1.17 g	**.649 L**	0.0100 osmolar
glucose C$_6$H$_{12}$O$_6$	**0.0281 moles**	**0.0281 osmoles**	**5.06 g**	0.375 L	0.0750 osmolar

Chapter 7 Worksheet:
Reactions in Solution

For each reaction below, determine if and what type of reaction will occur (under "REACTION TYPE" write either: precipitation, gas forming, or no reaction), **predict the products** for the reaction, and then write a **balanced chemical equation**. For those which do not react, indicate this by writing "No Reaction." for the products in the equation.

REACTION TYPE

iron (III) chloride + sodium carbonate

_____

copper (II) sulfate + ammonium hydroxide

_____

barium nitrate + lithium sulfate

_____

magnesium chloride + silver nitrate

_____

aluminum sulfate + calcium hydroxide

_____

lead (II) nitrate + sodium chloride

_____

Aluminum Nitrate + Potassium Iodide

_____

magnesium iodide + sodium carbonate

_____

sodium bicarbonate + hydrochloric acid

_____

KEY

Iron (III) chloride + sodium carbonate…………………………….............Precipitation

$2FeCl_3(aq) + 3Na_2CO_3(aq) \rightarrow Fe_2(CO_3)_3(s) + 6NaCl(aq)$

Copper (II) sulfate + ammonium hydroxide……………………….............Precipitation

$CuSO_4(aq) + 2 NH_4OH(aq) \rightarrow Cu(OH)_2(s) + (NH_4)_2SO_4 (aq)$
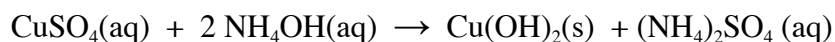
Barium nitrate + lithium sulfate……………………..………………............Precipitation

$Ba(NO_3)_2(aq) + Li_2SO_4 (aq) \rightarrow 2 LiNO_3(aq) + BaSO_4 (s)$
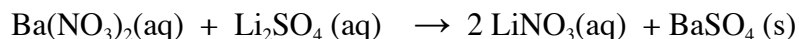
Magnesium chloride + silver nitrate……………………………….............Precipitation

$MgCl_2(aq) + 2 AgNO_3 (aq) \rightarrow Mg(NO_3)_2(aq) + 2 AgCl (s)$

Aluminum sulfate + calcium hydroxide……………………….................Precipitation

$Al_2(SO_4)_3(aq) + 3 Ca(OH)_2(aq) \rightarrow 2 Al(OH)_3(s) + 3CaSO_4 (aq)$
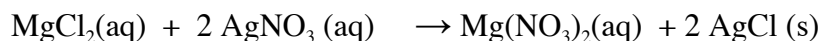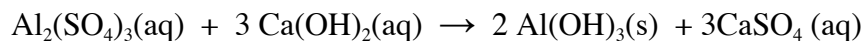
Lead (II) nitrate + sodium chloride………………….....…………............Precipitation

$Pb(NO_3)_2(aq) + 2 NaCl (aq) \rightarrow PbCl_2(s) + 2 NaNO_3 (aq)$
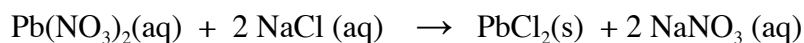
Aluminum Nitrate + Potassium Iodide…….….................................…….............NO REACTION
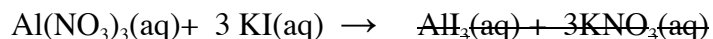
$Al(NO_3)_3(aq) + 3 KI(aq) \rightarrow$ ~~$AlI_3(aq) + 3KNO_3(aq)$~~

Magnesium iodide + sodium carbonate…………………….………..............Precipitation

$MgI_2(aq) + Na_2CO_3 (aq) \rightarrow 2 NaI(aq) + MgCO_3 (s)$
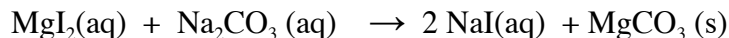
Sodium bicarbonate + hydrochloric acid…………………………..............Gas Forming

$NaHCO_3(aq) + HCl(aq) \rightarrow CO_2(g) + H_2O(l) + NaCl(aq)$
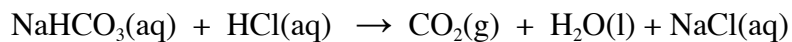
NOTE: initially forms $H_2CO_3(aq)$ but then it decomposes to $CO_2(g) + H_2O(l)$

Chapter 8 Lecture Notes: Acids, Bases, and pH

Educational Goals

1. Given a chemical equation, write the **law of mass action**.

2. Given the **equilibrium constant** (K_{eq}) for a reaction, predict whether the reactants or products are predominant.

3. Use **Le Châtelier's Principle** to explain how a chemical reaction at equilibrium responds when a change is made to the concentration of reactant or product.

4. Know the definitions of Bronsted-Lowry acids and bases.

5. Given the *acid form* or the *base form* of a **conjugate pair**, identify its conjugate.

6. List the properties of **acidic** and **basic solutions**.

7. Understand the term "**acid strength**," and know how acid strength is related to the **acidity constant** (K_a) value.

8. Given the $[H_3O^+]$, be able to calculate the $[OH^-]$ (and vice versa).

9. Given the $[H_3O^+]$, be able to calculate the pH (and vice versa).

10. Given the $[H_3O^+]$, $[OH^-]$, or pH, be able to characterize a solution as being **acidic**, **basic**, or **neutral**.

11. Given the reactants, predict the products of a **neutralization reaction**.

12. Given the pH of a solution and the pK_a for a particular acid, determine whether the acid or base form of a conjugate pair is predominant.

13. Define a **buffer**, and describe how a buffer solution is made.

In this chapter, you will learn what is meant by the terms **acid, base, acidic, basic, and pH.**

You will learn about the chemical system called a "*buffer*" that is used in nature to control the pH in plants and animals.

In order for you to adequately understand acids, bases, pH, and buffers, I must begin this chapter by discussing a concept called _____ _____.

Chemical Equilibrium

In chapter 6, you learned about **chemical reactions.**

You learned that in chemical reactions, new chemical bonds are made and/or existing chemical bonds are broken, and in doing so, *reactants* are converted to new substances that we called *products*.

You learned to represent chemical reactions with *chemical equations* by writing the formulas of the reactants, then an arrow, followed by the formulas of the products.

What I did not tell you in chapter 6 is that the **products** can be converted _____ into **reactants**!

Example:

Dinitrogen tetroxide (N_2O_4) can undergo a decomposition reaction to produce two nitrogen dioxide (NO_2) molecules:

$$N_2O_4\,(g) \quad \longrightarrow \quad 2\,NO_2\,(g)$$
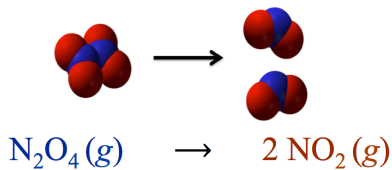
The **reaction** is _____; two NO_2 molecules can collide then bond with each other to form N_2O_4:

$$2\,NO_2\,(g) \quad \longrightarrow \quad N_2O_4\,(g)$$
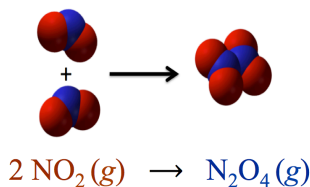
We use "double arrows" in **reversible** chemical reaction equations. For our example reaction, we write:

$$N_2O_4\,(g) \quad \rightleftarrows \quad 2\,NO_2\,(g)$$

forward reaction
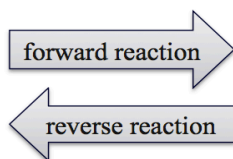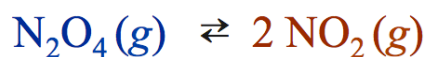
reverse reaction

Even though reversible reactions proceed in both *forward **and** reverse* directions, we use the convention of calling the substances on the left-hand side of the reaction arrows "reactants," and those on the right-hand side "products."

We call the process that occurs in the left-to-right direction (reactants to products) the " _____ **reaction**," and the process that occurs in the right-to-left direction (products to reactants) the " _____ **reaction**."

$$N_2O_4\,(g) \quad \rightleftarrows \quad 2\,NO_2\,(g)$$

The concentrations of N_2O_4 and NO_2 are **changing**.

Chemical Equilibrium: Concentrations of N_2O_4 and NO_2 are **no longer** changing.

N_2O_4

Amount Present: Concentrations of N_2O_4 and NO_2

NO_2

Time
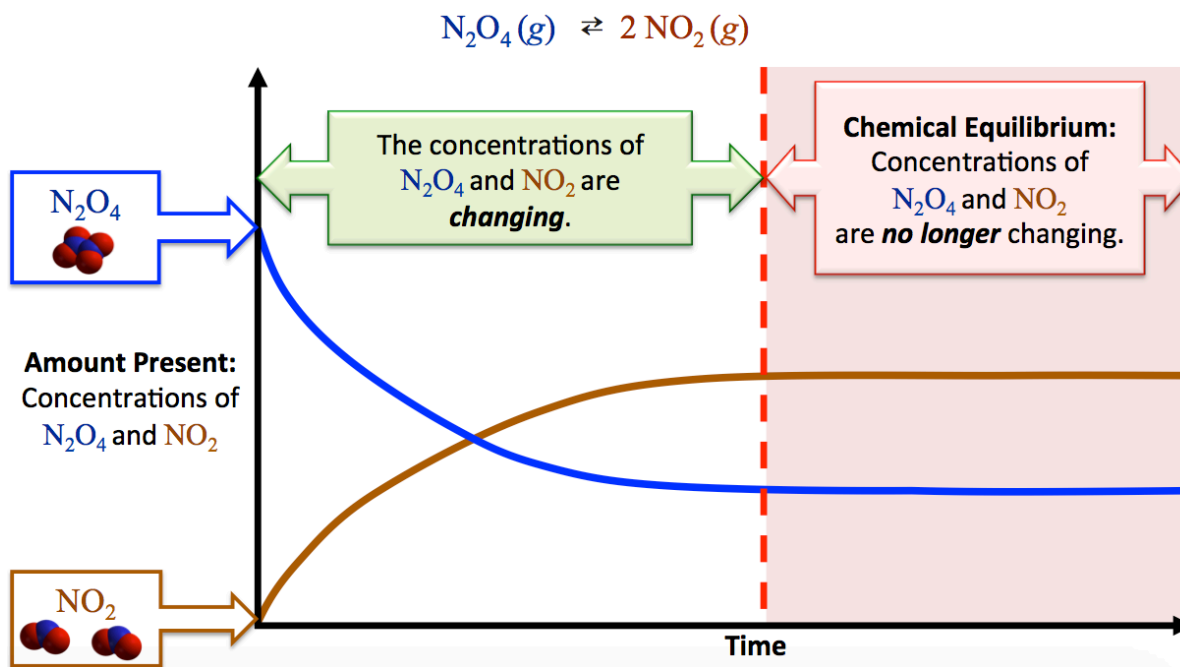
Chemical equilibrium is defined as the state in which the **rate** of the *forward reaction is* _____ to the rate of the *reverse reaction* and _____ of the reactants and products **do not change**.

2

Some chemical reactions reach equilibrium in a few seconds or less, others can take days (or longer).

Once chemical equilibrium has been reached, the concentrations of reactants and products remain constant unless a change is made to the system, such as adding or removing some products or reactants or changing the temperature.

If N_2O_4 (g) and NO_2 (g) are allowed to reach equilibrium and the equilibrium concentrations of each are measured, then the following will always be true:

$$\boxed{\text{concentrations in units of molarity}}$$

$$K_{eq} = \frac{[NO_2]^2}{[N_2O_4]}$$

$$\boxed{\text{equilibrium constant}}$$

Law of Mass Action

For any chemical reaction *at equilibrium*:

$$a\mathbf{A} \ + \ b\mathbf{B} \ \rightleftharpoons \ c\mathbf{C} \ + \ d\,\mathbf{D}$$

where *a*, *b*, *c*, and *d* are the *stoichiometric coefficients* for substances A, B, C, and D respectively, the concentrations of reactants and products must satisfy the *law of _____ _____*:

$$K_{eq} = \frac{[C]^c \ [D]^d}{[A]^a \ [B]^b} \quad \begin{array}{l} \boxed{\textit{products}} \\[4pt] \boxed{\textit{reactants}} \end{array}$$

The square brackets, **[ ]**, indicate concentration in _____, for example, "**[A]**" means "**molarity of substance A**."

The *law of mass action* is written by multiplying the concentration of the ***products*** (raised to their stoichiometric coefficient powers) in the _____, and multiplying the concentration of the ***reactants*** (raised to their stoichiometric coefficient powers) in the _____.

$\mathbf{K}_{eq}$ is called the _____ _____.

Each chemical reaction has its ***own*** equilibrium constant value.

- $\mathbf{K}_{eq}$ values for particular reactions are determined *experimentally* and are often tabulated in reference books or online.

- The value of the equilibrium constant for any particular reaction depends on temperature. Tabulated equilibrium constants usually indicate the temperature at which they were measured. The equilibrium constants used in the remainder of the book and videos are for reactions at (or close to) room temperature (25 °C).

The *law of mass action* is also referred to as the *equilibrium expression.*

IMPORTANT NOTE FOR EQUILIBRIUM EXPRESSIONS:

When solids (*s*) or liquids (*l*) are present as reactants and/or products, they are _____ *from the equilibrium expression*.

- The only substances that appear in the equilibrium expression are gases (*g*), aqueous (*aq*) solutes (or solutes dissolved in non aqueous solutions).

3

- **Example:**

  Write the *equilibrium expression* for the reaction of dissolved carbon dioxide and water:

  $$CO_2\,(aq)\ +\ H_2O\,(l)\ \rightleftharpoons\ H_2CO_3\,(aq)$$
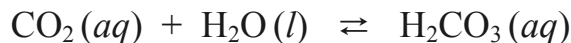
  NOTE: When solids (*s*) or liquids (*l*) are present as reactants and/or products, they are **omitted** *from the equilibrium expression*.

  $$K_{eq} = \frac{[H_2CO_3]}{[CO_2]}$$

Understanding Check: Write the *equilibrium expression* for the following reaction:

$$HCl\,(aq) + H_2O\,(l)\ \rightleftharpoons\ H_3O^+\,(aq) + Cl^-\,(aq)$$
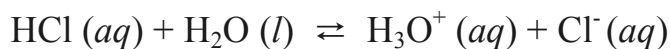
Equilibrium constants have been measured experimentally for many reactions. For example, in the reaction of boric acid (H_3BO_3) and water,

$$H_3BO_3\,(aq) + H_2O\,(l)\ \rightleftharpoons\ H_2BO_3^-\,(aq) + H_3O^+\,(aq)$$
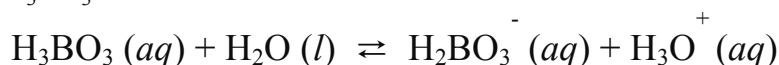
the equilibrium expression and the measured value of the equilibrium constant (K_{eq}) is:

$$K_{eq} = \frac{[H_2BO_3^-][H_3O^+]}{[H_3BO_3]} = 5.75 \times 10^{-10}\,M$$

The _____ of the equilibrium constant allows us to know the *relative* _____ of products vs. reactants that are present *at equilibrium* for a particular reaction.

If K_{eq} is *much greater* than **1**, then there are many more product species than reactant species present at equilibrium.

- In this case, we say that *the **products** are* _____ *at equilibrium*.

Conversely, if K_{eq} is *much less* than **1**, then there are many more reactant species than product species present at equilibrium.

- In this case, we say that *the **reactants** are **predominant** at equilibrium*.

Value of K_{eq}	Predominant Species
$K_{eq} \gg 1$	Products
$K_{eq} \ll 1$	Reactants

Understanding Check: For the reaction shown below, predict whether *the **reactants** or the **products** are **predominant** at equilibrium*.

$$HI\,(aq) + H_2O\,(l)\ \rightleftharpoons\ I^-\,(aq) + H_3O^+\,(aq) \qquad K_{eq} = 2.5 \times 10^{10}\,M$$

4
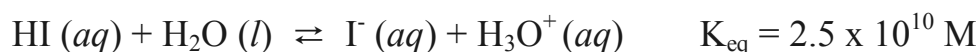
Le Châtelier's Principle

If a reaction is at equilibrium, and then *more* of one of the reactants is **added**, the system is *no longer in equilibrium*. Consider the general reaction:

$$A + B \rightleftarrows C + D$$

- When a reaction is *at equilibrium*, the forward rate *is equal to* the reverse rate, and the concentrations of reactants and products **are not changing**.

- If the concentration of reactant **A** or **B** is increased by *adding* more of substance **A** or **B,** this causes an increase in the rate of the *forward reaction* because there is now a greater probability of **A** colliding with **B** and then reacting.

- Upon the addition of substance **A** or **B**, substances **A** and **B** are converted to **C** and **D** at a faster forward rate than the reverse rate.

- This will continue to occur until enough of **C** and **D** are produced so that the reverse rate is once again equal to the forward rate and *equilibrium is reestablished*.

- A similar situation occurs if the concentration of one of the products (**C** or **D**) is increased; the reaction will then proceed faster in the reverse direction until enough **A** and **B** are formed so that the forward rate once again equals the reverse rate.

The *opposite* situation occurs if one of the reactants or products is **removed** from the system.

Reactants (or products) can be removed from the system if they are consumed by another chemical reaction, form a solid, or form a gas that is bubbled or evaporated from a liquid-phase reaction.

Consider the general reaction *at equilibrium*: $A + B \rightleftarrows C + D$

- If some of substance **A** or **B** is *removed*, this causes a significant decrease in the rate of the forward reaction relative to the reverse reaction simply because there is now a lower probability of **A** colliding with **B** and reacting.

- Substance **C** and **D** continue to be converted to **A** and **B** at a faster rate than the rate of the forward direction until enough of **A** and **B** are produced so that the forward rate is once again equal to the reverse rate and *equilibrium is reestablished*.

- An equivalent situation occurs if *products are removed*; the reaction will proceed faster in the forward direction until enough products are formed so that the reverse rate is equal to the forward rate and equilibrium is reestablished.

What I have just described is part of a law known as **Le Châtelier's Principle**.

- Predictions based on Le Châtelier's Principle of responses to changes in concentration of reactants or products for a reaction at equilibrium are summarized in the table below.

Change Made to a Reaction that was at Equilibrium:	Response:
Increase the concentration of a ***reactant.***	Rate of the **forward** reaction becomes **greater** than the rate of the reverse reaction until equilibrium is reestablished.
Increase the concentration of a ***product.***	Rate of the **reverse** reaction becomes **greater** than the rate of the forward reaction until equilibrium is reestablished.
Decrease the concentration of a ***reactant.***	Rate of the **forward** reaction becomes **less** than the rate of the reverse reaction until equilibrium is reestablished.
Decrease the concentration of a ***product.***	Rate of the **reverse** reaction becomes **less** than the rate of the forward reaction until equilibrium is reestablished.

The Ionization of Water

A reversible reaction that is very important in understanding the chemical behavior of biological solutions is the _____ of water.

$$2 \, H_2O \, (l) \quad \rightleftarrows \quad OH^- \, (aq) + H_3O^+ \, (aq)$$
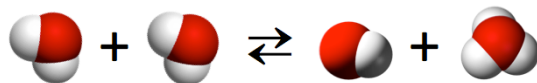
- The reactants are *two* water molecules.

- One water molecule transfers a hydrogen ion (H^+) to the other water molecule to produce a hydroxide ion (OH^-) and a _____ ion (H_3O^+).

The reason that this reaction is important in biological systems is that: (1) cells are filled with and surrounded by water, (2) hydronium and hydroxide ions are involved in many biological reactions and effect many biological processes. This reaction occurs wherever water is present, regardless of what other substance(s) may be present.

Ionization of water obeys the **law of mass action**, just like _____ other chemical reaction.

The *equilibrium expression* for this reaction is:

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

H_2O (*l*) does not appear in the equilibrium expression because *it is a* _____.

This equilibrium expression is so commonly used, that the symbol "K_w" is used for equilibrium constant (instead of K_{eq}).

- The value of the equilibrium constant has been measured experimentally for this reaction.
- The unit for K_w is M^2 because we are multiplying two molarity concentrations ($M \cdot M = M^2$).

I want to draw your attention to a few things about this equilibrium expression:

1) The **mathematical product** of the hydroxide ion concentration $[OH^-]$ and hydronium ion concentration $[H_3O^+]$ is always equal to $1.0 \times 10^{-14} M^2$; this is true whether the system is pure water *or* an aqueous solution containing one or more solutes.

mathematical product

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

2) The value of K_w is much less than **1**. There is always much *more water molecules present* (reactants) than hydroxide ions and hydronium ions (products).

3) In solutions (not pure water), there may be *other sources of hydroxide ions and hydronium ions*; therefore the hydroxide ion concentration *is not necessarily equal to* the hydronium ion concentration.

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The Concentration of Hydroxide and Hydronium Ions in *Pure Water*

In pure water, the ***only*** *source of hydroxide ions and hydronium ions* is from the ionization of water reaction:

$$2\ H_2O\ (l)\ \rightleftharpoons\ OH^-\ (aq)\ +\ H_3O^+\ (aq)$$

Every time this reaction proceeds in the forward direction ***exactly*** one hydroxide and one hydronium ion are formed. Therefore, ***in pure water*** the hydroxide ion concentration is always equal to the hydronium ion concentration.

If we solve the equilibrium expression to find which number multiplied by itself is equal to K_w (1.0×10^{-14} M^2), we can find the concentration of the hydroxide and hydronium ions in *pure water*:

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

$$(1.0 \times 10^{-7} M) \times (1.0 \times 10^{-7} M) = 1.0 \times 10^{-14} M^2$$

In ***pure water***, the ***hydroxide ion*** concentration ***and*** the ***hydronium ion*** concentration are both equal to 1.0×10^{-7} M.

The concentration of hydroxide and hydronium in aqueous solutions containing *other* solutes.

In aqueous *solutions* (not pure water), there may be *other sources of hydroxide ions and hydronium ions*; therefore the hydroxide ion concentration ***is not necessarily equal to*** the hydronium ion concentration.

- For example, a sodium hydroxide (NaOH) solution contains more hydroxide than pure water.
- In aqueous solutions, K_w does not give us enough information to determine the hydroxide ion (OH^-) and hydronium ion (H_3O^+) concentrations individually; we only know that their mathematical product, $[OH^-] \bullet [H_3O^+]$, is always equal to 1.0×10^{-14} M^2.

$$K_w = \boxed{[OH^-][H_3O^+]} = 1.0 \times 10^{-14} M^2$$

We know the equilibrium constant for *the ionization of water*.

That means whenever we know [OH⁻], we can calculate the concentration of _____.

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

$$[H_3O^+] = \frac{1.0 \times 10^{-14} M^2}{[OH^-]}$$

Also, whenever we know [H₃O⁺] we can calculate the concentration of _____.

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

$$[OH^-] = \frac{1.0 \times 10^{-14} M^2}{[H_3O^+]}$$

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Example:

What is the concentration of $[OH^-]$ in an aqueous solution when $[H_3O^+] = 1.0 \times 10^{-3}$ M?

$$\boxed{\text{Strategy:} \\ K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} \, M^2}$$

$$[OH^-] = \frac{1.0 \times 10^{-14} \, M^2}{[H_3O^+]} = \frac{1.0 \times 10^{-14} \, M^2}{1.0 \times 10^{-3} \, M} = \mathbf{1.0 \times 10^{-11} \, M}$$

Understanding Check

What is the concentration of $[H_3O^+]$ in an aqueous solution when $[OH^-] = 5.0 \times 10^{-11}$ M ?

Summary of the Ionization of Water

$$2 \, H_2O \; (l) \quad \rightleftarrows \quad OH^- \; (aq) \; + \; H_3O^+ \; (aq)$$

$$K_w = [OH^-][H_3O^+] = 1.0 \times 10^{-14} \, M^2$$

[OH⁻] ⟵ To convert use: $[H_3O^+][OH^-] = 1.0 \times 10^{-14} \, M^2$ ⟶ **[H₃O⁺]**
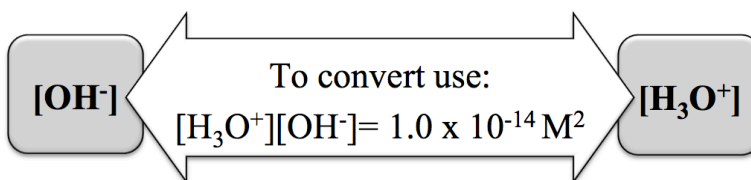
The ionization of water is a very important reaction in the chemical behavior of biological organisms and environments because hydronium and hydroxide ions are products or reactants in many biological reactions.

As described by Le Châtelier's Principle, changes in the hydronium or hydroxide ions can therefore affect the amounts of other products and/or reactants present in biological reactions such as the citric acid cycle and photosynthesis.

Acids and Bases

A compound can be classified as an "**acid**" or a "**base**" depending on its ability to _____ or _____ a hydrogen ion (H^+) *in a chemical reaction*.

We will use the definitions of acids and bases popularized and published by Johannes Brønsted and Thomas Lowry.

- An **acid** _____ an H^+ *in a chemical reaction*.

- A **base** _____ an H^+ *in a chemical reaction*.

Reactions in which an H^+ is transferred are called **acid-base reactions**.

If you are given a specific *acid-base reaction*, you can *only* determine which reactant is the *acid* and which reactant is the *base* by inspection of the products *and* reactants.

Let's consider the chemical reaction of aqueous hydrogen chloride and water:

$$HCl\ (aq)\ +\ H_2O\ (l)\ \rightleftharpoons\ Cl^-\ (aq)\ +\ H_3O^+\ (aq)$$

When discussing which reactant is the *acid* and which reactant is the *base*, we consider the reaction in the _____ *direction*.

- In the forward direction of this reaction, HCl is the *acid* because it _____ an H^+.

- The **water** molecule is the *base* in this reaction because it _____ an H^+.
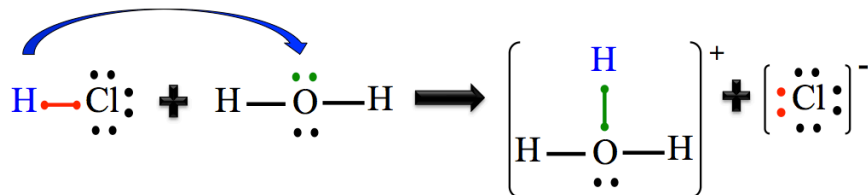
When a reactant molecule **donates** an H^+, its charge _____ by one charge unit.

- For example, the HCl in the reaction had *zero charge* as a reactant, however after donating the H^+, it is converted to Cl^-; the charge *decreased* by one charge unit.

$$HCl^0(aq)\ +\ H_2O\ (l)\ \rightleftharpoons\ Cl^-\ (aq)\ +\ H_3O^+\ (aq)$$

| zero charge | 1- charge |
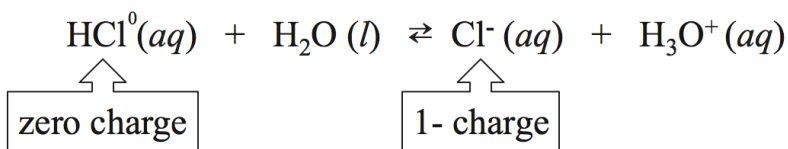
Conversely, when a reactant molecule **accepts** an H^+ in a reaction, its charge *__increases__* by one charge unit.

- For example, the H_2O in the reaction had *zero charge* as a reactant, however after accepting the H^+ and becoming H_3O^+, its charge *increased* by one charge unit.

$$HCl\ (aq)\ +\ H_2O^0(l)\ \rightleftharpoons\ Cl^-\ (aq)\ +\ H_3O^+\ (aq)$$

| zero charge | 1+ charge |
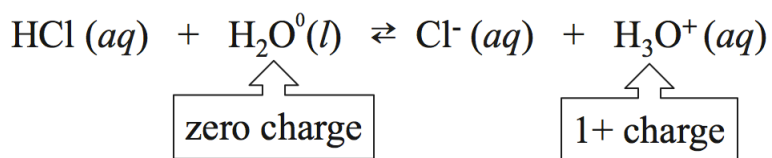
Understanding Check

Determine which reactant is the acid and which reactant is the base in each of the following reactions.

    a. $H_3BO_3\ (aq) + H_2O\ (l)\ \rightleftharpoons\ H_2BO_3^-\ (aq) + H_3O^+\ (aq)$

    b. $HSO_4^-\ (aq) + HNO_3\ (aq)\ \rightleftharpoons\ H_2SO_4\ (aq) + NO_3^-\ (aq)$

    c. $CN^-\ (aq) + H_2O\ (l)\ \rightleftharpoons\ HCN\ (aq) +\ OH^-\ (aq)$

Amphoteric Compounds

Did you notice that water acted as a **base** in problem (a) from the previous understanding check and as an **acid** in problem (c):

a. $H_3BO_3\ (aq) + H_2O\ (l) \rightleftarrows H_2BO_3^-\ (aq) + H_3O^+\ (aq)$
   acid   base

c. $CN^-\ (aq) + H_2O\ (l) \rightleftarrows HCN\ (aq) + OH^-\ (aq)$
   base   acid
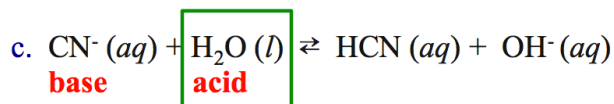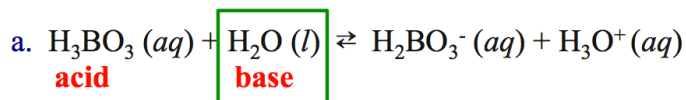
Compounds that can act as acids *or* as bases are called _____ **compounds**.

An example of another **amphoteric compound** is the bicarbonate ion (HCO_3^-).

Bicarbonate acts as an *acid* in this reaction:

$$HCO_3^- + CN^- \rightleftarrows CO_3^{2-} + HCN$$
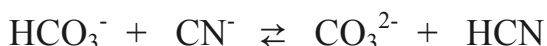
Bicarbonate acts as a *base* in this reaction:

$$HCO_3^- + HCl \rightleftarrows H_2CO_3 + Cl^-$$
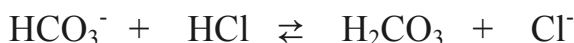
Conjugates

Pairs of chemical species, such as HCN and CN^- *or* H_3BO_3 and $H_2BO_3^-$, which differ only in the presence or absence of an H^+ are called _____ _____.

For each conjugate pair, the species that *contains the extra hydrogen* is called the "_____ _____" or the "*conjugate acid*," and the species *with one fewer hydrogen* is called the "_____ _____" or the "*conjugate base*."

Consider the chemical reaction of aqueous hydrogen chloride and water:

Conjugate Pair

$$HCl\ (aq) + H_2O\ (l) \rightleftarrows Cl^-\ (aq) + H_3O^+\ (aq)$$
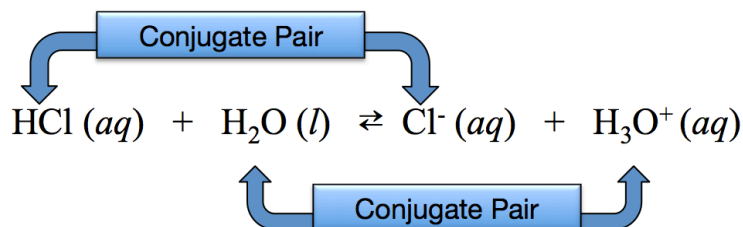
Conjugate Pair

There are _____ conjugate pairs in every acid-base reaction.

For the HCl/Cl^- conjugate pair, HCl is the *acid form* and Cl^- is the *base form*.

Understanding Check

For the H_2O/H_3O^+ conjugate pair, **label** the *acid form* and the *base form*.

$$HCl\ (aq) + H_2O\ (l) \rightleftarrows Cl^-\ (aq) + H_3O^+\ (aq)$$

Conjugate Pair

Identify the *acid form* and the *base form* in each of the conjugate pairs:

     a. H_3BO_3 and $H_2BO_3^-$

     b. H_2O and OH^-

     c. HSO_4^- and H_2SO_4

     d. HNO_3 and NO_3^-

Note that because the "*acid form*" in a conjugate pair has one more H^+, it will have **one unit greater charge** than the "*base form*."

pH

There are many applications, in both nature and laboratory settings, when it is important to measure and know the hydronium ion concentration. Since hydronium is a product or reactant in many chemical reactions, its concentration affects the amounts of other products and/or reactants involved in these reactions. An excess or deficiency of hydronium ions will hinder the ability of biological enzymes to catalyze crucial chemical reactions. The concentration of hydronium ions both affects, and is affected by, cellular metabolic activity. If the concentration of hydronium ions is too large or too small, irreversible damage to cells will occur. For these and many other reasons, much work has gone into enabling the experimental measurement of hydronium ion concentration.

The concentration of hydronium ions is determined experimentally and assigned a numeric value using the _____ _____.
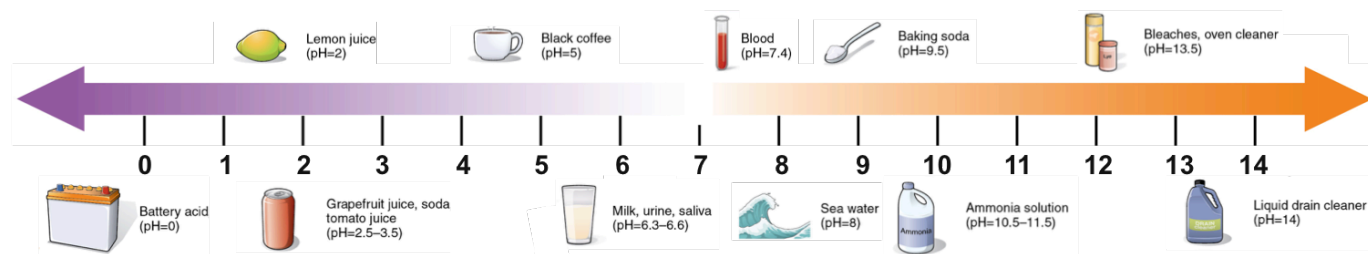
pH is most commonly defined as the "**negative logarithm of the *hydronium ion* concentration**."

- This definition can be written as a mathematical equation:

$$pH = -\log[H_3O^+]$$

- *pH is simply another way to express the _____ of _____ ions in a solution.*

Logarithms

If a value (number) changes by a factor of 10, then its logarithm changes by 1.

You may be familiar with the **Richter scale** used in describing the magnitude of earthquakes.
- The Richter scale is a logarithm scale. An earthquake that has a magnitude of 7 on the Richter scale is *ten times stronger* than an earthquake with a Richter scale value of 6. An earthquake with a Richter scale value of 8 is *one hundred times stronger* than a quake with a Richter scale value of 6.

A Quick Review of Logarithms

The log(10) is 1 because $10^1 = 10$
The log(100) is 2 because $10^2 = 100$
The log(1000) is 3 because $10^3 = 1000$
The log(.1) is -1 because $10^{-1} = .1$
The log(.01) is -2 because $10^{-2} = .01$
The log(3.4) is .53 because $10^{(.53)} = 3.4$ (We need to use a calculator for this one.)

Calculating the pH from the $[H_3O^+]$
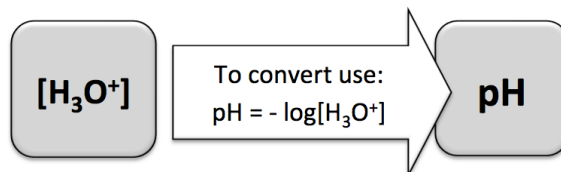
Example:
What is the pH of an aqueous solution with $[H_3O^+] = 6.3 \times 10^{-1}$M?

Strategy: pH = - log$[H_3O^+]$

$$pH = -\log[H_3O^+] = -\log[6.3 \times 10^{-1}] = -(-0.20) = \mathbf{0.20}$$

NOTE: pH is a _____ value.

Understanding Check: What is the pH of an aqueous solution with $[H_3O^+] = 8.1 \times 10^{-3}$M?

The rule for significant figures in pH values:

Numbers to the _____ of the *decimal point* are _____ significant in pH values.

- *Be careful*, **only** apply this rule to the **pH** value and not to $[H_3O^+]$ or $[OH^-]$.

$$pH = -\log[H_3O^+]$$

greater $[H_3O^+]$ $\quad [H_3O^+] = 6.3 \times 10^{-1}$M $\quad \longrightarrow \quad$ pH = **0.20**
(0.63 M)

lesser $[H_3O^+]$ $\quad [H_3O^+] = 8.1 \times 10^{-3}$M $\quad \longrightarrow \quad$ pH = **2.09**
(0.0081 M)
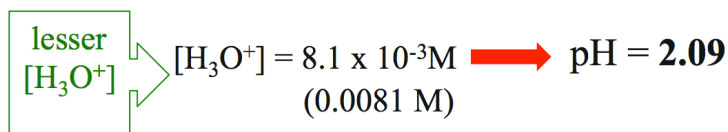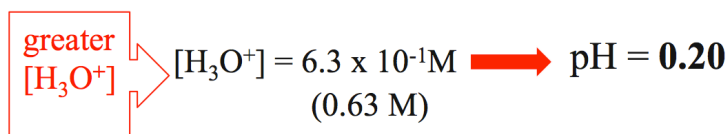
Because of the **negative sign** in our definition of pH, the _____ the **hydronium ion concentration**, the _____ the pH value.

Strategy:

$[OH^-]$ ⟵ To convert use: $[H_3O^+][OH^-] = 1.0 \times 10^{-14} M^2$ ⟶ $[H_3O^+]$ ⟵ To convert use: $pH = -\log[H_3O^+]$ ⟶ **pH**

Calculating the $[H_3O^+]$ from the pH

We calculated the pH from the $[H_3O^+]$ in the previous example and review problems. Since there are many devices that are used to experimentally measure pH, many applications require that the $[H_3O^+]$ be calculated from the measured pH value. In this case we must employ a mathematical operation called the *antilog*.

$[H_3O^+]$ ⟵ To convert use: $pH = -\log[H_3O^+]$ ⟶ **pH**
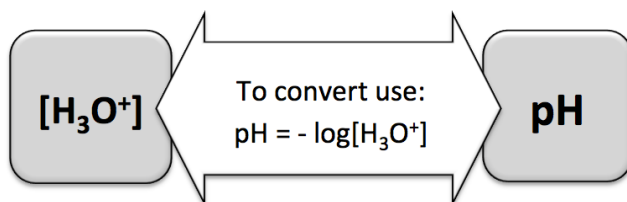
Example: What is the $[H_3O^+]$ of an aqueous solution with pH = 5.3?

Start with the definition of pH:

$$pH = -\log[H_3O^+]$$

$$5.3 = -\log[H_3O^+] \quad \longleftarrow \text{Multiply both sides by } (-1)$$

Take the antilog of both sides ⟶

$$-5.3 = \log[H_3O^+]$$

$$10^{(-5.3)} = [H_3O^+]$$

$$[H_3O^+] = 5 \times 10^{-6} M$$

Now that you know how to convert between the hydronium ion concentration and the hydroxide ion concentration, **_and_** convert between the $[H_3O^+]$ and the pH, if you are given *any **one** of these three quantities, $[H_3O^+]$, $[OH^-]$,or pH, you should be able to calculate **the other two**.*

| [OH⁻] | To convert use: $[H_3O^+][OH^-]= 1.0 \times 10^{-14} M^2$ | [H₃O⁺] | To convert use: $pH = - \log[H_3O^+]$ | pH |
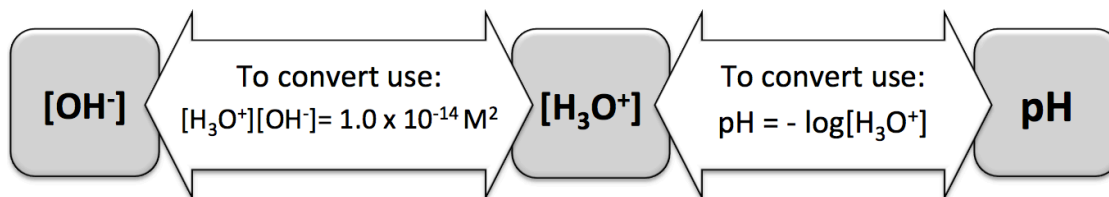
Understanding Check: Complete each row of the table:

$[OH^-]$	$[H_3O^+]$	pH
	1.1×10^{-3} M	
	1.0×10^{-7} M	
1.2×10^{-14} M		
1.4×10^{-3} M		
		1.0
		7.00
		9.3
		12.00

Acidic and Basic Solutions

_____ are characterized as **acids** or **bases** depending on whether they donate or accept H^+ in *a **particular** acid-base reaction*.

_____ are characterized as **acidic**, **basic**, or **neutral** by the relative amounts of H_3O^+ and OH^- that are present.

- Solutions that contain more H_3O^+ than OH^- are called _____ **solutions**.
- Solutions that contain more OH^- than H_3O^+ are called _____ **solutions**.
- Solutions that contain equal concentrations of H_3O^+ and OH^- are called _____ **solutions**.

Let's do an example problem to find the **pH** of a ***neutral solution***:

By definition, in neutral solutions, the $[H_3O^+] = [OH^-]$.

$$[OH^-][H_3O^+] = 1.0 \times 10^{-14} M^2$$

$$(1.0 \times 10^{-7} M) \times (1.0 \times 10^{-7} M) = 1.0 \times 10^{-14} M^2$$

In neutral solutions, the $[H_3O^+] = [OH^-]$, therefore they are both equal to 1.0×10^{-7} M.

Once the $[H_3O^+]$ is calculated, it can be used to calculate the pH:

$$pH = - \log[H_3O^+] = - \log(1.0 \times 10^{-7} M) = - (-7.00) = \textbf{7.00}$$

The pH of a *neutral solution* equals _____.

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Next, let's think about the pH range of **acidic** or **basic solutions**.

In **acidic solutions,** $[H_3O^+] > [OH^-]$, therefore $[H_3O^+] > 1.0 \times 10^{-7}$ M.

- When the hydronium ion concentration is *greater* than 1.0×10^{-7} M, then the pH is *less than* 7.00.
- Note that as the *hydronium ion* concentration *increases*, the pH *decreases*; this is because of the *negative sign* in the definition of pH.

In **basic solutions,** $[OH^-] > [H_3O^+]$, therefore $[H_3O^+] < 1.0 \times 10^{-7}$ M.

- When the hydronium ion concentration is *less* than 1.0×10^{-7} M, then the pH is *greater than* 7.00.
- Note that as the *hydronium ion* concentration *decreases*, the pH *increases*.

Solution Characterization	pH	$[H_3O^+]$	$[OH^-]$
Acidic	less than 7.00	greater than 1.0×10^{-7} M	less than 1.0×10^{-7} M
Neutral	7.00	1.0×10^{-7} M	1.0×10^{-7} M
Basic	greater than 7.00	less than 1.0×10^{-7} M	greater than 1.0×10^{-7} M

Understanding Check:

For each of the following, write whether it describes an acidic, basic, or neutral solution.

a) pH = 8.9

b) $[H_3O^+] = 1 \times 10^{-9}$ M

c) $[H_3O^+] = 1 \times 10^{-7}$ M

d) $[OH^-] > [H_3O^+]$

e) $[H_3O^+] > [OH^-]$

f) pH = 1.7

g) pH = 12.0

h) $[OH^-] = 6.8 \times 10^{-2}$ M

i) pH = 0.06

j) $[H_3O^+] = [OH^-]$

k) pH = 7.00

l) $[OH^-] = 1.0 \times 10^{-7}$ M

Properties of Acidic Solutions

Acidic solutions will turn a plant pigment molecule (in blue litmus) from blue to red.

Molecules such as litmus are often used as pH indicators.

- The color of the pH indicator, after being placed in contact with the test solution, indicates that the solution is in a certain pH range.

A more precise way to measure the pH of a solution is to use a pH meter.

- A pH meter is an electronic device with an electrode that is sensitive to the *hydronium ion concentration*.

Acidic solutions taste *sour*.

- The juice from lemons has a relatively high concentration of citric acid, (about 5%(w/v),) which gives lemons their sour taste.
- Many solutions are so acidic (pH much less than 7.00) that they will damage your mouth and digestive tract, and can result in death if enough is ingested.

Some molecules contain the word "*acid*" in their name based on the fact that they act as acids when they react with water.

Carboxylic *acids* are examples of this.

An **acidic solution** can be prepared by the addition into water of a compound that acts as an acid when reacting with the water.

- For example, when acetic acid (a carboxylic *acid*) is added to pure water, a reaction occurs and an equilibrium is established:

$$\underset{\substack{\text{acetic acid} \\ \text{(a carboxylic acid)}}}{CH_3\overset{\displaystyle :O:}{\overset{\|}{C}} - \ddot{\underset{..}{O}}H}\ (aq) + H_2O\ (l) \ \rightleftarrows\ \underset{\text{acetate ion}}{CH_3\overset{\displaystyle :O:}{\overset{\|}{C}} - \ddot{\underset{..}{O}}:^-}\ (aq) + H_3O^+\ (aq)$$
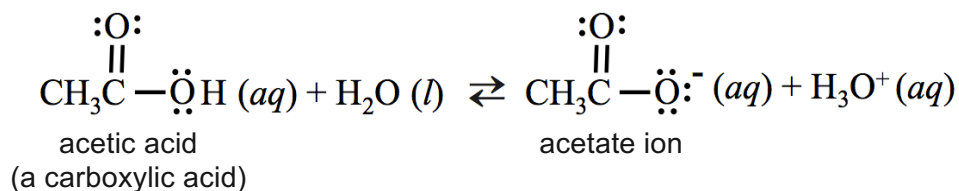
Before the acetic acid was added to pure water, the $[H_3O^+]$ was equal to the $[OH^-]$. When the acetic acid was added, **more** H_3O^+ was produced and the $[H_3O^+]$ increased.

The resulting acetic acid solution is **acidic** (pH < 7) because $[H_3O^+] > [OH^-]$.

The pH of a solution that is prepared by adding an **acid** into pure water is determined by two factors:

1) The _____ of the compound that was added.

2) The extent to which the compound _____ (donates H^+ and thereby produces its **base form** and H_3O^+).

The extent to which an acid dissociates when reacting with water is referred to as "**acid strength**."

When a "_____ _____" is placed in water and reacts with it, there is very little of the **acid form** present and much more of the **base form** present **at equilibrium**.

- An example of a **strong acid** is HCl (often referred to as hydrochloric acid).
- When hydrogen chloride is in water, it dissociates as shown in the chemical equation below:

$$HCl\ (aq) + H_2O\ (l)\ \rightleftarrows\ Cl^-\ (aq) + H_3O^+\ (aq)$$
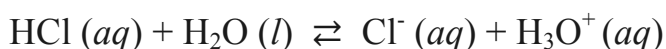
Recall that the value of the equilibrium constant (K_{eq}) for a reaction indicates the relative amounts of products and reactants that exist at equilibrium.

> If K_{eq} is much greater than 1, then, at equilibrium, the concentrations of the products are much greater than those of the reactants.
>
> > - In this case we say *the products are predominant at equilibrium.*
>
> Conversely, if K_{eq} is much less than 1, at equilibrium, the concentrations of the reactants are much greater than those of the products.
>
> > - In this case we say *the reactants are predominant at equilibrium.*

When writing the equilibrium constant for the reaction of an acid with water, we use the symbol _____ instead of K_{eq}.

K_a is referred to as the **acidity constant** or the **acid dissociation constant**.

- Keep in mind that it is just the **equilibrium constant** for the reaction of the acid with water.

K_a for the reaction of HCl and water is about 1×10^7 M.

$$\text{HCl } (aq) + \text{H}_2\text{O } (l) \rightleftharpoons \text{Cl}^- (aq) + \text{H}_3\text{O}^+ (aq) \qquad K_a \approx 1 \times 10^7 \text{ M}$$
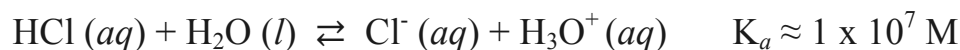
The equilibrium expression for this reaction is:

$$K_a = \frac{[\text{Cl}^-][\text{H}_3\text{O}^+]}{[\text{HCl}]} \approx 1 \times 10^7 \text{ M}$$

Because K_a is approximately 1×10^7 M, at equilibrium there are about about **ten million** Cl⁻ ions and **ten million** H_3O^+ ions for every **one HCl** molecule.

- Almost all of the HCl that is added to pure water is converted to Cl⁻ and H_3O^+.

When a "_____ _____" is placed in water and reacts with it, at equilibrium, there is very little of its **base form** and much more of the **acid form** present.

An example of a **weak acid** is boric acid (H_3BO_3).

- When boric acid is in water, it dissociates as shown in the chemical equation below:

$$\text{H}_3\text{BO}_3 (aq) + \text{H}_2\text{O } (l) \rightleftharpoons \text{H}_2\text{BO}_3^- (aq) + \text{H}_3\text{O}^+ (aq)$$
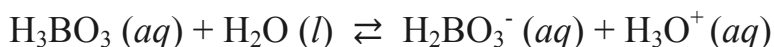
K_a for the reaction of H_3BO_3 and water is 5.75×10^{-10} M.

The equilibrium expression for this reaction is:

$$K_{eq} = \frac{[\text{H}_2\text{BO}_3^-][\text{H}_3\text{O}^+]}{[\text{H}_3\text{BO}_3]} = 5.75 \times 10^{-10} \text{ M}$$

K_a for this reaction is much less than 1, and *the reactant* (H_3BO_3) *is predominant at equilibrium.*

- At equilibrium, there are about about 25000 H_3BO_3 molecules for every *one* H_2BO_3^- or H_3O^+ ion present.

Summary of Acid Strength

Strong acids have K_a values ***much*** _____ than 1.

- When ***strong acids*** are placed in pure water, they react with water and an equilibrium is establish in which there is much more of the **base form** and H_3O^+ than the **acid form** present.

Weak acids have K_a values ***much*** _____ than 1.

- When ***weak acids*** are placed in pure water, they react with water and an equilibrium is establish in which there is much more of the **acid form** than the **base form** *and* H_3O^+ present.

The greater the K_a, the stronger the acid.

Various Acids and Their Acidity Constants		
Acid Name	**Acid Formula**	**K_a**
Perchloric acid	HClO_4	1×10^9 M (estimated)
Hydrochloric acid	HCl	1×10^7 M (estimated)
Chloric acid	HClO_3	1×10^3 M (estimated)
Phosphoric acid	H_3PO_4	7.5×10^{-3} M
Hydrofluoric acid	HF	6.6×10^{-4} M
Acetic acid	$\text{CH}_3\text{CO}_2\text{H}$	1.8×10^{-5} M
Carbonic acid	H_2CO_3	4.4×10^{-7} M
Dihydrogen phosphate ion	H_2PO_4^-	6.2×10^{-8} M
Boric acid	H_3BO_3	5.7×10^{-10} M
Ammonium ion	NH_4^+	5.6×10^{-10} M
Hydrocyanic acid	HCN	4.9×10^{-10} M
Bicarbonate ion	HCO_3^-	5.6×10^{-11} M
Methylammonium ion	CH_3NH_3^+	2.4×10^{-11} M
Hydrogen phosphate ion	HPO_4^-	4.2×10^{-13} M

Properties of Basic Solutions

Basic solutions *feel slippery*, have a *bitter* taste, and will turn litmus pH indicator from red to blue.

Basic solutions can be prepared by dissolving an ionic compound that contains hydroxide in water.

For example, the addition of sodium hydroxide to pure water will result in dissociation of the sodium hydroxide crystals to produce sodium ions and hydroxide ions:

$$NaOH\ (s)\ \rightleftarrows\ Na^+\ (aq) + OH^-\ (aq)$$
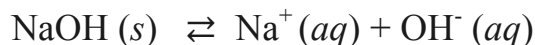
When the NaOH was added, the $[OH^-]$ increased.

The resulting NaOH solution is *basic* (pH >7) because $[OH^-] > [H_3O^+]$.

Neutralization Reactions

An *acid* will react with a *hydroxide-containing base* compound to produce _____ and *an* _____ *compound* in a reaction called_____.

An example of a *neutralization reaction* is the reaction of perchloric acid and sodium hydroxide:

$$HClO_4\ (aq) +\ NaOH\ (aq)\ \rightleftarrows\ H_2O\ (l) + NaClO_4\ (aq)$$
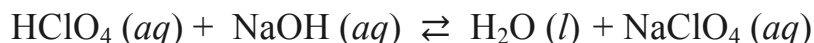
In *neutralization reactions*, the H^+ from the *acid* bonds to the OH^- to produce H_2O.

The (anionic) *base form* of the acid (ClO_4^- in this case) combines with the cationic part of the base (Na^+ in this case) to make an *ionic compound* called a _____.

- Although sodium chloride is commonly called "salt," the chemical definition of salt states that a *salt* is an ionic compound *formed in a neutralization reaction*.

Understanding Check: Predict the products of the following *neutralization reactions*:

$$HCl\ (aq)\ +\ NaOH\ (aq)\ \rightleftarrows\ \underline{\hspace{2cm}}\ +\ \underline{\hspace{2cm}}$$

$$HCl\ (aq)\ +\ KOH\ (aq)\ \rightleftarrows\ \underline{\hspace{2cm}}\ +\ \underline{\hspace{2cm}}$$

The Henderson-Hasselbalch Relationship

There is a unique relationship between the **pH** of a solution and the relative amounts of *acid* and *base forms* of a conjugate pair that is present in the solution.

The **general form** of a chemical equation for an acid reacting with water to produce its base form and hydronium can be written as:

$$HA\ (aq)\ +\ H_2O\ (l)\ \rightleftarrows\ A^-\ (aq)\ +\ H_3O^+\ (aq)$$
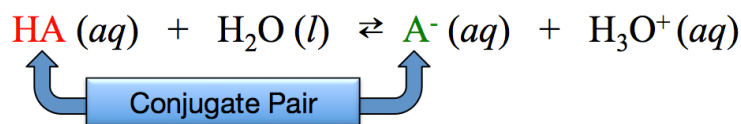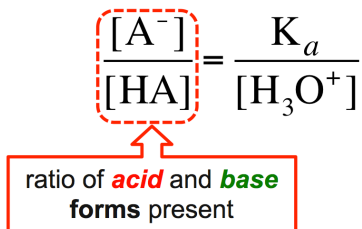
Conjugate Pair

HA represents the *acid form*, and A⁻ represents the *base form* of any **conjugate pair.**

The equilibrium expression for this general reaction is:

$$K_a = \frac{[A^-][H_3O^+]}{[HA]}$$

We can rearrange this equation to get the ratio of the equilibrium concentration of the acid and base form of a conjugate pair.

$$\frac{[A^-]}{[HA]} = \frac{K_a}{[H_3O^+]}$$

ratio of *acid* and *base*
forms present

The important thing to see here is that the relative amounts (ratio) of the *base form* and *acid form* of a conjugate pair at equilibrium depends on the K_a value for the particular acid *and* $[H_3O^+]$.

Since pH is used as a measure of $[H_3O^+]$, it is more practical to use pH instead of $[H_3O^+]$.

- The **$[H_3O^+]$** in equation can be replaced with **pH** by taking the *negative logarithm* of both sides of the equation and doing some other algebraic steps.

$$pH = -\log(K_a) + \log\left(\frac{[A^-]}{[HA]}\right)$$

The "-log(K_a)" term in this equation above is written as "pK_a."

Doing so yields what is known as the **Henderson-Hasselbalch Equation**:

$$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$$

For a particular conjugate pair, the **Henderson-Hasselbalch Equation** gives the relationship between the relative amounts of the *acid and base forms* present at equilibrium and the **pH** of the solution.

Henderson-Hasselbalch Equation

$$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$$

The Henderson-Hasselbalch Equation is used so often that K_a values for acids are sometimes tabulated as pK_as.

Do not be confused by the use of pK_a; it is simply the $-\log(K_a)$.

Acid Name	Acid Formula	K_a	pK_a $pK_a = -\log(K_a)$
Perchloric acid	$HClO_4$	1×10^9 M (estimated)	-9.0 (estimated)
Hydrochloric acid	HCl	1×10^7 M (estimated)	-7.0 (estimated)
Chloric acid	$HClO_3$	1×10^3 M (estimated)	-3.0 (estimated)
Phosphoric acid	H_3PO_4	7.5×10^{-3} M	2.12
Hydrofluoric acid	HF	6.6×10^{-4} M	3.18
Acetic acid	CH_3CO_2H	1.8×10^{-5} M	4.74
Carbonic acid	H_2CO_3	4.4×10^{-7} M	6.36
Dihydrogen phosphate ion	$H_2PO_4^-$	6.2×10^{-8} M	7.21
Boric acid	H_3BO_3	5.7×10^{-10} M	9.24
Ammonium ion	NH_4^+	5.6×10^{-10} M	9.25
Hydrocyanic acid	HCN	4.9×10^{-10} M	9.31
Bicarbonate ion	HCO_3^-	5.6×10^{-11} M	10.25
Methylammonium ion	$CH_3NH_3^+$	2.4×10^{-11} M	10.62
Hydrogen phosphate ion	HPO_4^{2-}	4.2×10^{-13} M	12.38

We will not use the Henderson-Hasselbalch Equation to do calculations; but we will take advantage of its *implications* in order to _____ whether the *acid form* or the *base form* of a **particular conjugate pair** is *predominant* at equilibrium.

A solution containing a conjugate pair can be at *any* pH; other species that are in the solution (or might be added) can affect the pH. However, the K_a, and therefore pK_a, for a particular conjugate pair *does not change*.

In order to solve problems in this course, you should know and understand the following three statements that are *implied* by the **Henderson-Hasselbalch Equation**.

- When the **pH** of a solution is _____ than the **pK_a** of an acid, then the concentration of the *acid form*, [HA], is *greater than* the concentration of the *base form*, [A⁻].
    - In this case, we say that *the acid form is predominant*.

- When the **pH** of a solution is _____ than the **pK_a** of an acid, then the concentration of the *base form*, [A⁻], is *greater than* the concentration of the *acid form*, [HA].
    - In this case, we say that *the base form is predominant*.

- When the **pH** of a solution is _____ *to* the **pK_a** of an acid, then the concentration of the *acid form*, [HA], is *equal to* the concentration of the *base form*, [A⁻].

Solution Condition	Relative Amounts of Acid and Base Forms
$pH < pK_a$	[HA] > [A⁻]
$pH > pK_a$	[A⁻] > [HA]
$pH = pK_a$	[HA] = [A⁻]

Buffer Solutions

Predicting, measuring, and controlling the pH of a solution or biological environment are important.

Nature and certain laboratory applications employ a chemical system, called a _____, that helps to **maintain a narrow pH range** in bodily fluids or other aqueous solutions.

A _____ is a solution that resists changes in pH when **small amounts** of acid or base are added.

A buffer solution contains fairly high concentrations of the **acid and base forms of a conjugate pair**.

Solution Condition	Relative Amounts of Acid and Base Forms
pH < pK_a	[HA] > [A⁻]
pH > pK_a	[A⁻] > [HA]
pH = pK_a	[HA] = [A⁻]

A high concentration of **both** the **acid and base form** of the conjugate pair is needed; this occurs when the pH is equal to, or very close to, the pK_a.

How does a buffer work?   **Example of a Buffer Solution: Blood Plasma.**

The pH of your blood normally ranges between 7.35 and 7.45.

A blood pH below the normal range is called **acidosis**, while a blood pH above this range is called **alkalosis**, either one of which is potentially fatal.

Blood is kept in this narrow range (pH = 7.35 – 7.45) with the help of buffers.

Adding Acid to a Buffer Solution

If acid (hydronium ions) is added to the carbonic acid (H_2CO_3)/bicarbonate (HCO_3^-) **buffer in blood,** the excess hydronium ions would cause an *increase in the reverse reaction rate of the buffer conjugate pair equilibrium*, shown below, as predicted by Le Chatalier's Principle.

$$H_2CO_3\,(aq) \; + \; H_2O\,(l) \; \rightleftharpoons \; HCO_3^-\,(aq) \; + \; H_3O^+\,(aq)$$

The excess hydronium ions that are added and bicarbonate (HCO_3^-) are converted to carbonic acid (H_2CO_3) + H_2O (l) in the reverse direction of the reaction, and therefore there is **not** a significant change in the pH.

The removal of the excess hydronium will continue until most of the *base form* of the conjugate pair is depleted.

- It is for this reason that buffers are made of relatively **high concentrations** of the buffering conjugate pairs, and that we say, "a buffer is a solution that will resist pH changes when **small** amounts of acid or base are added."

Addition of Base to a Buffer Solution

If a small amount base was added to a _____ **buffered solution**, it would increase the pH.

- The pH would increase because the hydroxide ion concentration would increase, and therefore *the concentration of **hydronium ions** will **decrease***.

However, if a small amount of base was added to a **buffered solution, the hydronium ion concentration would be maintained because of a decrease in the reverse reaction rate** of the *buffer conjugate pair equilibrium*, as predicted by Le Châtelier's Principle.

$$\text{HA } (aq) + H_2O \ (l) \quad \longleftarrow \quad A^- \ (aq) + H_3O^+ \ (aq)$$

The concentration of **hydronium ions** will be **maintained** because it is replenished by the greater rate of the forward reaction.

Biological Buffers

An important _____ (within cells) buffer is the dihydrogen phosphate/hydrogen phosphate conjugate pair:

$$H_2PO_4^- \ (aq) + H_2O \ (l) \ \rightleftarrows \ HPO_4^{2-} \ (aq) + H_3O^+ \ (aq)$$

Conjugate Pair
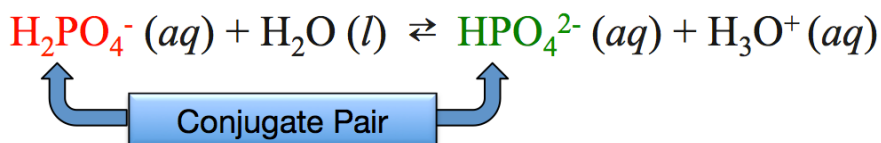
Proteins also act as *intracellular* buffers.
- In chapter 13 you will learn how proteins can donate or accept H^+.

Important _____ (outside of cells) buffers, in solutions such as blood or interstitial fluids, are the carbonic acid (**H_2CO_3**)/bicarbonate (**HCO_3^-**) and the ammonium (**NH_4^+**)/ammonia (**NH_3**) conjugate pairs.

In blood, the carbonic acid (**H_2CO_3**)/bicarbonate (**HCO_3^-**) buffering pair is especially useful because the buffer conjugate pair concentrations ([**H_2CO_3**] *and* [**HCO_3^-**]) are replenished through cellular respiration and can be controlled through breathing.

- To understand how this happens, we must consider these two reactions:

Reaction 1

$$CO_2(aq) + H_2O \ (l) \ \rightleftarrows \ H_2CO_3 \ (aq) + H_2O \ (l) \ \rightleftarrows \ HCO_3^- \ (aq) + H_3O^+ (aq)$$
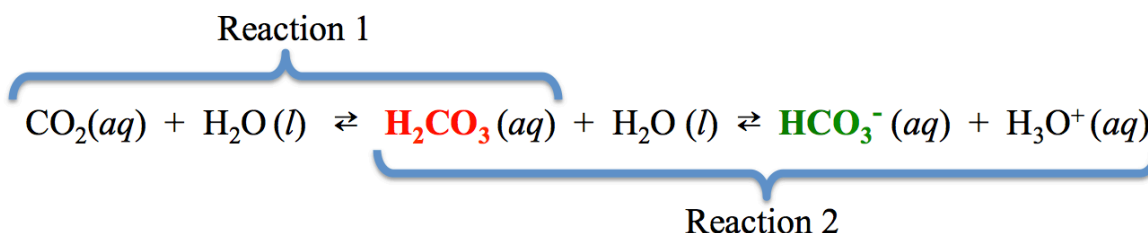
Reaction 2

- The CO_2 in Reaction 1 is constantly produced in the body during cellular respiration. Most of the CO_2 produced is exhaled; however, there is always some CO_2 dissolved in the blood.
- Reaction 2 is the carbonic acid/bicarbonate equilibrium, which acts as a **buffer**.

pH and Equilibrium Worksheet and Key

1. If the $[H_3O^+]$ = 1.7 x 10^{-4}, what is the $[OH^-]$?

2. If the $[H_3O^+]$ = 5.4 x 10^{-9}, what is the $[OH^-]$?

3. If the $[OH^-]$ = 9.7 x 10^{-2}, what is the $[H_3O^+]$?

4. If the $[OH^-]$ = 4.3 x 10^{-12}, what is the $[H_3O^+]$?

5. Fill in the table:

$[OH^-]$	$[H_3O^+]$	pH
	1.1 x 10^{-3} M	
	1.0 x 10^{-7} M	
	8.3 x 10^{-1} M	
	7.2 x 10^{-12} M	
		1.0
		7.00
		9.3
		12.00

Le Chatelier's Principle and Equilibrium Shifts

1. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$2CO_{(g)} + O_{2(g)} \rightleftarrows 2CO_{2(g)}$$
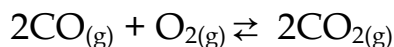
a. The amount of O_2 is increased.
b. The amount of CO_2 is decreased?
c. The amount of oxygen gas is decreased.

2. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$C_{(s)} + H_2O_{(g)} \rightleftarrows CO_{(g)} + H_{2(g)}$$

a. adding **$H_2O_{(g)}$**

b. removing carbon

c. removing H_2

d. adding carbon

3. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$PCl_{5(g)} \rightleftarrows PCl_{3(g)} + Cl_{2(g)}$$

a. adding PCl_3

b. removing Cl_2

c. removing PCl_3

d. adding Cl_2

pH and Equilibrium Key

1. If the $[H_3O^+]$ = 1.7 x 10^{-4}, what is the $[OH^-]$? **5.9 x 10^{-11} M**

2. If the $[H_3O^+]$ = 5.4 x 10^{-9}, what is the $[OH^-]$? **1.9 x 10^{-6} M**

3. If the $[OH^-]$ = 9.7 x 10^{-2}, what is the $[H_3O^+]$? **1.0 x 10^{-13} M**

4. If the $[OH^-]$ = 4.3 x 10^{-12}, what is the $[H_3O^+]$? **2.3 x 10^{-3} M**

5. Fill in the table:

$[OH^-]$	**$[H_3O^+]$**	**pH**
9.1 x 10^{-12} M	1.1 x 10^{-3} M	**2.96**
1.0 x 10^{-7} M	1.0 x 10^{-7} M	**7.00**
1.2 x 10^{-14} M	8.3 x 10^{-1} M	**0.081**
1.4 x 10^{-3} M	7.2 x 10^{-12} M	**11.14**
1 x 10^{-13} M	.1 M	1.0
1.0 x 10^{-7} M	**1.0 x 10^{-7} M**	7.00
2 x 10^{-5} M	**5 x 10^{-10} M**	9.3
1.0 x 10^{-2} M	**1.0 x 10^{-12} M**	12.00

Le Chatelier's Principle and Equilibrium Shifts

1. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$2CO_{(g)} + O_{2(g)} \rightleftarrows 2CO_{2(g)}$$

a. The amount of O_2 is increased.   **forward**
b. The amount of CO_2 is decreased? **forward**
c. The amount of oxygen gas is decreased. **reverse**

2. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$C_{(s)} + H_2O_{(g)} \quad \rightleftarrows \quad CO_{(g)} + H_{2(g)}$$
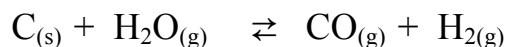
a. adding **$H_2O_{(g)}$** **forward**

b. removing carbon   **reverse**

c. removing H_2 **forward**

d. adding carbon **forward**

3. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$PCl_{5(g)} \rightleftarrows PCl_{3(g)} + Cl_{2(g)}$$

a. adding PCl_3 **reverse**

b. removing Cl_2 **forward**

c. removing PCl_3 **forward**

d. adding Cl_2 **reverse**

Chapter 8 Review Worksheet

Topics:

- Definition of equilibrium
- K_{eq}: law of mass action
- Le Chatelier's Principle

- Properties of acids & bases
- Brønstead-Lowry Acids & Bases definition
- K_w & calculating $[H_3O^+]$, $[OH^-]$, pH

1. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: **forward, reverse, or no change.**

$$H_{2(g)} + Cl_{2(g)} \rightleftarrows 2\ HCl_{(g)}$$
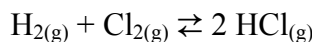
   a. the amount of H_2 is increased
   b. the amount of HCl is decreased
   c. the amount of Cl_2 is decreased

2. If the reaction below is initially at equilibrium, and then more NH_4^+ is added, predict which direction the reaction rate will be fastest until equilibrium is once again established**: forward, reverse, or no change**.

$$NH_4^+ + H_2O \rightleftarrows NH_3 + H_3O^+$$
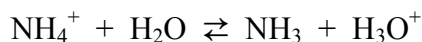
3. Define (a) **reversible reaction** and (b) **equilibrium**.

4. For the reaction below:
$$2NO_{2\ (g)} + O_{2\ (g)} \rightleftarrows 2NO_{3\ (g)}$$
   a. Write the law of mass action (the equilibrium expression for K_{eq})
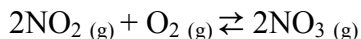
   b. If gas concentrations are as follows, 2.10 M NO_2, 1.75 M O_2, and 1.00 M NO_3, calculate K_{eq}

   c. Using K_{eq} from part b, are the **reactants** <u>or</u> **products** *predominant* (predominant means that there is a greater amount present)?

   d. Using K_{eq} from part b, calculate **[NO_3]** if $[NO_2] = [O_2] = 4.3 \times 10^{-6}$ M

Acids and Bases

5. For each of the following, write whether it describes acids/acidic (**A**), bases/basic (**B**), or both (**A & B**):

    a. $pH = 9.7$ f. $[H_3O^+] > [OH^-]$ k. sour

    b. $[H_3O^+] = 1 \times 10^{-9}$ M   g. $pH = 2.7$ l. slippery

    c. bitter   h. $pH = 13.0$

    d. $pH = 1.0$ i. gains/accepts an H^+ in a reaction

    e. $[OH^-] = 6.8 \times 10^{-2}$ M   j. electrolytes

6. For each of the following ***neutralization reactions***, predict the products AND balance the equation:

    a. $HCl + KOH \rightleftharpoons$

    b. $HCN + Ca(OH)_2 \rightleftharpoons$

7. Identify the acid and the base (for the forward direction) in each of the following reactions:

    a. $BH_3 + H_2O \rightarrow BH_4^+ + OH^-$

    b. $CH_3COOH + H_2O \rightarrow CH_3COO^- + H_3O^+$

    c. $HCO_3^- + H_2O \rightarrow CO_3^{-2} + H_3O^+$

    d. $HCN + H_2O \rightarrow CN^- + H_3O^+$

    e. $HNO_3 + H_2O \rightarrow NO_3^- + H_3O^+$

8. What is the conjugate acid of...
    a. NH_3
    b. HCO_3^-
    c. H_2O

9. What is the conjugate base of...
    a. H_2O
    b. HF
    c. HPO_4^{-2}

10. a. In a neutral solution, what is the concentration of H_3O^+?

    b. In a neutral solution, what is the concentration of OH^-?

11. Solutions in which the...

       a. $[H_3O^+]$ is greater than 1×10^{-7} M are _____ [**Choose one:** acidic, basic, or neutral]

       b. $[H_3O^+]$ is less than 1×10^{-7} M are _____ [**Choose one:** acidic, basic, or neutral]

       c. $[OH^-]$ is greater than 1×10^{-7} M are _____[**Choose one:** acidic, basic, or neutral]

       d. $[OH^-]$ is less than 1×10^{-7} M are _____[**Choose one:** acidic, basic, or neutral]

       e. $[H_3O^+]$ is equal to 1×10^{-7} M are _____[**Choose one:** acidic, basic, or neutral]

12. What is the concentration of H_3O^+ and OH^- for each of the following conditions?

    a. pH = 8.0

    b. pH = 6.50

    c. pH = 10.60

13. If the pH > pK_a in a buffer solution, which is larger, the concentration of the acid form or the concentration of base form.

1. If the reaction below is initially at equilibrium, and then each of the following changes are made, predict which direction the reaction rate will be fastest until equilibrium is once again established: forward, reverse, or no change.

$$H_{2(g)} + Cl_{2(g)} \rightleftarrows 2\ HCl_{(g)}$$
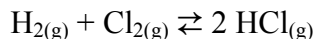
a. If the amount of H_2 is increased, then the **forward** reaction will be fastest until equilibrium is re-established.

b. If the amount of HCl is decreased, then the **forward** reaction will be fastest until equilibrium is re-established.

c. If the amount of Cl_2 is decreased, then the **reverse** reaction will be fastest until equilibrium is re-established.

2. If the reaction below is initially at equilibrium, and then more NH_4^+ is added, predict which direction the reaction rate will be fastest until equilibrium is once again established: forward, reverse, or no change.

$$NH_4^+ + H_2O \rightleftarrows NH_3 + H_3O^+$$
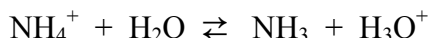
Answer: If more NH_4^+ is added, then the **forward** reaction will be fastest until equilibrium is re-established.

3. Define (a) **reversible reaction** and (b) **equilibrium**:
   SEE YOUR LECTURE NOTES

4. For the reaction below:

$$2NO_{2\ (g)} + O_{2\ (g)} \rightleftarrows 2NO_{3\ (g)}$$
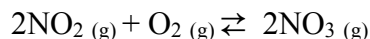
a. Write the law of mass action (the equilibrium expression for K_{eq})

$$K_{eq} = \frac{[NO_3]^2}{[O_2][NO_2]^2}$$

b. If gas concentrations are as follows, 2.10 M NO_2, 1.75 M O_2, and 1.00 M NO_3, calculate K_{eq}

$$K_{eq} = \frac{[1.00\ M]^2}{[1.75\ M][2.10\ M]^2} = 0.130\ M^{-1} \quad \textbf{(NOTE: "M^{-1}" is another way to write "1/M")}$$

c. Using K_{eq} from part b, are the reactants or products *predominant*?
   REACTANTS: K_{eq} is much less than 1

d. Using K_{eq} from part b, calculate **[NO₃]** if $[NO_2] = [O_2] = 4.3 \times 10^{-6}$

$$K_{eq} = \frac{[NO_3]^2}{(4.3 \times 10^{-6}M)(4.3 \times 10^{-6}M)^2} = 0.130\ M^{-1}$$

SOLVING THIS EQUATION FOR **[NO₃]** GIVES:

$$[NO_3] = \sqrt{(0.130\ M^{-1})(4.3 \times 10^{-6}\ M)(4.3 \times 10^{-6}M)^2} = 3.2 \times 10^{-9}\ M$$

5. For each of the following, write whether it describes acids/acidic (A), bases/basic (B), or both (A & B):

   a. B   f. A   k. A

   b. B   g. A   l. B

   c. B   h. B

   d. A   i. B

   e. B   j. A & B

6. For each of the following neutralization reactions, predict the products & balance the equation:
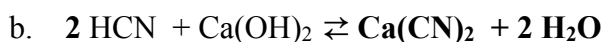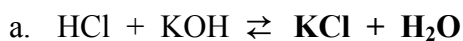
   a. $HCl + KOH \rightleftarrows KCl + H_2O$

   b. $2\ HCN + Ca(OH)_2 \rightleftarrows Ca(CN)_2 + 2\ H_2O$

7. Identify the acid and the base (for the forward direction) in each of the following reactions:

   a. $BH_3 + H_2O \rightarrow BH_4^+ + OH^-$
         Base   Acid

   b. $CH_3COOH + H_2O \rightarrow CH_3COO^- + H_3O^+$
           Acid   Base

   c. $HCO_3^- + H_2O \rightarrow CO_3^{-2} + H_3O^+$
         Acid   Base

   d. $HCN + H_2O \rightarrow CN^- + H_3O^+$
         Acid   Base

   e. $HNO_3 + H_2O \rightarrow NO_3^- + H_3O^+$
         Acid   Base

8. What is the conjugate acid of...
   a. NH_3 Conjugate acid = NH_4^+
   b. HCO_3^- Conjugate acid = H_2CO_3
   c. H_2O Conjugate acid = H_3O^+

9. What is the conjugate base of...
   a. H_2O Conjugate base = OH^-
   b. HF Conjugate base = F^-
   c. HPO_4^{-2} Conjugate base = PO_4^{-3}
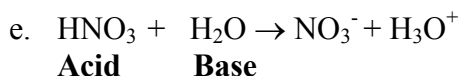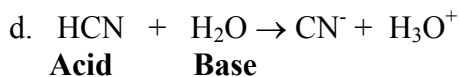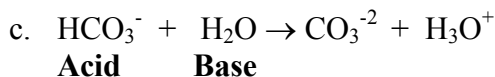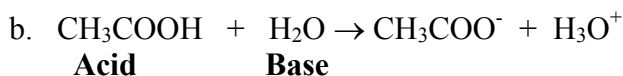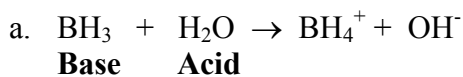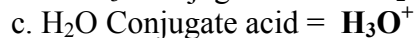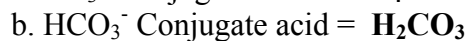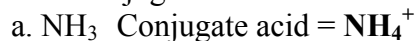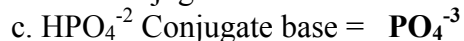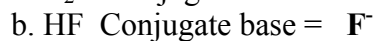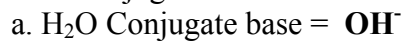
10. a. In a neutral solution, what is the concentration of H_3O^+?

   1.0 x 10^{-7} M

   b. In a neutral solution, what is the concentration of OH$^-$?

   1.0 x 10^{-7} M

11. Solutions in which the...

   a. $[H_3O^+]$ is greater than 1 x 10^{-7} M are **acidic**

   b. $[H_3O^+]$ is less than 1 x 10^{-7} M are **basic**

   c. $[OH^-]$ is greater than 1 x 10^{-7} M are **basic**

   d. $[OH^-]$ is less than 1 x 10^{-7} M are **acidic**

   e. $[H_3O^+]$ is equal to 1 x 10^{-7} M are **neutral**

12. What is the concentration of H_3O^+ and OH$^-$ for each of the following conditions?

   a. pH = 8.0 **H$_3$O$^+$= 1 x 10^{-8} M   OH= 1 x 10^{-6} M**

   b. pH = 6.50 **H$_3$O$^+$= 3.2 x 10^{-7} M   OH= 3.1 x 10^{-8} M**

   c. pH = 10.60 **H$_3$O$^+$= 2.5 x 10^{-11} M   OH= 4.0 x 10^{-4} M**

13. If the pH > pK$_a$, for a buffer, which is larger, the concentration of the acid [HA] or the concentration of the base [A$^-$].
   Base form [A$^-$]

Chapter 9 Lecture Notes: Carboxylic Acids, Amines, and Amides

Educational Goals

1. Given the structure of a **carboxylic acid**, **carboxylate ion**, **ester**, **amide**, **or amine molecule**, be able to give the systematic names and vice versa.

2. Know and understand the intermolecular forces that attract carboxylic acid, amine, or amide molecules to one another, and how these forces affect boiling points and melting points.

3. Identify **amines** as primary (1°), secondary (2°), or tertiary (3°). Compare and contrast **amines** and **quaternary ammonium ions**.

4. Predict the products for the reactions of carboxylic acids with water, alcohols, amines, ammonia, or with strong bases.

5. Predict the products for the reactions of amines with water or with strong acids.

6. Predict the products for the acid-catalyzed **hydrolysis of an amide**.

7. Identify **chiral carbon** atoms in structural formulas. Given the number of chiral carbons in a molecule, determine the number of **stereoisomers**.

8. Define the term **enantiomer**. Compare and contrast **enantiomers** and **diastereomers**.

Organic compounds are categorized into various _____ by the presence of distinct *functional groups*.

A **functional group** is an _____, _____ *of atoms*, **or** _____ that gives a compound a particular set of physical and chemical properties.

Carboxylic Acids

The Structure of Carboxylic Acids

Carboxylic acids contain a _____ *functional* group attached to a hydrocarbon (alkyl group) part.

Carboxyl groups contain both a _____ *group*, which is a carbon double bonded to an oxygen (**C=O**), *and* a _____ *group* (**-OH**) that are connected to each other and the hydrocarbon part as shown below.
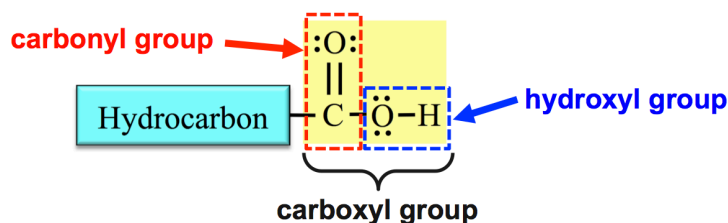
The *carboxyl group* is sometimes drawn as "**COOH**" or "**CO₂H**" in condensed structures:

Chemists use the letter "**R**" in the general structures to represent either a hydrocarbon/alkyl group part *or* any other organic group of atoms.
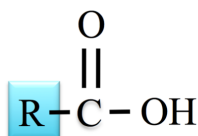
general form of a carboxylic acid molecule

A specific example of a carboxylic acid is **acetic acid**.

- White vinegar is a mixture composed of 95% water and 5% acetic acid.

The hydrocarbon part (**R**) in acetic acid is a methyl group (**CH₃**).

condensed structural formula
of **acetic acid**

ball-and-stick model
of **acetic acid**

black sphere = carbon
red sphere = oxygen
white sphere = hydrogen
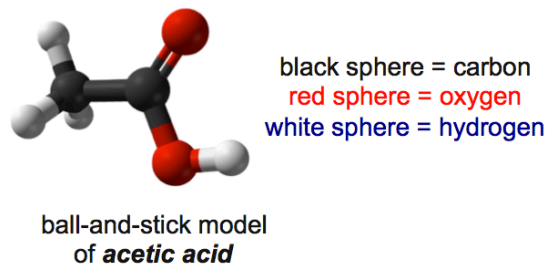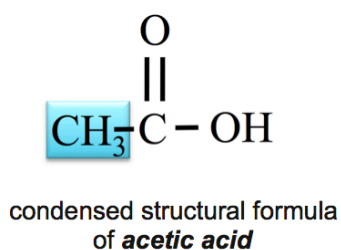
The skeletal structure of *acetic acid* is shown below. I have added dots to indicate the carbon atom positions.

skeletal structure of **acetic acid**
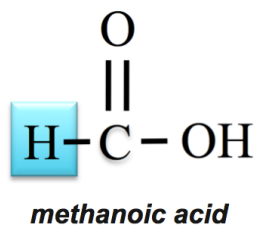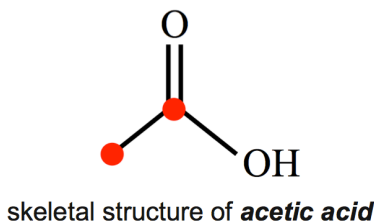
Although **methanoic acid**, contains a hydrogen (**H**) bonded to the carbonyl group instead of an alkyl group (**R**) it is still classified as carboxylic acid.

Methanoic acid is the molecule that is responsible for the stinging sensation caused by some ant bites.

methanoic acid

Naming Carboxylic Acids

We will use the IUPAC system for naming carboxylic acid molecules. The systematic naming of carboxylic acids is based on the hydrocarbon naming method.

Step 1: Find and name the **parent chain**.

The parent chain of a carboxylic acid is the longest continuous chain of carbon atoms that _____ the **carbonyl carbon**. The **carbonyl carbon** is the carbon in the carbonyl group (**C=O**).
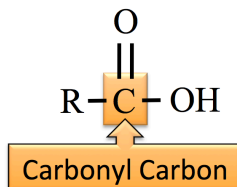
Carbonyl Carbon

Count the number of carbon atoms in the parent chain (*include the carbonyl carbon*). Starting with the alkane name that corresponds to the number of carbon atoms in the parent chain, replace the "**e**" at the end of the alkane name with "**oic acid**."

Example: the parent chain of a carboxylic acid that contains *three* carbons is called propan**oic acid**.
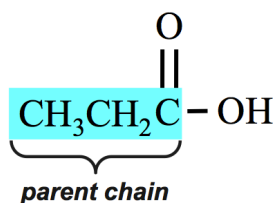
propan**e** ⟶ propan***oic acid***

If there are *no substituents on the parent chain*, the naming is complete. In this case the name of the molecule (above) would be **propanoic acid**.

parent chain

If there are substituents on the parent chain, you will need to continue with the steps that follow.

2

Step 2: Name any alkyl group **substituents**.

Alkyl groups are named in the same way as we did for hydrocarbons.

   Example:
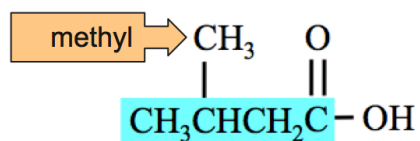
Step 3: Determine the *point of attachment* of alkyl group(s) to the parent chain.

In order to assign "position numbers" to the substituents, the carbons *in the parent chain* are numbered.

_____ *numbering at the* _____ *carbon*.

Example: the carbons in the parent chain of the molecule shown below are assigned position numbers:
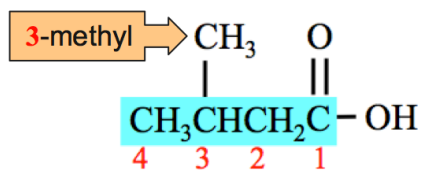
Step 4: Construct the name of the carboxylic acid by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

Use a ***dash*** between position *numbers* and *letters*.

Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) *identical* substituents are present.

   Example:

3-methylbutanoic acid
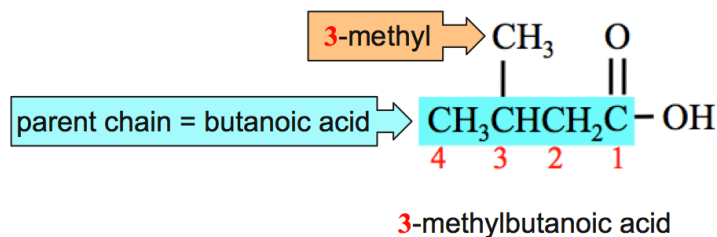
Naming Carboxylic Acids Example: Name the molecule that is shown below.
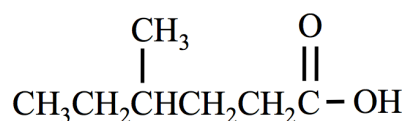
Step 1: Find and name the **parent chain**.
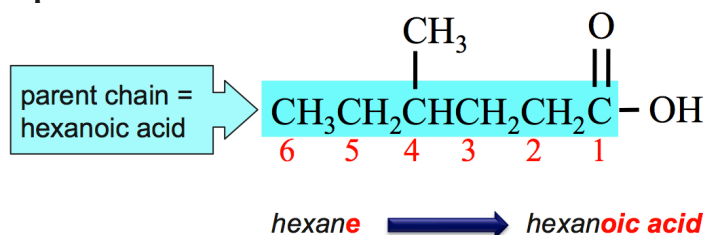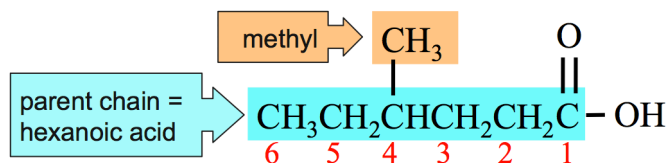
hexane ➡ *hexanoic acid*

Step 2: Name any alkyl group **substituents**.

methyl ⟶ CH_3

parent chain = hexanoic acid ⟶

$$CH_3CH_2CHCH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-OH$$

6 5 4 3 2 1

Step 3: Determine the *point of attachment* of alkyl group(s) to the parent chain.

Step 4: Construct the name of the carboxylic acid by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

4-methyl ⟶ CH_3

parent chain = hexanoic acid ⟶

$$CH_3CH_2CHCH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-OH$$

6 5 4 3 2 1

4-methylhexanoic acid

Understanding Check: Name the molecule that is shown below.

CH_2CH_3

$$CH_3CH_2CH_2CHCH_2CH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-OH$$
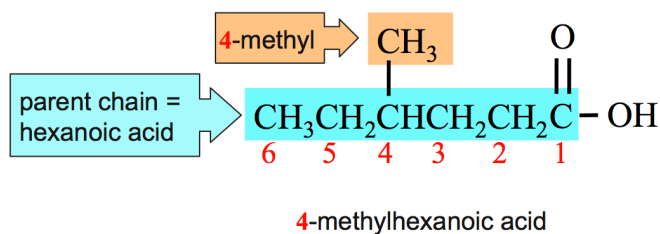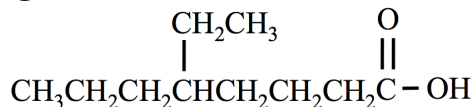
Understanding Check

The *common name* of the molecule shown below is acetic acid. What is the IUPAC systematic name for acetic acid?

$$CH_3\overset{\overset{\displaystyle O}{||}}{C}-OH$$
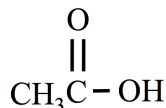
Let's do a problem in which we are given the name of a carboxylic acid and wish to draw its structural formula.

Example: Draw the *line bond structure* of 2-methylpropanoic acid.

For comparison, the *condensed and skeletal structure* of 2-methylpropanoic acid are shown below.

$$CH_3CH\overset{\overset{\displaystyle O}{||}}{C}-OH$$
$$|$$
$$CH_3$$
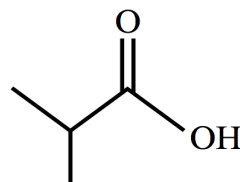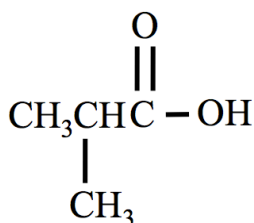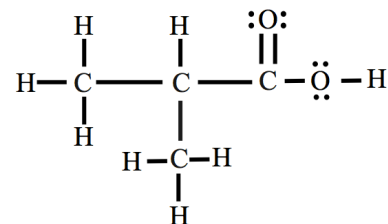
Understanding Check

Draw the line bond, condensed, and skeletal structural formulas of *decanoic acid.*

Hydroxyl, Fluorine, Chlorine, and Bromine Substituents

So far, you have only seen alkyl group substituents. It is not uncommon to see carboxylic acids that contain other *atoms* or *groups of atoms* that are named as substituents.

A hydroxyl group (-OH), fluorine atom, chlorine atom, or bromine atom that is bonded to *the parent chain* of a carboxylic acid is named as a substituent.

The table below list the names used for these substituents.

Names of Non Alkyl Substituents	
Substituent	**Name**
OH	hydroxy
F	fluoro
Cl	chloro
Br	bromo

Use position numbers and alphabetize these substituents, along with any alkyl group substituents, when naming carboxylic acids.

Examples:

3-chlorobutanoic acid

3-hydroxy-5-methylhexanoic acid

5
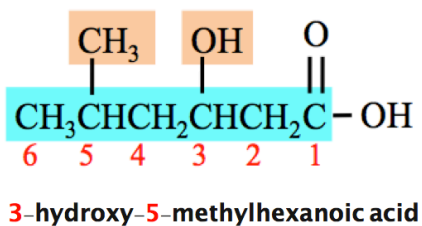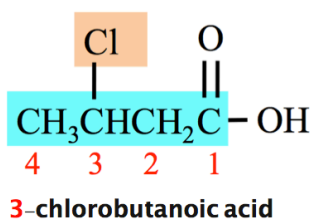
Alpha (*α*) and Beta (*β*) Carbons

Two of the carbon positions in the parent chain of carboxylic acids are designated as "***α***" or "***β***."

- The *α* and *β* designations are not part of the IUPAC naming system, however they are commonly used.

The carbons that are designated as carbon number **2** and **3** in the IUPAC system are often referred to as the *α* carbon and *β* carbon, respectively.

>   **Example:** The *α* carbon and *β* carbon are labeled in the structure of *butanoic acid* shown below.

$$CH_3-\underset{4}{CH_2}-\underset{3}{\overset{\beta}{CH_2}}-\underset{2}{\overset{\alpha}{CH_2}}-\underset{1}{\overset{\overset{\displaystyle O}{\|}}{C}}-OH$$
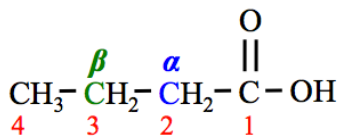
>   **Example:** The IUPAC systematic name of the molecule shown below is **3**-hydroxybutanoic acid. It is named ***β***-hydroxybutanoic acid when using the *α*/*β* designation.

$$CH_3\underset{\beta}{CH}\underset{\alpha}{CH_2}\overset{\overset{\displaystyle O}{\|}}{C}-OH$$
(with OH above the β carbon)
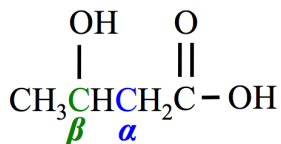
Understanding Check

Lactic acid is another name for *α*-hydroxypropanoic acid.

a. Draw the condensed structure of **lactic acid**.

b. What is the IUPAC systematic name for lactic acid?

Water Solubility of Carboxylic Acids

The water solubility of an organic compound depends on the compound's ability to interact with water.

All carboxylic acid molecules have a significantly strong attraction to water through hydrogen bonding and dipole-dipole interactions.

Small carboxylic acid molecules have significant water solubility.

As the _____ region (hydrocarbon part) of carboxylic acids gets larger, their water solubility _____; this is true not only for carboxylic acids, but for all organic molecules.

Water Solubility of Carboxylic Acids

Molecule Name	Condensed Structure	Water Solubility (g/100 mL)
methanoic acid	HCOOH	miscible*
ethanoic acid	CH_3COOH	miscible
propanoic acid	CH_3CH_2COOH	miscible
butanoic acid	$CH_3CH_2CH_2COOH$	miscible
pentanoic acid	$CH_3CH_2CH_2CH_2COOH$	3.7
hexanoic acid	$CH_3CH_2CH_2CH_2CH_2COOH$	1.0

*miscible indicates that the substance will mix/dissolve at any carboxylic acid to water ratio.

Names, Structural Formulas, and Natural Sources of Various Carboxylic Acids

Number of Carbons	IUPAC Name	Common Name	Condensed Structure	Source(s)
1	methanoic acid	formic acid	HCOOH	insect stings
2	ethanoic acid	acetic acid	CH_3COOH	bacterial fermentation
3	propanoic acid	propionic acid	CH_3CH_2COOH	bacterial production
4	butanoic acid	butyric acid	$CH_3(CH_2)_2COOH$	butter
5	pentanoic acid	valeric acid	$CH_3(CH_2)_3COOH$	valerian (an herb)
6	hexanoic acid	caproic acid	$CH_3(CH_2)_4COOH$	goat fat
7	heptanoic acid	enanthic acid	$CH_3(CH_2)_5COOH$	rancid oils
8	octanoic acid	caprylic acid	$CH_3(CH_2)_6COOH$	coconuts and breast milk
9	nonanoic acid	pelargonic acid	$CH_3(CH_2)_7COOH$	pelargonium (a genus of flowering plants)
10	decanoic acid	capric acid	$CH_3(CH_2)_8COOH$	coconuts and palm kernel oil
12	dodecanoic acid	lauric acid	$CH_3(CH_2)_{10}COOH$	coconut oil
16	hexadecanoic acid	palmitic acid	$CH_3(CH_2)_{14}COOH$	palm oil
18	octadecanoic acid	stearic acid	$CH_3(CH_2)_{16}COOH$	chocolate
20	icosanoic acid	arachidic acid	$CH_3(CH_2)_{18}COOH$	peanut oil

Chemical Reactions of Carboxylic Acids

1) Reaction of Carboxylic Acids with Water

Carboxylic acids have the word "_____" in their names because they readily donate an H^+ in acid-base reactions.

When placed in water, a carboxylic acid molecule acts as an acid and water acts as a base. An H^+ from the hydroxyl group (OH) of the carboxylic acid is donated to H_2O.
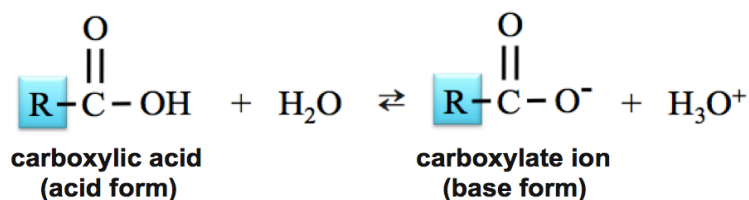
The **base form** of a carboxylic acid is called a _____ _____.

- A carboxylate ion has a charge of (1-) because of the _____ *charge* on the single-bonded oxygen. Recall that an oxygen atom with just one single bond has a (1-) formal charge.

A specific example of the reaction of a carboxylic acid and water is the reaction ethanoic acid and water.
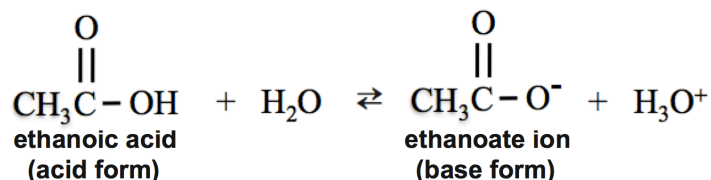
The **base form** of ethanoic acid is named **ethanoate ion**.

7

Carboxylate ions are named by replacing the "-__ _____" suffix of their *acid form* name with "-__ ___."

Examples:

ethano**ic acid** $\longrightarrow$ ethano**ate ion**

acet**ic acid** $\longrightarrow$ acet**ate ion**

3-methylpentano**ic acid** $\longrightarrow$ 3-methylpentano**ate ion**

When a carboxylic acid is placed in water, a reaction occurs between the acid and the water, and an equilibrium is established.

$$R-\overset{\overset{\displaystyle O}{\|}}{C}-OH \;+\; H_2O \;\rightleftarrows\; R-\overset{\overset{\displaystyle O}{\|}}{C}-O^- \;+\; H_3O^+$$
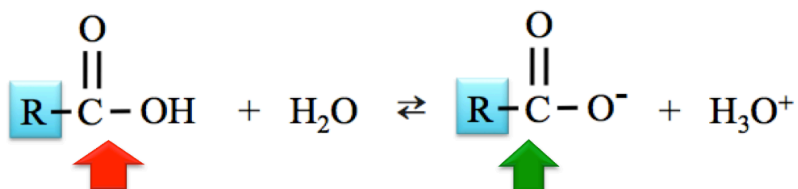
There is some of the *acid form* present and some of the *base form* present at equilibrium.

Carboxylic acids are considered to be "*weak acids*" because their K_a values are much less than 1.

Acid Name	Acid Formula	K_a	pK_a $pK_a = -\log(K_a)$
Acetic acid	CH_3COOH	1.8×10^{-5} M	4.74
2-hydroxypropanoic acid (lactic acid)	$CH_3CH_2(OH)COOH$	1.4×10^{-4} M	3.86
propanoic acid	CH_3CH_2COOH	1.3×10^{-5} M	4.88

When carboxylic acid/carboxylate ion conjugate pairs are in a solution, even if the solution contains other dissolved species, the relative amounts of the *acid form* and *base form* can be predicted by the Henderson-Hasselbalch Equation.

- The implications of the Henderson-Hasselbalch Equation are shown in the table below.

Solution Condition	Relative Amounts of Acid and Base Forms
$pH < pK_a$	$[HA] > [A^-]$
$pH > pK_a$	$[A^-] > [HA]$
$pH = pK_a$	$[HA] = [A^-]$

Understanding Check

Add the products for the following reaction:

$$\underset{CH_3}{\overset{\displaystyle CH_3}{|}}$$

CH$_3$CHCH$_2$CH$_2$C—OH   + H$_2$O $\rightleftarrows$
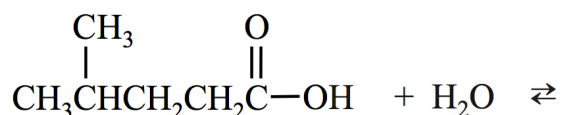
Draw the **condensed structure** *of the base form* (carboxylate ion) for each of the following carboxylic acids *and* write the name of each carboxylate ion.

a. octanoic acid

b. 3-methylbutanoic acid

c. 5-methylhexanoic acid

Understanding Check

When a carboxylic acid is placed in water, it reacts with water and an equilibrium is established. For example, butanoic acid reacts with water as shown here:

$$CH_3CH_2CH_2\overset{\overset{\displaystyle O}{\|}}{C}-OH + H_2O \rightleftarrows CH_3CH_2CH_2\overset{\overset{\displaystyle O}{\|}}{C}-O^- + H_3O^+$$

butanoic acid　　　　　　　　　　**butanoate ion**
(acid form)　　　　　　　　　　　**(base form)**
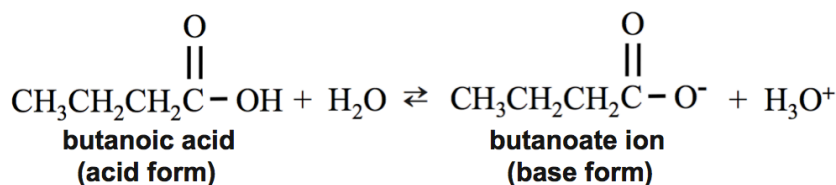
In many biochemical applications, it is of interest to understand whether the *acid form* or the *base form* of a species is predominant. We use the implications of the Henderson-Hasselbalch Equation to predict the predominant species at any particular pH.

The pK_a of butanoic acid is about 4.8. Is the *acid form* or *base form* of butanoic acid predominant at physiological pH (~7.4)?

---

2) Neutralization: Reaction of a Carboxylic Acid and a Hydroxide Ion

In a **neutralization reaction**, a carboxylic acid will react with a *hydroxide-containing* base compound to produce H_2O and *a carboxylic acid salt*.

$$R-\overset{\overset{\displaystyle O}{\|}}{C}-OH + NaOH \rightleftarrows R-\overset{\overset{\displaystyle O}{\|}}{C}-O^-Na^+ + H_2O$$

carboxylic acid　　　　　　　　carboxylic acid *salt*
　　　　　　　　　　　　　　　　(an ionic compound)
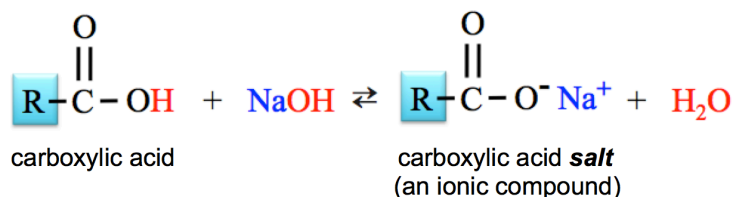
This is the same neutralization reaction that you learned in a previous chapter; the H^+ from the acid bonds to the OH^- to produce H_2O.

The _____ *ion* and the _____ *from the base* make an *ionic compound* called a *carboxylic acid* _____.

A specific example of the **neutralization** of a carboxylic acid is the reaction of propanoic acid and sodium hydroxide:

$$CH_3CH_2\overset{\overset{\displaystyle O}{\|}}{C}-OH + NaOH \rightleftarrows CH_3CH_2\overset{\overset{\displaystyle O}{\|}}{C}-O^-Na^+ + H_2O$$

propanoic acid　　　　　　　　carboxylic acid *salt*
　　　　　　　　　　　　　　　　(sodium propanoate)
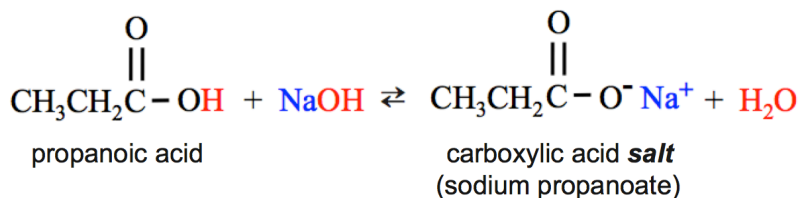
Water Solubility of Carboxylate Ions

A *carboxylic acid salt* formed from a carboxylate anion and a Na^+ or K^+ cation is water **soluble** if its "**R**" group contains less than twelve carbon atoms.

If its "**R**" group contains twelve or more carbons, then it is _____.

- The attraction of water to the _____
_____ of the carboxylate ion makes the salts more water soluble than their carboxylic acid conjugates.

A carboxylic acid salt formed from a *carboxylate anion* and a Ca^{2+} or Mg^{2+} cation is water **insoluble**.

It is the Ca^{2+} and Mg^{2+} ions that are responsible for the build up of **soap scum** in bathtubs and showers.

The Water Solubility of Carboxylic Acids and the Carboxylate Ions of Their Na^+ or K^+ Salts

Carboxylic Acid	Carboxylate Ion
$$\begin{array}{c} O \\ \| \\ R-C-OH \end{array}$$	$$\begin{array}{c} O \\ \| \\ R-C-O^- \end{array}$$
Acid Form	Base Form
When **R** gets to **five** carbons, the water solubility decreases dramatically.	If **R** < 12: water soluble
	If **R** ≥ 12: amphipathic (forms monolayers or micelles)

Water with significant amounts of Ca^{2+} and/or Mg^{2+} ions is called **hard water**.

The long-chain carboxylate ions in soap combine with Ca^{2+} or Mg^{2+} to form *insoluble solids* (precipitates) called *soap scum*.

In order to prevent the formation of soap scum and other Ca^{2+} and Mg^{2+} precipitates, Ca^{2+} and Mg^{2+} can be removed from water, in a device called a **water softener** before the water is distributed throughout a home's plumbing system. Water softeners operate by exchanging Na^+ ions for Ca^{2+} and Mg^{2+} ions.

Understanding Check: Add the products for the following neutralization reaction.

$$\begin{array}{c} CH_3 \qquad\quad O \\ | \qquad\qquad \| \\ CH_3CHCH_2CH_2C-OH \end{array} \quad + \quad NaOH \quad \rightleftarrows$$

---
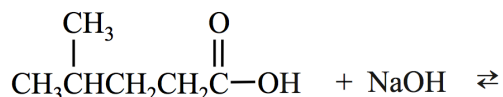
3) Esterification: The Reaction of a Carboxylic Acid and an Alcohol

In an ***esterification reaction,*** a carboxylic acid reacts with an alcohol to produce an _____ and water.

The general form for the esterification reaction is:

$$\underset{\text{carboxylic acid}}{\begin{array}{c} O \\ \| \\ R-C-OH \end{array}} \quad + \quad \underset{\text{alcohol}}{H-OR'} \quad \rightleftarrows \quad \underset{\text{ester}}{\begin{array}{c} O \\ \| \\ R-C-OR' \end{array}} \quad + \quad \underset{\text{water}}{H_2O}$$
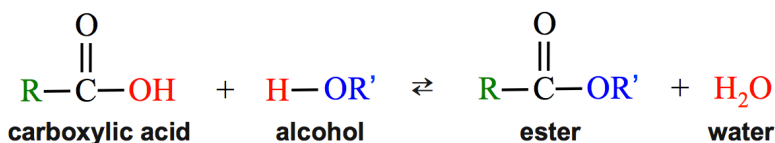
In order to keep track of them in the general reaction, we use "**R**" for the hydrocarbon part of the carboxylic acid, and "**R'** " for the hydrocarbon part of the alcohol.

- **R** and **R'** may, or may not, be identical.

An ester is produced when the **OH** from the carboxylic acid is replace with the **OR'** from the alcohol.

The **OH** from the carboxylic acid combines with the **H** from the alcohol to produce H_2O.

Replace this OH with this OR'

$$\underset{\text{carboxylic acid}}{\begin{array}{c} O \\ \| \\ R-C-\boxed{OH} \end{array}} \quad + \quad \underset{\text{alcohol}}{\boxed{H}-OR'} \quad \rightleftarrows \quad \underset{\text{ester}}{\begin{array}{c} O \\ \| \\ R-C-OR' \end{array}} \quad + \quad \underset{\text{water}}{\boxed{H_2O}}$$
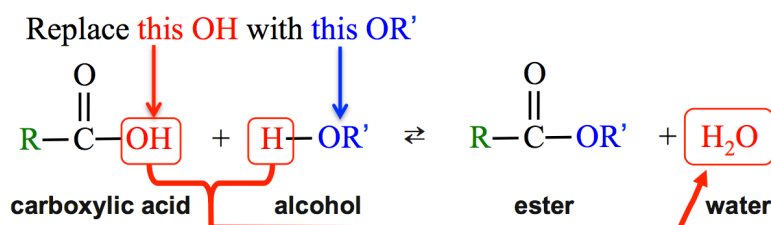
Esterification reactions can be done in the lab by heating a carboxylic acid and alcohol mixture in the presence of a strong acid catalyst.

A specific example of an esterification reaction is the reaction of ethanoic acid and pentanol (an alcohol):

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OH \;+\; H-OCH_2CH_2CH_2CH_2CH_3 \;\underset{\Delta}{\overset{H_3O^+}{\rightleftharpoons}}\; CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_2CH_2CH_2CH_2CH_3 \;+\; H_2O$$

| ethanoic acid | pentanol | pentyl ethanoate | water |
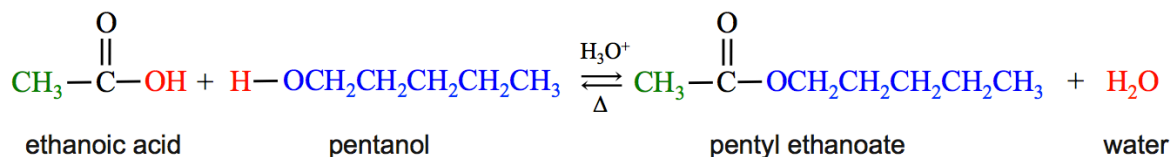
The *ester formed in the reaction above*, pentyl ethanoate, has the distinct aroma of bananas.

Many esters have pleasant aromas and flavors, and occur naturally in foods. Esters are often added to foods as artificial flavors. They are also used in perfumes.

The Greek delta symbol (Δ) is written below the arrows in the chemical equation when heat is used to increase the rate of a reaction, as shown in the equation above.

Likewise, when catalysts, such as H_3O^+, are used, the formula or name of the catalyst is written above the arrows.

Understanding Check

Add the products for the following esterification reactions:

a.

$$CH_3CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OH \;+\; H-OCH_2CH_2CH_3 \;\rightleftharpoons$$

b.

$$CH_3CH_2CH_2CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OH \;+\; H-OCH_3 \;\rightleftharpoons$$
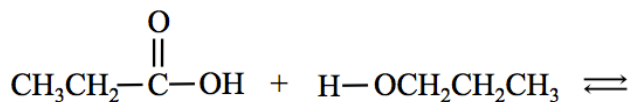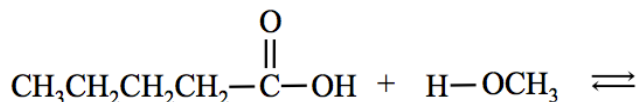
Naming Esters

The IUPAC method for naming esters involves naming the **R'** alkyl group part first, followed by the "*carboxylate-like*" part.
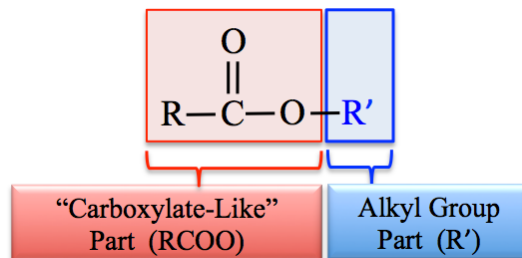
Example: Name the ester shown below:

$$CH_3CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-O-CH_2CH_3$$

11
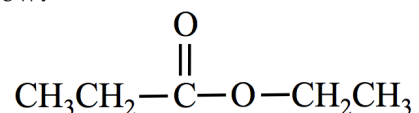
SOLUTION:

1) Identify the alkyl group (**R'**) part and the carboxylate-like part.

2) The ester is named by writing the alkyl group (**R'**) part name first, then a space, followed by the name that the "carboxylate-like" part would have *if it were an actual carboxylate ion*.

In this example, the "carboxylate-like" part contains three carbons, therefore its name would be *propanoate* if it were an *actual* carboxylate ion. The alkyl group (**R'**) is an **ethyl** group. The name of this ester is **ethyl propanoate**.
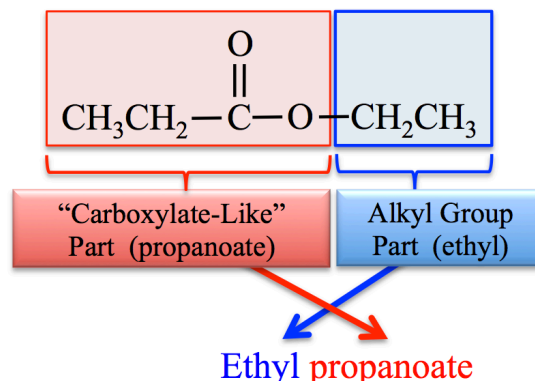
Many naturally-occurring esters contain alkyl groups composed of more than four carbons. In chapter 4, you learned the names of alkyl groups with four or fewer carbons (i.e. methyl, ethyl, propyl, butyl).

The table below lists the names and structures of nonbranched alkyl groups composed of 5-10 carbons.

Names and Structures of Some Alkyl Groups		
Number of Carbons	Alkyl Group Name	Condensed Structure
5	pentyl	$-CH_2CH_2CH_2CH_2CH_3$
6	hexyl	$-CH_2CH_2CH_2CH_2CH_2CH_3$
7	heptyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
8	octyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
9	nonyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
10	decyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

Understanding Check

Write the name of each of the esters shown below:
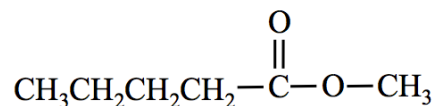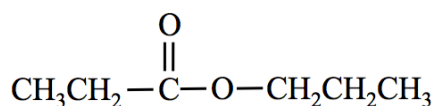
Understanding Check

Draw the condensed structure of **octyl butanoate**.

4) Decarboxylation of Carboxylic Acids

Carboxylic acids undergo a decomposition reaction called _____.

This reaction is very important in the citric acid cycle and other biological processes.

- The carbon dioxide that we exhale is produced by decarboxylation reactions in two of the reactions of the citric acid cycle.

In decarboxylation reactions, a _____ *group* (COOH) is _____ and *replaced by a hydrogen atom*.

The general form for the decarboxylation reaction is:
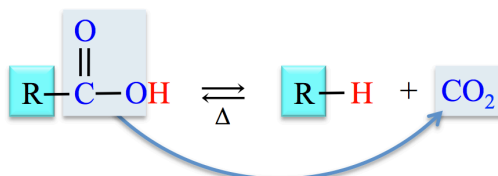
Decarboxylation reactions require heat and/or a catalyst.

The enzymes in biological systems that catalyze decarboxylation reactions are called *decarboxylases*.

Carboxylic acids with an **R** group composed of an alkyl group *only* do not readily undergo decarboxylation reactions. However, when the alpha (α) or beta carbon (β) of the **R** group is double bonded to an oxygen, then decarboxylation reactions readily occur.

- **Example:** the decarboxylation of pyruvic acid (an important reaction in yeast):
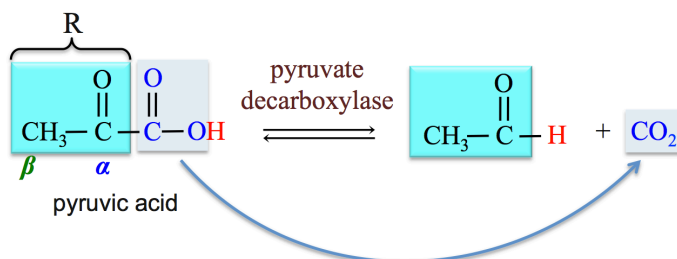
Note that we have expanded our definition of the "**R**" group to be *any organic group* that is unchanged in a reaction. The carbonyl group at pyruvate's α-carbon is unchanged in this decarboxylation reaction.

Decarboxylation is not only an important reaction in yeast, it also take place in cellular respiration in other animals.

Understanding Check

The production of molecules called *ketone bodies* occurs in humans when large amounts of stored fat are used to produce energy. This can occur during dieting, starvation conditions, or other conditions in a process called **ketosis**. The production of ketone bodies is useful since cells in the brain *cannot* get energy from molecules other than sugars or ketone bodies. When *acetoacetic acid* (one of the three ketone body molecules) is produced in ketosis, it is subsequently converted to another ketone body molecule in a *decarboxylation reaction*.

Predict (draw) the products of this decarboxylation reaction of acetoacetic acid (shown below).
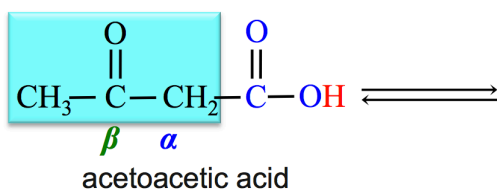
NOTE: The *carbonyl* (C=O) *group* at the β-carbon of *acetoacetic* acid is not affected by the reaction; it is considered to be part of the R group.

- The *carboxyl group* (**COOH**) is removed and replaced with a hydrogen.

Summary of the Reactions of Carboxylic Acids

1) Reaction of Carboxylic Acids with Water

When placed in water, a carboxylic acid molecule acts as an acid and water acts as a base. An H^+ from the hydroxyl group (OH) of the carboxylic acid is donated to H_2O.

$$R-\overset{\overset{\textstyle O}{\|}}{C}-OH \;+\; H_2O \;\rightleftharpoons\; R-\overset{\overset{\textstyle O}{\|}}{C}-O^- \;+\; H_3O^+$$

carboxylic acid (acid form)   **carboxylate ion** (base form)

2) Neutralization: Reaction of a Carboxylic Acid and a Hydroxide Ion

In a **neutralization reaction**, a carboxylic acid will react with a *hydroxide-containing* base compound to produce **H_2O** and *a carboxylic acid salt*.

$$R-\overset{\overset{\textstyle O}{\|}}{C}-OH \;+\; NaOH \;\rightleftharpoons\; R-\overset{\overset{\textstyle O}{\|}}{C}-O^- Na^+ \;+\; H_2O$$

carboxylic acid   carboxylic acid **salt** (an ionic compound)

3) Esterification: The Reaction of a Carboxylic Acid and an Alcohol

In an *esterification reaction,* a carboxylic acid reacts with an alcohol to produce an *ester* and water.

Replace this OH with this OR'

$$R-\overset{\overset{\textstyle O}{\|}}{C}-\boxed{OH} \;+\; \boxed{H}-OR' \;\rightleftharpoons\; R-\overset{\overset{\textstyle O}{\|}}{C}-OR' \;+\; \boxed{H_2O}$$
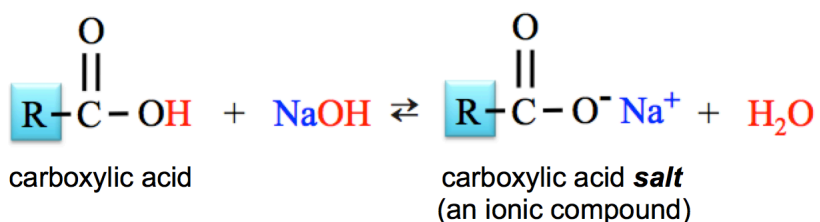
carboxylic acid   alcohol   ester   water
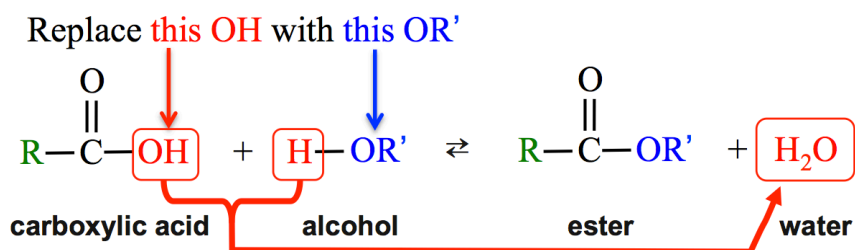
4) Decarboxylation of Carboxylic Acids

In decarboxylation reactions, a *carboxyl group* (COOH) is *removed* and *replaced by a hydrogen atom*.

$$R-\overset{\overset{\textstyle O}{\|}}{C}-OH \;\underset{\Delta}{\rightleftharpoons}\; R-H \;+\; CO_2$$
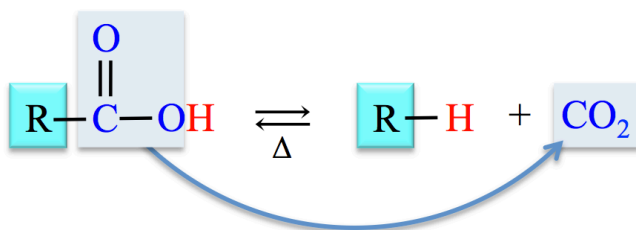
Amines

The Structure of Amines

Amines contain a _____ *atom* with *one* lone pair and *three* single bonds to **R** groups or hydrogens.

Amines are classified as primary (1°), secondary (2°), or tertiary (3°) based on the number of **R** groups that they contain.

The general forms of the three categories of amines are:
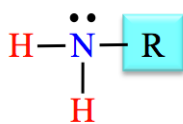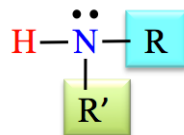
primary (1°) amine	secondary (2°) amine	tertiary (3°) amine
NH_2R	NHR_2	NR_3
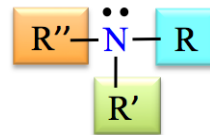
In _____ **(1°)** *amines*, a nitrogen is bonded to _____ **R** group and _____ hydrogen atoms.

An example of a **primary amine** is methanamine. The structural formula and ball-and-stick model for methanamine are shown below (blue sphere = nitrogen, black sphere = carbon, and white sphere = hydrogen).
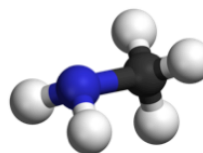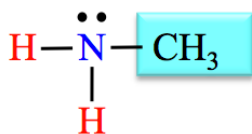
methanamine

In _____ **(2°)** *amines*, a nitrogen is bonded to _____ **R** groups and _____ hydrogen atom.

secondary (2°) amine

NHR_2
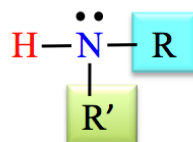
One **R** group is written as **R**, and the other as **R'**, to indicate that *they are not necessarily the same alkyl group*.

An example of a **secondary amine** is *N*-methylethanamine:
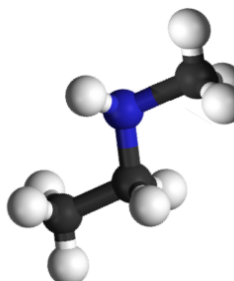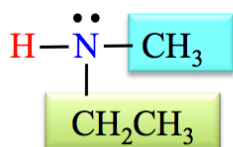
N-methylethanamine

In *tertiary* (**3°**) *amines*, a nitrogen is bonded to *three* **R** groups.

$$R'' - \overset{\cdot\cdot}{N} - R$$
$$|$$
$$R'$$

tertiary (3°) amine

$$NR_3$$
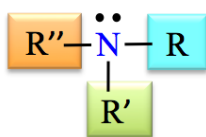
An example of a *tertiary amine* is *N,N*-dimethylmethanamine:

$$CH_3 - \overset{\cdot\cdot}{N} - CH_3$$
$$|$$
$$CH_3$$
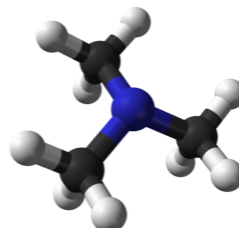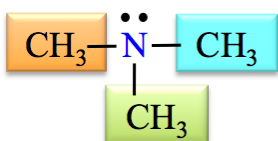
N,N-dimethylmethanamine

Understanding Check

Identify each of the amines shown below as either primary (1°), secondary (2°), or tertiary (3°).

a. $H - N - CH_3$
    $\quad\quad |$
    $\quad CH_3CHCH_3$

b. $CH_3CHCH_2CH_3$
    $\quad\quad\quad |$
    $\quad\quad\; NH_2$

c. $CH_3 - N - CH_3$
    $\quad\quad\quad |$
    $\quad CH_3CHCH_2CH_3$

d. $\quad\quad NH_2 \quad CH_2CH_3$
    $\quad\quad\quad |\quad\quad\;\; |$
    $CH_3CHCHCH_2CHCH_2CH_3$
    $\quad\quad\quad\quad\quad |$
    $\quad\quad\quad\quad\; CH_3$

e. $CH_2CH_2CH_3$
    $\quad |$
    $\; NH_2$

f. $\quad\quad\quad H - N - CH_2CH_3$
    $\quad\quad\quad\quad\quad\; |$
    $\quad CH_3CHCH_2CHCH_3$
    $\quad\quad\quad\quad\quad |$
    $\quad\quad\quad\quad\; CH_3$
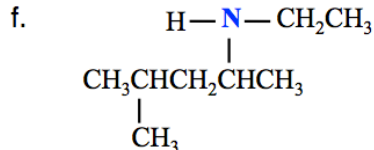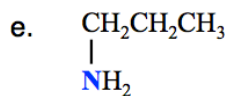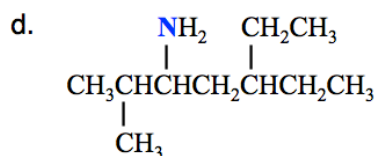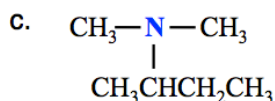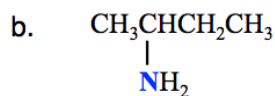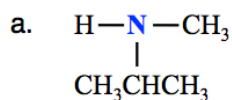
Understanding Check

Draw the **skeletal structure** of each of the *amines* shown below:

a. $CH_2CH_2CH_3$
    $\quad |$
    $\; NH_2$

b. $CH_3CHCH_2CH_3$
    $\quad\quad |$
    $\quad\; NH_2$

c. $\quad\quad H - N - CH_2CH_3$
    $\quad\quad\quad\quad\; |$
    $\quad CH_3CHCH_2CHCH_3$
    $\quad\quad\quad\quad\; |$
    $\quad\quad\quad\; CH_3$
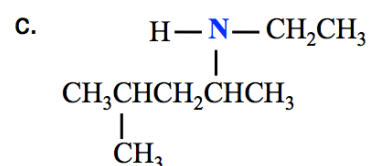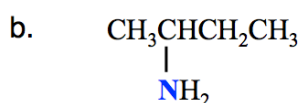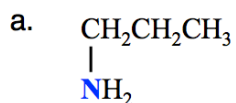
A **quaternary ammonium ion** is formed when *an* _____ hydrogen *or* alkyl group (**R**) is added to an amine.

The **nitrogen** in a quaternary ammonium ion *does not have a lone pair* and, therefore has a _____ _____ of **1+**.
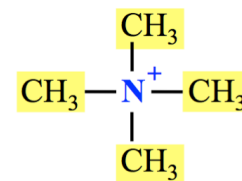
An example of a **quaternary ammonium ion** is the tetramethylammonium ion, which occurs naturally in some animals.

$$CH_3-\overset{\underset{\displaystyle |}{CH_3}}{\overset{\displaystyle |}{N^+}}-CH_3$$
$$|$$
$$CH_3$$

tetramethylammonium ion

Some molecules contain **more than one** type of functional group.

For example, molecules called **amino acids** contain both an **amino group** (**-NH₂**) *and* a carboxyl group (**-COOH**).

An example of an **amino acid** is alanine:

carboxyl group

amino group
(**-NH₂**)

$$H_2N-\underset{\underset{\displaystyle CH_3}{|}}{CH}-\overset{\overset{\displaystyle O}{\|}}{C}-OH$$

alanine
an amino acid
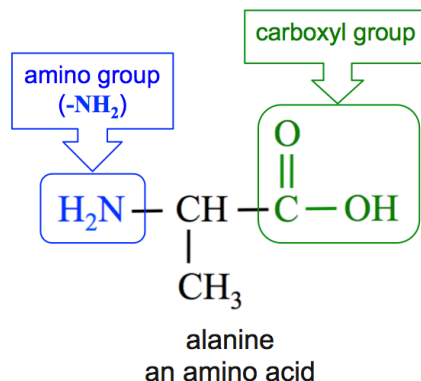
Amino acids are the precursors to **proteins**.

Naming Amines

The *systematic method* that we will use for naming amines is based on the hydrocarbon naming method.

Step 1. Find and name the *parent chain*.

The *parent chain is the longest, continuous chain of carbon atoms that **contains the point of** _____ **to the nitrogen**.*

- Starting with the alkane name that corresponds to the number of carbon atoms in the ***parent chain***, replace the "**e**" at the end of the alkane name with "**amine**."

Example: if the parent chain of an amine contains two carbons, it would be called *ethanamine.*

ethan**e** ➡️ ethan***amine***

For amines with ***more than two carbons***, the position of *the point of attachment to the **nitrogen*** must be indicated by adding a number ***before the parent chain name***, as described below.

Assign *position numbers* to the carbons in the parent chain. Position number **1** is assigned to the carbon at the *end of the parent chain* that is **nearest to the point of attachment to the** _____.

If the nitrogen is bonded to carbon number **1** of the parent chain, then "**1-**" is used as a prefix to the parent chain name.

- For example, in the molecule below, the parent chain is called **1-**pentanamine.
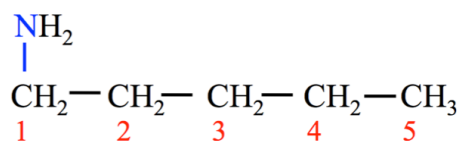
$$\overset{\overset{\displaystyle NH_2}{|}}{\underset{1}{CH_2}}-\underset{2}{CH_2}-\underset{3}{CH_2}-\underset{4}{CH_2}-\underset{5}{CH_3}$$

1-pentanamine

17

If the nitrogen is bonded to carbon number **2** of the parent chain, then "**2-**" is used as a prefix to the parent chain name.

- For example, in the molecule below, the parent chain is called **2-pentanamine**.

$$\begin{array}{c}
NH_2 \\
| \\
CH_3-CH_2-CH_2-CH-CH_3 \\
54321
\end{array}$$

2-pentanamine
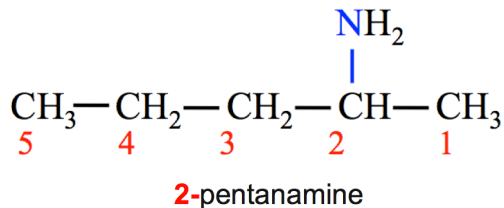
This is analogous to the numbers that you used as prefixes for the parent chain names of alkenes to indicate the position of the double bond.

Step 2. Name any alkyl group substituents.

Alkyl group substituents that are attached to the parent chain are named in the same way as you did for alkanes.

For secondary and tertiary amines, the *nonparent chain* **R** group(s) *attached to the nitrogen* are named as substituents.

- "**N-**" is written in front of the **R** group substituent name, instead of a position *number,* in order to indicate that the **R** group is ***attached to the*** _____.

- For example, the amine shown below has a ***methyl*** substituent attached to the ***parent chain*** *and* an ***ethyl*** substituent attached to the **nitrogen**.

$$\begin{array}{c}
H-N-CH_2CH_3 \Leftarrow \boxed{\textit{N}\text{-ethyl}} \\
123|4567 \\
CH_3CHCHCH_2CH_2CH_2CH_3 \\
| \\
CH_3 \Leftarrow \boxed{2\text{-methyl}}
\end{array}$$
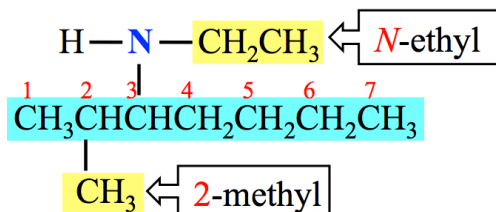
Step 3. Construct the name of the amine by placing the alkyl groups in alphabetical order and specifying their position, followed by the name of the parent chain.

- This is done the same way as you did for hydrocarbons and carboxylic acids.
- Remember to use a dash between position numbers (or "*N*") and letters.

The name of the amine **shown below** is: **N-ethyl-2-methyl-3-heptanamine**.

$$\begin{array}{c}
H-N-CH_2CH_3 \Leftarrow \boxed{\textit{N}\text{-ethyl}} \\
123|4567 \\
CH_3CHCHCH_2CH_2CH_2CH_3 \\
| \\
CH_3 \Leftarrow \boxed{2\text{-methyl}}
\end{array}$$

18
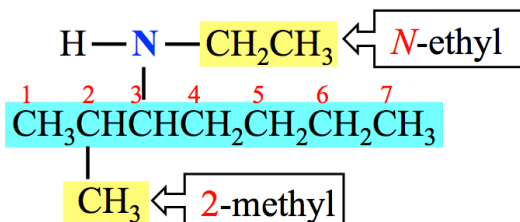
Other Examples:

Names and Structures of Primary (1°) Amines

$\overset{1}{\text{CH}_3}\overset{2}{\text{CH}}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_3}$

$|$

NH_2

2-butanamine

$\overset{1}{\text{CH}_2}\overset{2}{\text{CH}_2}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_3}$

$|$

NH_2
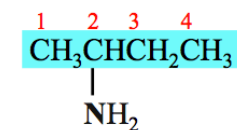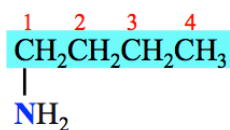
1-butanamine

also drawn as:

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$

or

$\text{NH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$

$\text{NH}_2 \quad \text{CH}_2\text{CH}_3 \Leftarrow \boxed{\text{5-ethyl}}$

$\overset{1}{\text{CH}_3}\overset{2}{\text{CH}}\overset{3}{\text{CH}}\overset{4}{\text{CH}_2}\overset{5}{\text{CH}}\overset{6}{\text{CH}_2}\overset{7}{\text{CH}_2}\overset{8}{\text{CH}_3}$

$|$

$\text{CH}_3 \Leftarrow \boxed{\text{2-methyl}}$
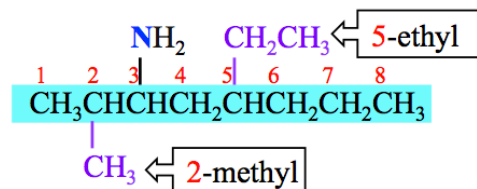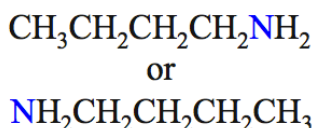
5-ethyl-2-methyl-3-octanamine

Names and Structures of Secondary (2°) Amines

$\text{H}-\text{N}-\boxed{\text{CH}_3} \Leftarrow \boxed{\textit{N}\text{-methyl}}$

$|$

$\overset{1}{\text{CH}_3}\overset{2}{\text{CH}}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_3}$

N-methyl-2-butanamine

$\text{H}-\text{N}-\boxed{\text{CH}_2\text{CH}_3} \Leftarrow \boxed{\textit{N}\text{-ethyl}}$

$|$

$\overset{5}{\text{CH}_3}\overset{4}{\text{CH}}\overset{3}{\text{CH}_2}\overset{2}{\text{CH}}\overset{1}{\text{CH}_3}$

$|$

$\boxed{\text{CH}_3} \Leftarrow \boxed{\text{4-methyl}}$
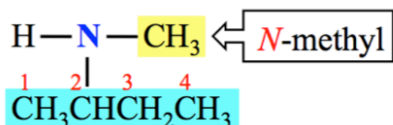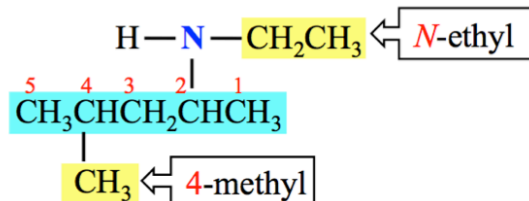
N-ethyl-4-methyl-2-pentanamine

Names and Structures of Tertiary (3°) Amines

$\boxed{\textit{N}\text{-methyl}} \quad \boxed{\textit{N}\text{-methyl}}$

$\boxed{\text{CH}_3}-\text{N}-\boxed{\text{CH}_3}$

$|$

$\overset{1}{\text{CH}_3}\overset{2}{\text{CH}}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_3}$

N,N-dimethyl-2-butanamine

$\boxed{\textit{N}\text{-methyl}} \quad \boxed{\textit{N}\text{-ethyl}}$

$\boxed{\text{CH}_3}-\text{N}-\boxed{\text{CH}_2\text{CH}_3}$

$|$

$\overset{1}{\text{CH}_2}\overset{2}{\text{CH}_2}\overset{3}{\text{CH}_2}\overset{4}{\text{CH}_3}$
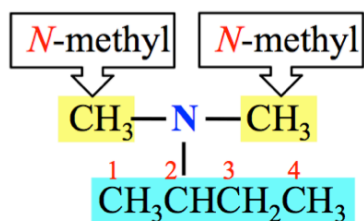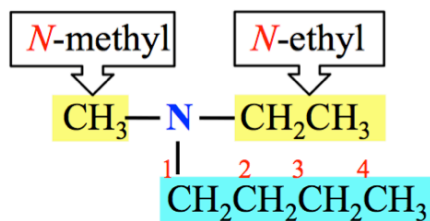
N-ethyl-*N*-methyl-1-butanamine

Common Names for Amines

Simple amines, those with a relatively few number of carbon atoms, are often identified by ***common names*** by placing "amine" after the names of the alkyl group(s) that are attached to the nitrogen.

Examples:

CH_3NH_2

methylamine

$\text{CH}_3\text{CH}_2\text{NH}_2$

ethylamine

$\text{NH}(\text{CH}_3)_2$

dimethylamine

$\text{N}(\text{CH}_3)_3$

trimethylamine
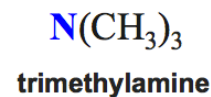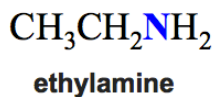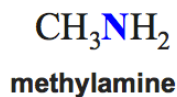
Understanding Check

Write the **systematic names** for each of the amines shown below:

a. CH_3CH_2
    |
    NH_2

b. $CH_3CH_2CH_2-N-CH_2CH_3$
                     |
                    CH_3

c. $H-N-CH_2CH_3$
         |
        CH_3

d. $H-N-CH_2CH_3$
         |
    $CH_3CHCHCH_2CH_2CH_3$
         |
        CH_3

e. CH_3CHCH_3
         |
        NH_2

f. CH_2CH_3 NH_2
         | |
    $CH_3CH_2CCH_2CH_2CHCH_2CH_3$
         |
        CH_3
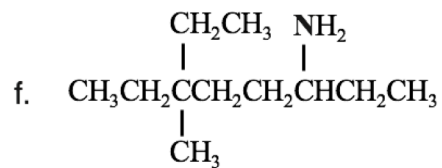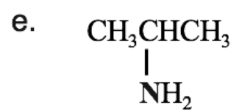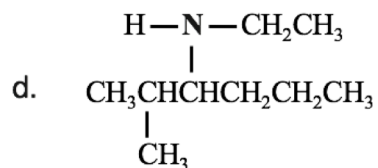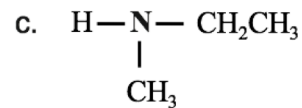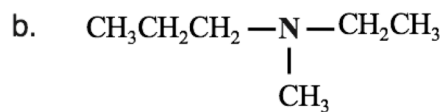
Understanding Check

Draw the condensed **and** skeletal structure of each of the amines listed below.

2-methyl-3-hexanamine   *N*-methyl-2-propanamine   *N,N*-diethylethanamine

Heterocyclic Compounds

You have seen cyclic compounds such as cyclohexane and cyclopentane. The rings of the cyclic compounds that you have seen so far have contained *only carbon atoms*.

Cyclic compounds that contain atoms _____ _____ carbon are known as **heterocyclic compounds**.

Examples of heterocyclic compounds are:
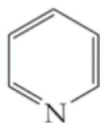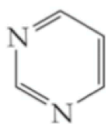
pyridine   pyrimidine   purine
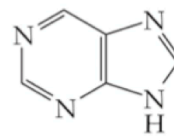
Heterocyclic, *nitrogen-containing* rings are very common in plants and animals.

- **Example:** Nicotine is a naturally occurring, nitrogen-containing heterocyclic molecule from the tobacco plant.
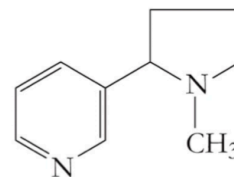
nicotine

Adenosine triphosphate (ATP), used by nature in both plants and animals, is an important compound for energy storage.

ATP has *nitrogen-containing* heterocyclic rings **and** an *oxygen-containing* heterocyclic ring.
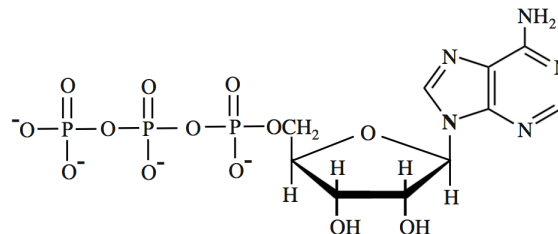
adenosine triphosphate (**ATP**)

DNA and RNA have both *nitrogen-containing* and *oxygen-containing* heterocyclic ring structures.

A structural formula for a *small portion* of DNA is shown here.
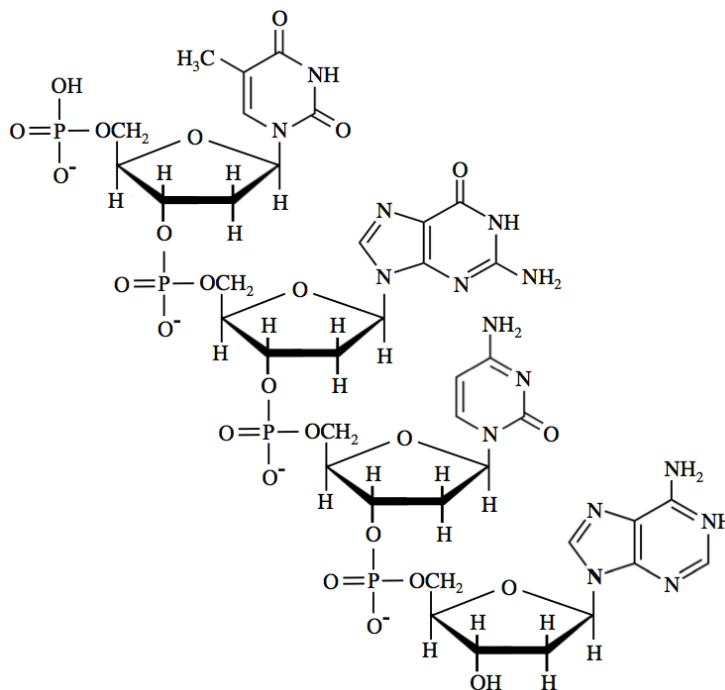
Properties of Amines

Many amines have the foul odor of decomposing fish.

Amines frequently occur in plants and animals.

_____ amines can irritate skin, eyes, and mucous membrane and are toxic when ingested.

Many synthetic and naturally occurring amines are _____ active.

- Examples of physiologically active amines:
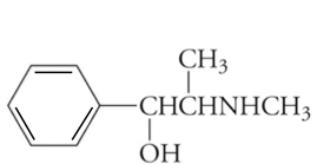
pseudoephedrine
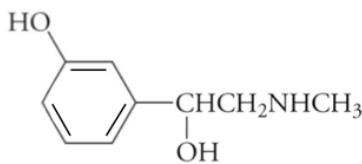
phenylephrine
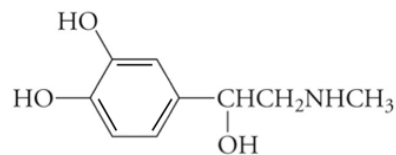
epinephrine
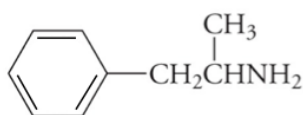
amphetamine
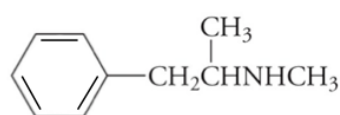
methamphetamine

Pseudoephedrine and **phenylephrine** cause vasoconstriction and are used as a nasal decongestant.

Epinephrine (also called *adrenaline*) is a naturally occurring hormone and neurotransmitter that is associated with the stimulation of the fight-or-flight response.

Amphetamine and **methamphetamine** are strong stimulators of the central nervous system.

- **Amphetamine** is used as a treatment for attention deficit hyperactivity disorder (ADHD), obesity, and narcolepsy.
- **Methamphetamine** has widespread use as an illegal "recreational" psychostimulant and was the focus of the popular TV drama "Breaking Bad." Methamphetamine is rarely prescribed as a therapeutic drug because of its many undesirable side effects.

The term "_____" is used for physiologically active amines that occur in nature (i.e. bacteria, fungi, plants, and animals).

- Some examples of *alkaloids* are shown below.
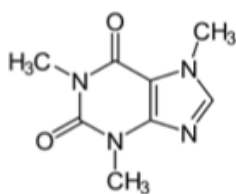
caffeine
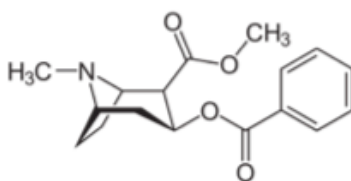
cocaine

Caffeine is a stimulant that is produced in high concentration by coffee plants and is also found in seeds, leaves, nuts, and berries of other plants. It serves as a natural insecticide.

Cocaine is a very strong, central nervous system stimulant that is produced in the leaves of the coca plant.
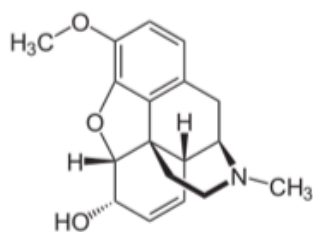
codeine
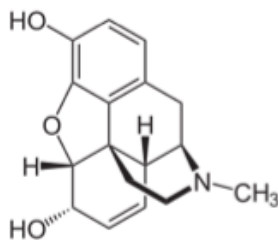
morphine

Codeine and **morphine** are the two most abundant psychoactive components of opium, the dried extract of opium poppy seeds. **Codeine** is used as a pain reliever and to treat coughs. **Morphine** is used to treat severe pain. It is highly addictive.

Heroin is produced *from morphine* by a chemical reaction that replaces the hydrogens of the hydroxyl (**-OH**) groups with *acetyl groups* (CH₃C=O, highlighted in blue).

morphine → heroin
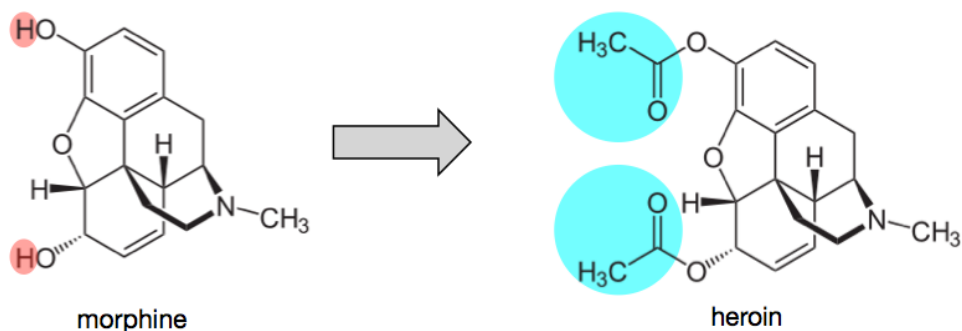
Water Solubility of Amines

All *amine* molecules have the ability to interact with water through hydrogen bonding and dipole-dipole interactions.

Small amines have significant water solubility.

As the *hydrocarbon parts* of amines get *larger*, their water solubility *decreases*; as is the case for all organic molecules.

Boiling and Melting Points of Amines

Amines are polar and can interact with each other through dipole-dipole forces, therefore they have higher boiling and melting points than hydrocarbon molecules of similar size.

Tertiary amines do not have **N-H** bonds, and are therefore _____ of hydrogen bonding with each other.

Only the 1º and 2º Amines Exhibit Hydrogen Bonding Between their Molecules.
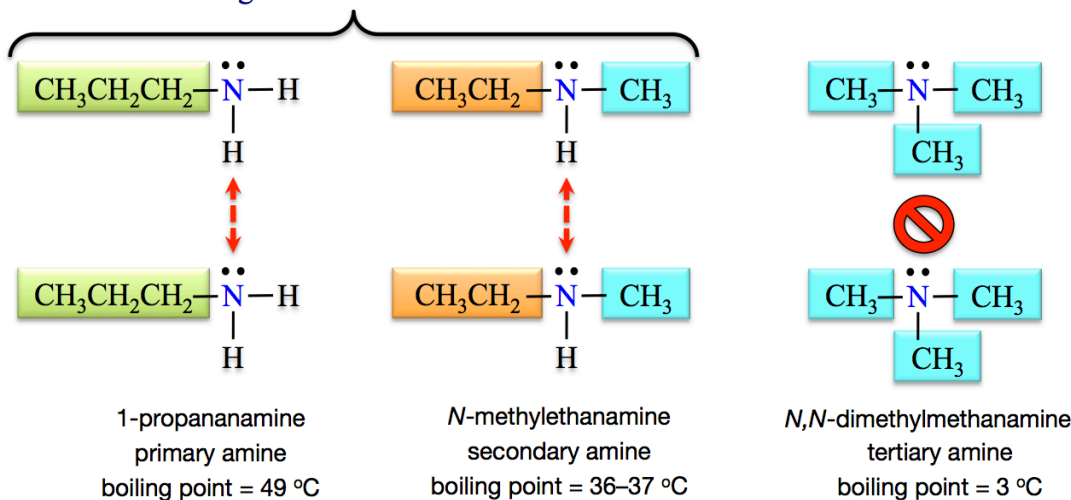
For this reason, primary and secondary amines have higher boiling points than tertiary amines of similar size.

1-propananamine
primary amine
boiling point = 49 ºC

N-methylethanamine
secondary amine
boiling point = 36–37 ºC

N,N-dimethylmethanamine
tertiary amine
boiling point = 3 ºC

Chemical Reactions of Amines

1) Reactions of Amines with Water

An amine acts as a _____ when it reacts with **water** to produce a **quaternary ammonium ion** *and a* **hydroxide ion.**

- The general form of the reaction of an amine with water is shown below.

$$R''\ or\ H-\overset{\cdot\cdot}{\underset{R'\ or\ H}{N}}-R\ +\ H_2O\ \rightleftharpoons\ R''\ or\ H-\overset{\overset{H}{|}}{\underset{R'\ or\ H}{\overset{+}{N}}}-R\ +\ OH^-$$

1°, 2°, or 3° amine   quaternary ammonium ion   +   hydroxide
(NH_2R or NHR_2 or NR_3)
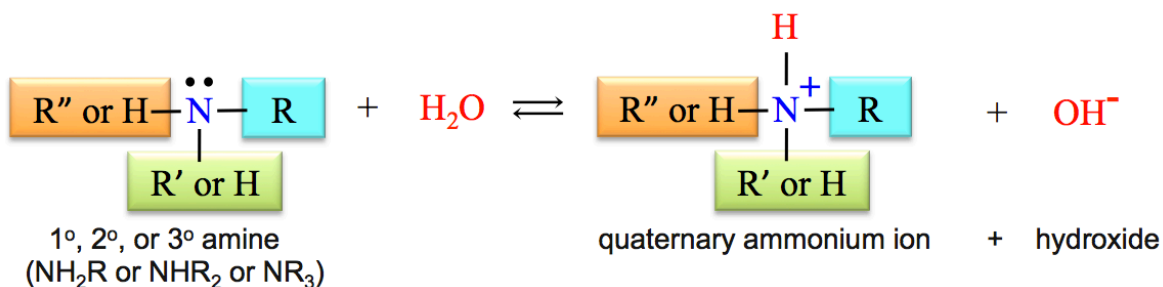
The lone pair on the amine **nitrogen** forms a bond to the H^+ from water.

When amines are put into *pure water*, the pH is _____ since hydroxide ions are produced in this reaction.

The **amine** and the **quaternary ammonium ion** are a _____ *pair*.

- The *amine* is the **base form** and the *quaternary ammonium ion* is the **acid form**.

- When an amine/quaternary ammonium ion conjugate pair is in a mixture that contains other dissolved species, the relative amounts of the *acid form* and *base form* can be predicted by the Henderson-Hasselbalch Relationship.

A specific example of the reaction of an amine with water is the reaction of ethanamine with water:

$$CH_3CH_2-\overset{\cdot\cdot}{\underset{H}{N}}-H\ +\ H_2O\ \rightleftharpoons\ CH_3CH_2-\overset{\overset{H}{|}}{\underset{H}{\overset{+}{N}}}-H\ +\ OH^-$$

Understanding Check
Add the products for the following reaction: $CH_3\overset{\overset{CH_3}{|}}{C}HCH_2CH_2\overset{}{\underset{H}{N}}-H\ +\ H_2O\ \rightleftharpoons$
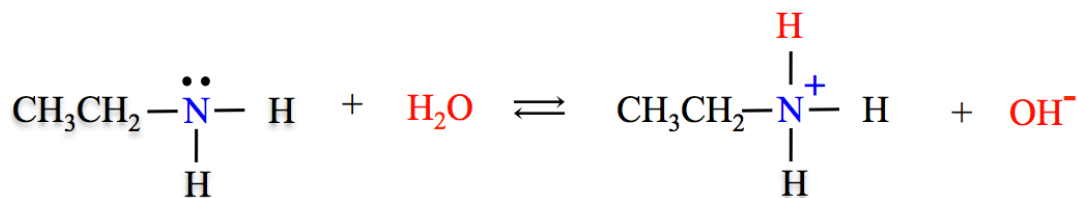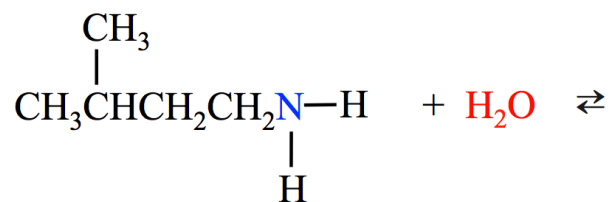
2) Reaction of Amines with Acids

An amine will react with an *acid* to produce *a **quaternary ammonium compound*** in a _____ *reaction*.

- The general form of the equation for the reaction of an amine with an acid is shown below:
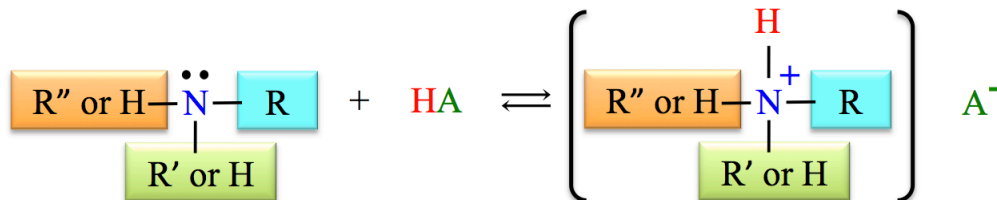
The lone pair on the amine **nitrogen** forms a bond to the H^+ from the acid.

Amines that are used as medications, both legal and illegal, are often administered as quaternary ammonium ions in order to increase their water-solubility.

- For example, pseudoephedrine hydrochloride, used in the decongestant sold as ***Allegra D*** by Bayer Healthcare, and as ***Benadryl*** by Johnson and Johnson, can be prepared by the reaction of pseudoephedrine and HCl.
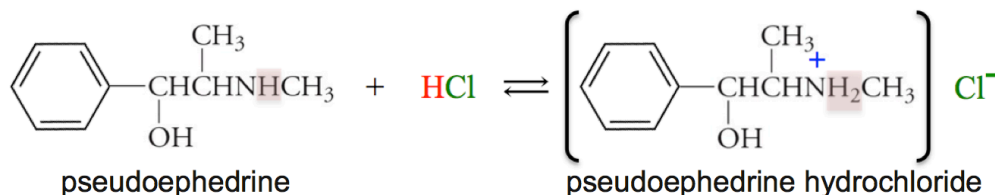
- Pseudoephedrine sulfate, used in ***Claritin D***, can be prepared by the reaction of pseudoephedrine and sulfuric acid (H_2SO_4).
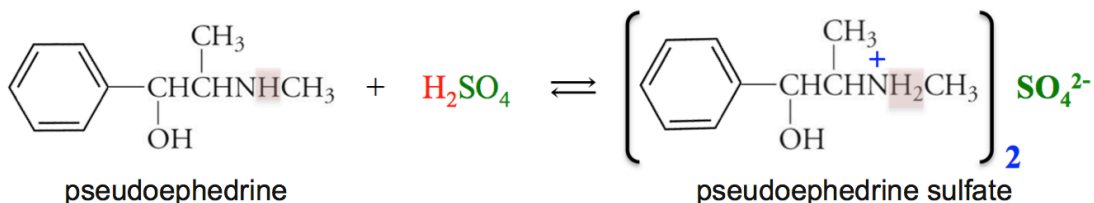
Understanding Check

Add the product for the following reaction:

$$CH_3CH_2 - \overset{\cdot\cdot}{\underset{H}{N}} - H \ + \ HCl \ \rightleftharpoons$$
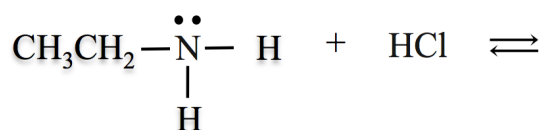
Amides

The Structure of Amides

Amides contain both a ***carbonyl group*** (**C=O**), *and* a nitrogen (**N**), with the nitrogen bonded to the *carbonyl* carbon. The general form of an amide is shown below.
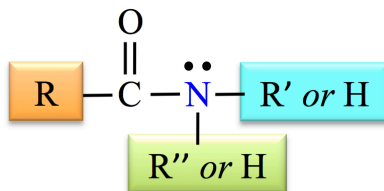
A specific example of an amide is *ethanamide*. The condensed structural formula, skeletal formula, and a ball-and-stick model for *ethanamide* are shown below.
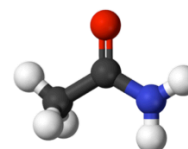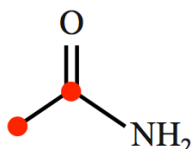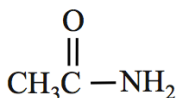
black sphere = carbon, red sphere = oxygen, blue sphere = nitrogen, and white sphere = hydrogen

The amide bonding pattern occurs in nature in the structure of proteins.

Naming Amides

We will use the IUPAC system for naming amide molecules. The systematic method for naming amides is based on the hydrocarbon naming method.

Step 1: Find and name the parent chain.

The parent chain of an amide is the longest continuous chain of carbon atoms that includes the

_____ *carbon* - *just as we did with carboxylic acids.*

Starting with the alkane name that corresponds to the number of carbon atoms in the parent chain, replace the "**e**" at the end of the alkane name with "**amide**."

- For example, if the parent chain of an amide contains *three* carbons, it is called propan*amide*.

propan*e* ➡ propan*amide*

Step 2: Name any alkyl group substituents.

Alkyl groups are named in the same way as was done for hydrocarbons.

Step 3: Determine the *point of attachment* of any alkyl groups.

Substituents are assigned positions based on their point of attachment to the parent chain or to the nitrogen. Begin numbering the parent chain at the *carbonyl carbon*.

- For example, the amide shown below has a "**3-methyl**" substituent.
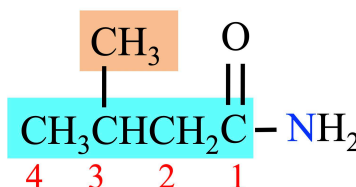
Step 4: Construct the name of the amide by placing the alkyl groups in alphabetical order and specifying their positions, followed by the name of the parent chain.

- Use a *dash* between positions and *letters*.
- Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) identical substituents are present.

$$CH_3CHCH_2C-NH_2$$
with CH_3 above carbon 3, O (double bond) above the carbonyl carbon

4   3   2   1

3-methylbutanamide
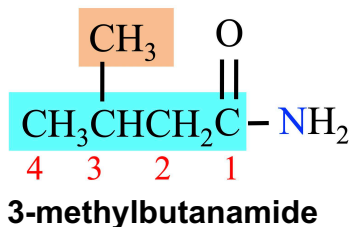
Example: Name the amide shown below.

$$CH_3CH_2CHCH_2CH_2C-NH_2$$
with CH_3 above carbon 4, O (double bond) above the carbonyl carbon

6   5   4   3   2   1
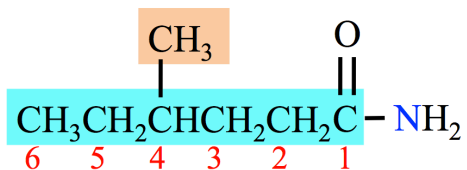
Step 1: Find and name the parent chain. **hexanamide**

Step 2: Name any alkyl group substituents. **methyl**

Step 3: Determine the *point of attachment* of any alkyl groups. **4-methyl**

Step 4: Construct the name of the amide by placing the alkyl groups in alphabetical order and specifying their positions, followed by the name of the parent chain.

4-methylhexanamide

Understanding Check: Name the molecules that are shown below.

$$CH_3CH_2C-NH_2$$
with O (double bond) above the carbonyl carbon

$$CH_3CH_2CH_2CHCH_2CH_2CH_2C-NH_2$$
with CH_2CH_3 above carbon 4, O (double bond) above the carbonyl carbon

---
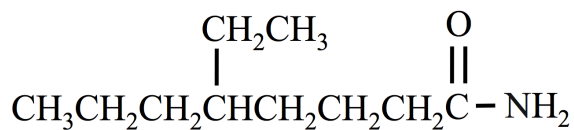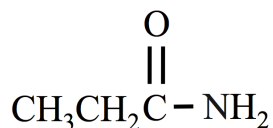
Understanding Check:
Draw the *line bond*, *condensed*, **and** the *skeletal* structural formula of **pentanamide**.

Formation of Amides: The Reaction of Carboxylic Acids with Amines

An **amide** is produced when a _____ _____ reacts with an _____ or **ammonia** (NH_3).

The general form of this reaction is shown below.
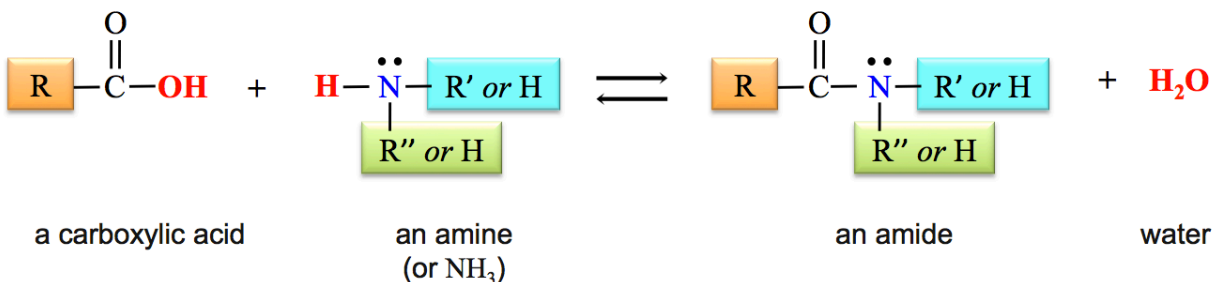
An easy way to predict and draw the products of this reaction is to:

1) Draw the structures of the carboxylic acid and the amine (or ammonia) with the (**OH**) from the carboxylic acid and an **H** from the amine (or ammonia) *adjacent* to each other.

2) Remove the (**OH**) from the carboxylic acid and an **H** from the amine (or ammonia), and then combine the **H** and **OH** to make **H_2O**.

3) Bond the **nitrogen** and its remaining groups to the *carbonyl carbon* of the carboxylic acid.
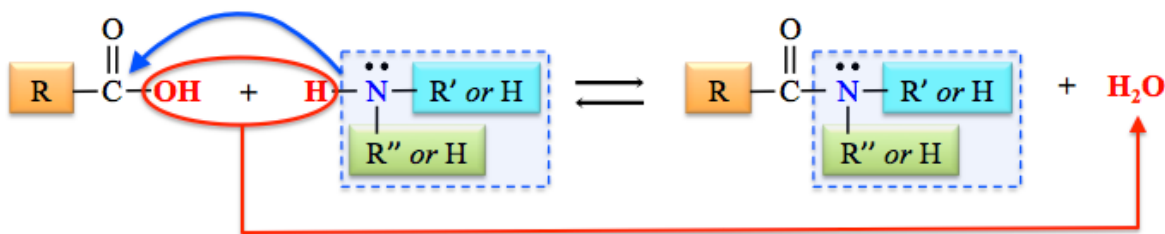
An amide can form when a carboxylic acid reacts with ammonia, with a primary, or with a secondary amine.

- **Examples:**

   a) Formation of an amide by the reaction of a carboxylic acid and *ammonia*.
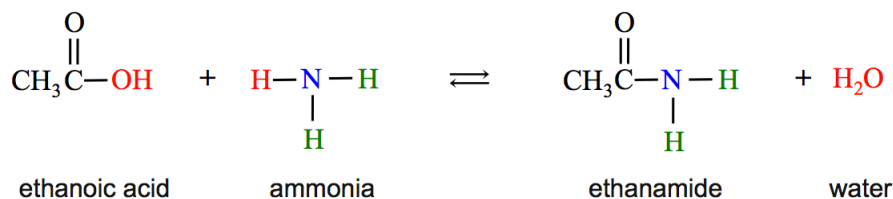
   b) Formation of an amide by the reaction of a carboxylic acid and a 1° amine.
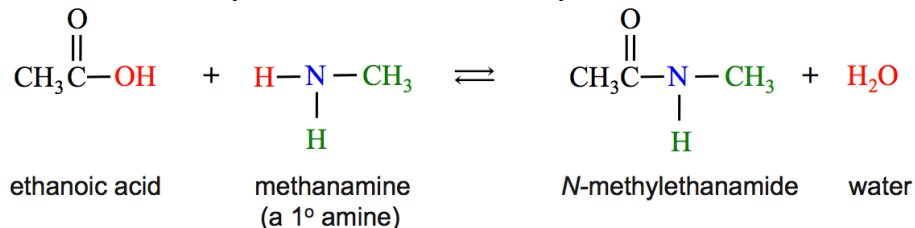
The "*N*-methyl" in "*N*-methylethanamide" indicates that there is a *methyl* substituent bonded to the nitrogen.

c) Formation of an amide by the reaction of a carboxylic acid and a 2° amine.

$$CH_3\overset{\overset{\displaystyle O}{||}}{C}-OH \quad + \quad H-\underset{\underset{\displaystyle CH_3}{|}}{N}-CH_3 \quad \rightleftharpoons \quad CH_3\overset{\overset{\displaystyle O}{||}}{C}-\underset{\underset{\displaystyle CH_3}{|}}{N}-CH_3 \quad + \quad H_2O$$

ethanoic acid   N-methylmethanamine   N,N-dimethylethanamide   water
                   (a 2° amine)
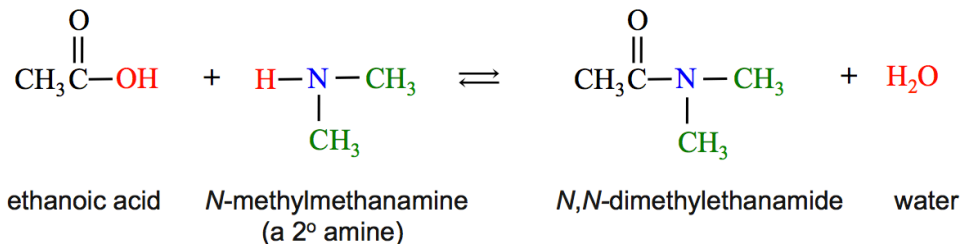
The "N,N-dimethyl" in "N,N-dimethylethanamide" indicates that there are two *methyl* substituents bonded to the nitrogen.

Amides are not formed from 3° amines because 3° amines do not have a _____ attached to the nitrogen.

$$R''-\overset{\cdot\cdot}{\underset{\underset{\displaystyle R'}{|}}{N}}-R$$
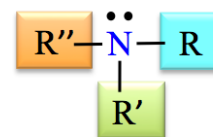
tertiary (3°) amine

$$NR_3$$

Understanding Check:

Add the products for the following reaction *and* **name** the *amide* that is produced:

$$CH_3CH_2-\overset{\overset{\displaystyle O}{||}}{C}-OH \ + \ H-\underset{\underset{\displaystyle H}{|}}{N}-CH_2CH_2CH_3 \ \rightleftharpoons$$
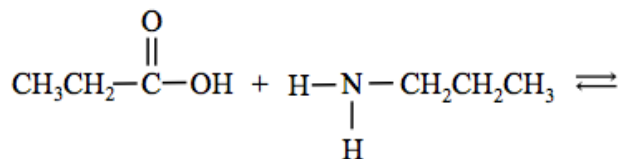
Naming Hint: There will be a substituent attached to the nitrogen (not the parent chain). You will use "N-" in the name to indicate that a substituent is bonded to the nitrogen.

Hydrolysis of Amides

The _____ of the *amide formation* reaction is the **hydrolysis of amides**.

With heat and an acid catalyst, an amide can be hydrolyzed to produce a **carboxylic acid** and an **amine** (or ammonia).

$$R-\overset{\overset{\displaystyle O}{||}}{C}-\overset{\cdot\cdot}{\underset{\underset{\displaystyle R'' \ or \ H}{|}}{N}}-R' \ or \ H \ + \ H-OH \ \underset{\Delta}{\overset{H_3O^+}{\rightleftharpoons}} \ R-\overset{\overset{\displaystyle O}{||}}{C}-OH \ + \ H-\overset{\cdot\cdot}{\underset{\underset{\displaystyle R'' \ or \ H}{|}}{N}}-R' \ or \ H$$

an amide   water   a carboxylic acid   an amine
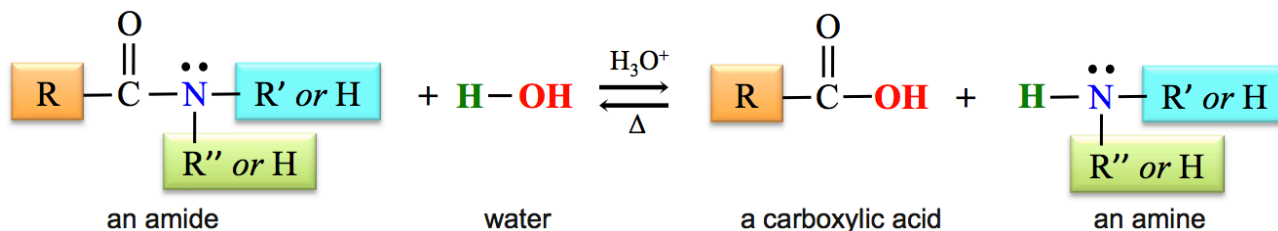
A specific example of this reaction is the hydrolysis of N-methylpropanamide.

$$CH_3CH_2\overset{\overset{\displaystyle O}{||}}{C}-\underset{\underset{\displaystyle H}{|}}{N}-CH_3 \ + \ H_2O \ \underset{\Delta}{\overset{H_3O^+}{\rightleftharpoons}} \ CH_3CH_2\overset{\overset{\displaystyle O}{||}}{C}-OH \ + \ H-\underset{\underset{\displaystyle H}{|}}{N}-CH_3$$

29
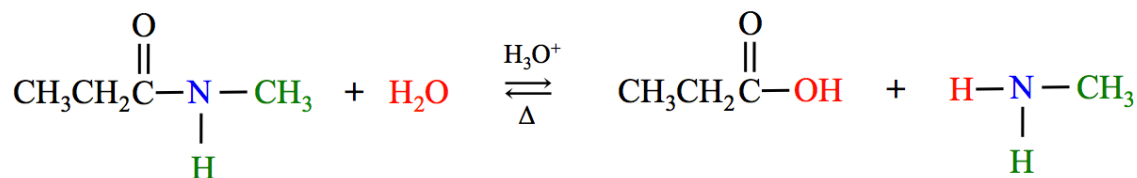
Beginning with the structure of **any** amide and water, an ***easy way to predict and draw the products*** of this reaction is to:

1) Break the bond between the **carbonyl group** and the **nitrogen**.
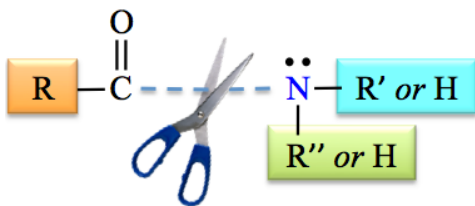
2) Bond the **OH** from water to the **carbonyl carbon**, and bond the **H** from **water** to the **nitrogen**.
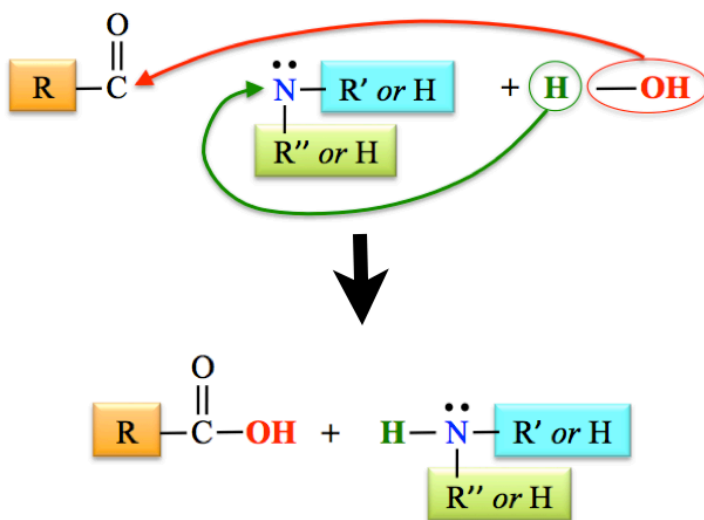
Understanding Check:

Add the products for the following amide hydrolysis reaction *and* name ***both*** of the products:
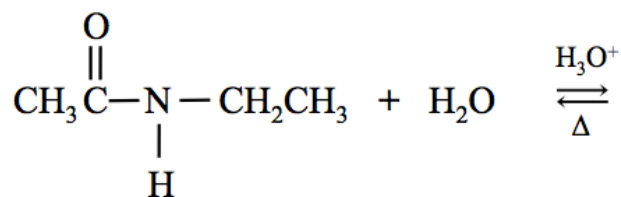
Enantiomers and Diastereomers

Stereoisomers are molecules that have the *same* molecular formula, have the *same* atomic connections, but have *different* three-dimensional arrangements of the atoms.

We have seen some examples of stereoisomers in the past (chapter 4) - **geometric isomers**.

When *stereoisomers* exist because of *limited bond rotation*, they are called **geometric isomers**.

You saw that geometric isomers could occur for certain cycloalkanes and alkenes.
- We designated the geometric isomers as either *cis* or *trans*.

Another type of stereoisomers occurs when _____ _____ *groups are bonded to the* _____ *atom*.
- In these cases, there are two distinct, three-dimensional arrangements of the atoms.

For our purposes, we will be concerned with the pairs of stereoisomers that result whenever four different groups are bonded to the same *carbon atom*.

A carbon atom that carries *four different groups* is called a "_____ _____."

The two distinct, three-dimensional arrangements of the atoms around the chiral carbon are *mirror images* of each other.

When four different groups are arranged in the tetrahedral geometry (we called it AB$_4$), the mirror images *are* _____ identical.

- Another way to describe nonidentical mirror images is with the term "*nonsuperimposable mirror images*."

Stereoisomers such as these, which are nonsuperimposable mirror images of each another, are called

_____.

An example of a pair of stereoisomers (*an enantiomer pair*) that results from the presence of a *chiral carbon* is shown below.
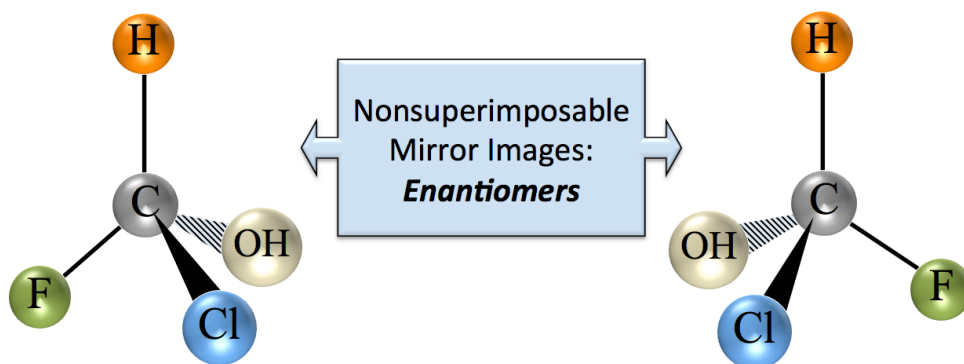
Recall that in *wedge and dash* illustrations of three-dimensional objects, *solid wedges* indicate bonds that would be coming *out and above* the page (toward the viewer). *Dashed shapes* indicate bonds that would be coming *out and behind* the page (away from the viewer). Regular lines (neither wedge nor dash) indicate bonds that would exist *on the plane* of the page.

The image shown here may help you to visualize and understand that the two molecules shown in the previous slide are not identical.

I have graphically depicted the failed attempt to superimpose the pair of enantiomers.
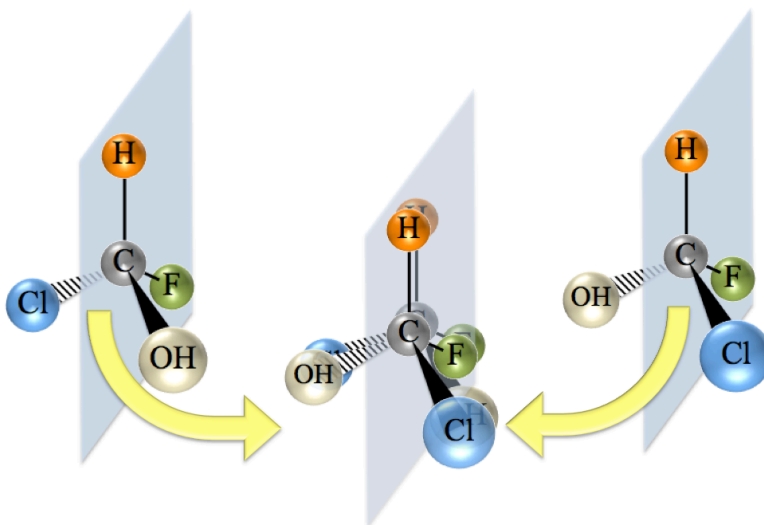
Pairs of enantiomers have very _____ *physical properties*.

- For this reason, they are very difficult to separate (purify) from each other. For example, their boiling points are so similar that separation by distillation is not possible.

They do _____ in a couple of important ways.

- Since enantiomers' arrangements of electrons are mirror images of each other, they interact with light in different ways. It is for this reason that enantiomers are sometimes called "optical isomers."
- Another important difference in enantiomers is the way they behave in *biological systems*.
- Since enantiomers do not have identical three-dimensional shapes, they do not behave identically when interacting with biomolecules such as enzymes or the receptors that are responsible for taste.

- **Example:** One of the enantiomers of asparagine (L-asparagine) has a sweet taste. The other enantiomer (D-asparagine) has a bitter taste.

L-asparagine
(tastes sweet)

D-asparagine
(tastes bitter)
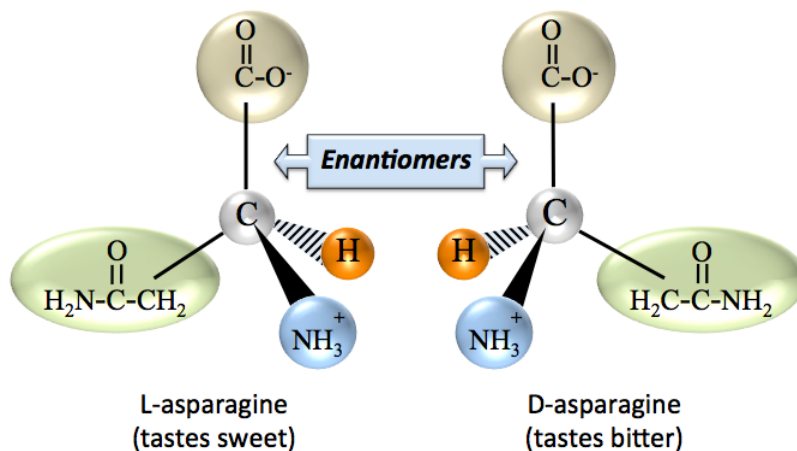
Many enzymes are "**stereospecific**." This means that they will catalyze a reaction for only *one* particular enantiomeric reactant and/or will catalyze the formation of only one enantiomeric product.

For example, when the antibiotic that we call penicillin is made by enzymatic reactions by mold, only one of the enantiomers (penicillin) is produced.

Plants produce only one enantiomer of the glucose molecule (D-glucose). It is therefore understandable that all organisms - with only one known exception of particular bacterium - will only metabolize the D-glucose enantiomer.

Let's do an example problem in order to help you identify **chiral carbons**.

Example: The line bond structure of 2-bromo-3-chlorobutane is shown below. How many **chiral carbons** are in this molecule?
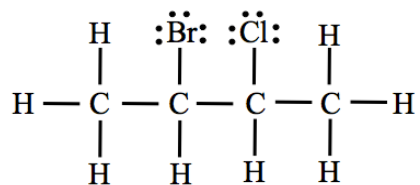
Solution: Consider each carbon individually. A carbon is **chiral** if it is bonded to *four different groups*.

Carbon number 1 is **not** chiral. It is bonded to four groups, however, the four groups are not all *different* from each other. I have highlighted the four groups that are bonded to carbon number **1** in the structure shown below. Three of the groups are hydrogens.
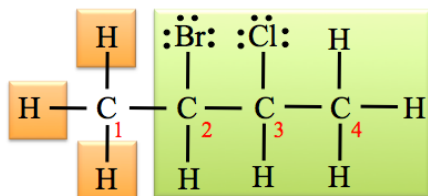
Carbon number 2 is chiral; it is bonded to *four different groups*
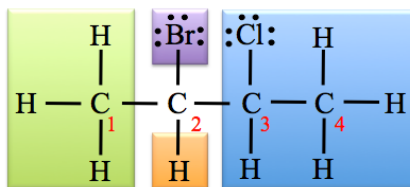
> **IMPORTANT:** A mistake that chemistry students sometimes make is to consider only the four *atoms* to which a carbon is bonded. If you were to do that with this molecule, you might think that **carbon number 2** is *not* chiral since it is bonded to *two other carbons* (carbon number **1** and **3**). Be careful; you must consider the entire *group of atoms to which a carbon is bonded in order to determine if that carbon is chiral*. It is for this reason that I highlighted the *entire groups* that are bonded to carbon number **2** in the structure shown above.

Carbon number 3 is chiral; it is bonded to *four different groups*.
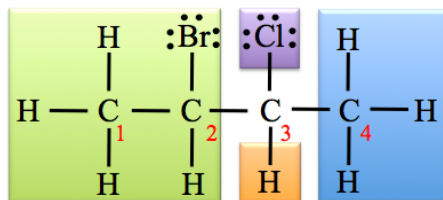
Carbon number 4 is not chiral. Three of the groups are the same - three hydrogens.
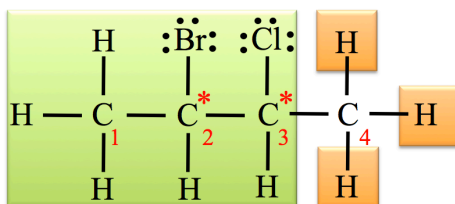
There are *two* **chiral carbons** in 2-bromo-3-chlorobutane - carbons number **2** and **3**.

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Diastereomers

When _____ *than one chiral carbon* is present in a molecule, then more than one pair of enantiomers will exist.

The **number of stereoisomers** that can exist depends on the **number of** _____ **carbons**.

If we let "**n**" represent *the number of chiral carbons* in a molecule, then the maximum number of stereoisomers is calculated as follows:

Maximum Number of Stereoisomers = 2^n

Example: In our previous example problem, we determined that 2-bromo-3-chlorobutane contained *two chiral carbons*.
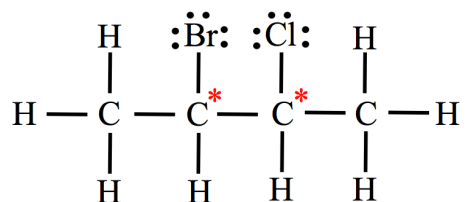
Therefore the *maximum number of stereoisomers* that 2-bromo-3-chlorobutane has is:

Maximum Number of Stereoisomers = 2^n = 2^2 = 4

The **four** stereoisomers of 2-bromo-3-chlorobutane, **two pairs** of mirror images, are shown on the right.

You learned about the relationship between nonsuperimposable mirror image molecules, called **enantiomers**.

Nonsuperimposable molecules **that are not mirror images of each other,** *but are* in the group of 2^n stereoisomers, are called

_____.

- The **enantiomer** relationships are indicated with blue arrows.

- The **diastereomer** relationships are indicated with yellow arrows.
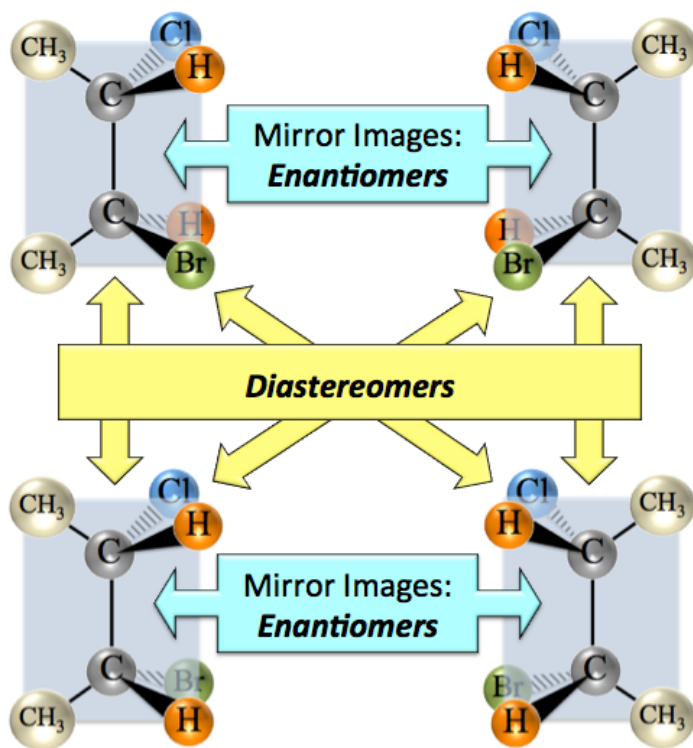
It may be helpful for you to compare and contrast *enantiomers* and *diastereomers* by using a "family relationship" analogy of *siblings* (for enantiomers) and *cousins* (for diastereomers).

You will see more enantiomers, diastereomers, and geometric isomers in the biochemistry chapters of this course.

Understanding Check:

What is the *maximum number of stereoisomers* that can exist for each of the molecules shown below?

$$CH_3 — CH — CH_2 — CH — CH_3$$

$$\qquad\quad | \qquad\qquad\quad |$$

$$\qquad\quad NH_2 \qquad\qquad CH_3$$

$$CH_3 — CH — CH — CH_3$$

$$\qquad\quad | \qquad | $$

$$\qquad\quad NH_2 \quad OH$$
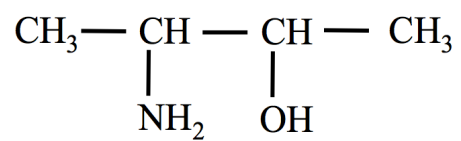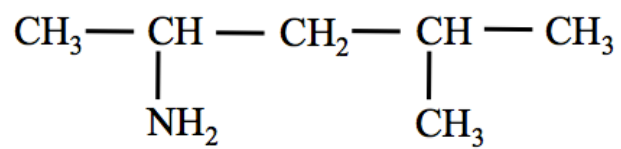
Naming the Organic Molecules of Chapter 9 Worksheet and Key

1) Write the names of the following organic molecules:

NOTE: If you are having a hard time with these, you may wish to try drawing them as line bond structures.

$$O$$
$$\|$$
$$CH_3CH_2 - C - OH$$

_____

$$CH_3NH_2$$

_____

$$CH_3 - N - H$$
$$|$$
$$CH_2CH_3$$

_____

$$O$$
$$\|$$
$$CH_3 \; CH_2 \; C - O^-$$

_____

$$O$$
$$\|$$
$$CH_3CH_2 \; CHCH_2 - C - O - H$$
$$|$$
$$CH_3$$

_____

$$O$$
$$\|$$
$$CH_3CH_2 - C - O - CH_2CH_2 \; CH_2 \; CH_3$$

_____

$$H - N - CH_2CH_3$$
$$|$$
$$CH_3CHCH_2CH_2CH_3$$

_____
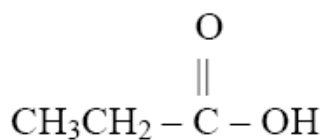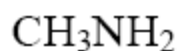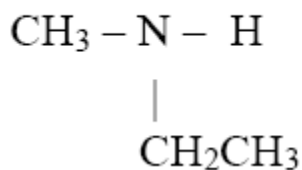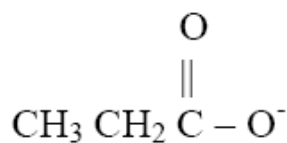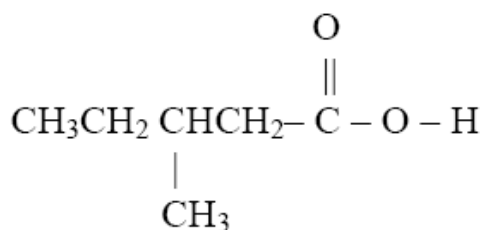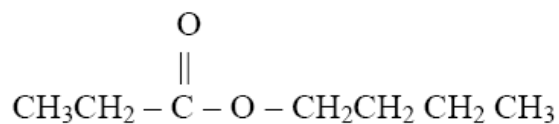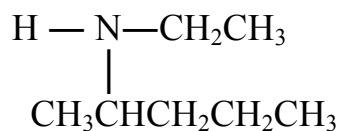
2) Write the condensed formula for the following compounds

NOTE: If you are having a hard time with these, try drawing the Line Bond Structure, then convert it to a condensed structure.

a) 1- butanamine

b) pentanoic acid
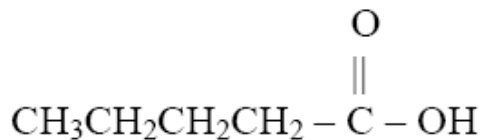
c) N-ethylethanamine
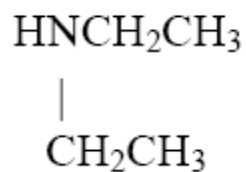
d) pentanoate ion
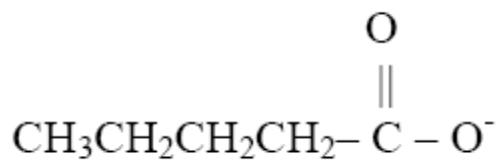
e) methyl pentanoate

f) 5-methylhexanoic acid

g) N-methyl-2-propanamine

1) Write the names of the following organic molecules:

$$\underset{}{CH_3CH_2} - \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - OH$$

.... propanoic acid

$$CH_3NH_2$$

.... methanamine

$$CH_3 - N - H$$
$$\quad\quad |$$
$$\quad CH_2CH_3$$

.... N-methylethanamine

$$CH_3\ CH_2\ \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - O^-$$

.... propanoate ion

$$CH_3CH_2\ CHCH_2 - \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - O - H$$
$$\quad\quad\quad |$$
$$\quad\quad CH_3$$

.... 3-methylpentanoic acid

$$CH_3CH_2 - \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - O - CH_2CH_2\ CH_2\ CH_3$$

.........butyl propanoate

$$H - N - CH_2CH_3$$
$$\quad\quad |$$
$$CH_3CHCH_2CH_2CH_3$$

.... N-ethyl-2-pentanamine

3

2) Write the condensed formula for the following compounds

a) 1- butanamine

$CH_3 CH_2CH_2CH_2NH_2$

b) pentanoic acid

$$CH_3CH_2CH_2CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH$$

c) N-ethylethanamine

$$HNCH_2CH_3$$
$$|$$
$$CH_2CH_3$$

d) pentanoate ion

$$CH_3CH_2CH_2CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O^-$$

e) methyl pentanoate

$$CH_3CH_2CH_2CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - CH_3$$

f) 5-methylhexanoic acid

$$CH_3CH \; CH_2CH_2CH_2\overset{\overset{\displaystyle O}{\|}}{C} -OH$$
$$|$$
$$CH_3$$

g) N-methyl-2-propanamine

$$H - N - CH_3$$
$$|$$
$$CH_3CHCH_3$$

Summary of the Reactions of Chapter 9:

1) Reactions of Carboxylic Acids

    a)   Reaction of a Carboxylic acid and water.

        •   When placed in water, a carboxylic acid molecule acts as an acid and water acts as a base. An H^+ from the hydroxyl group (OH) of the carboxylic acid is donated to H_2O.
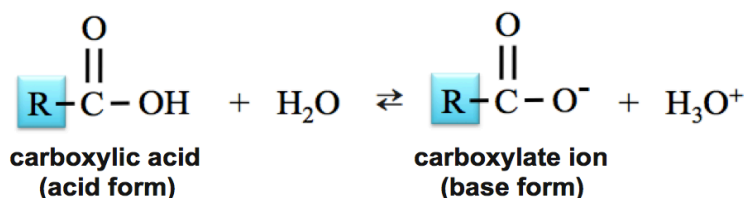
    b)   Neutralization: Reaction of a Carboxylic Acid and a Hydroxide Ion

        •   In a **neutralization reaction**, a carboxylic acid will react with a ***hydroxide-containing*** *base* compound to produce **H_2O** and *a **carboxylic acid salt***.
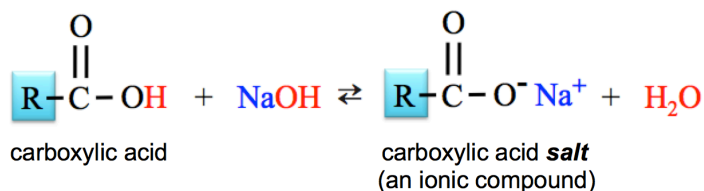
    c)   Esterification: The Reaction of a Carboxylic Acid and an Alcohol

        •   In an ***esterification reaction,*** a carboxylic acid reacts with an alcohol to produce an ***ester*** and water.
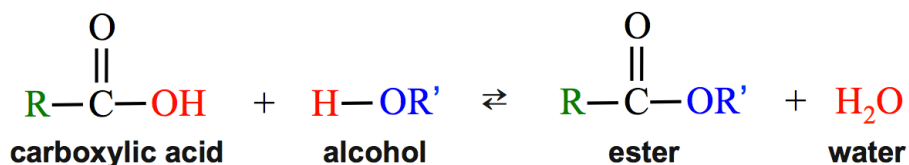
    d)   Decarboxylation of Carboxylic Acids

        •   In decarboxylation reactions, ***carboxyl group*** (COOH) is removed and ***replaced by a hydrogen atom***.
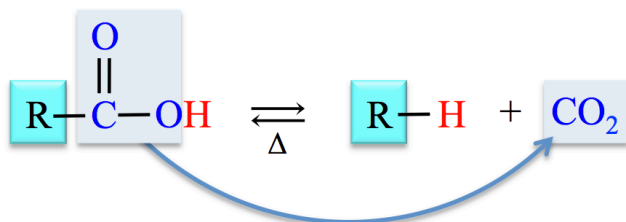
2) Chemical Reactions of Amines

a) Reactions of Amines with Water

- An amine acts as a *base* when it reacts with *water* to produce a *quaternary ammonium ion* and a *hydroxide ion.*

1°, 2°, or 3° amine
(NH_2R or NHR_2 or NR_3)

quaternary ammonium ion + hydroxide
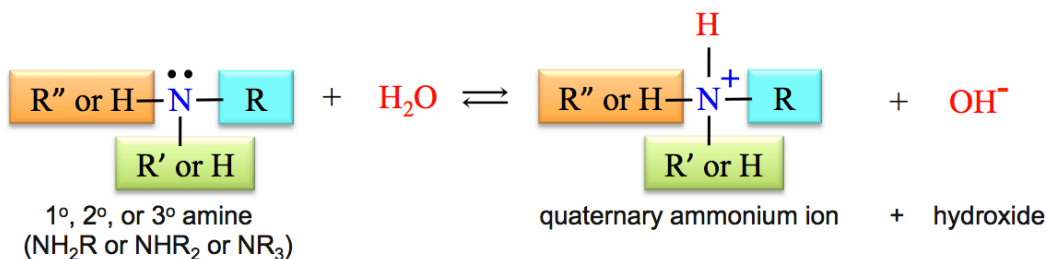
b) Reaction of Amines with Acids

- An amine will react with an *acid* to produce *a quaternary ammonium compound* in a *neutralization reaction*.
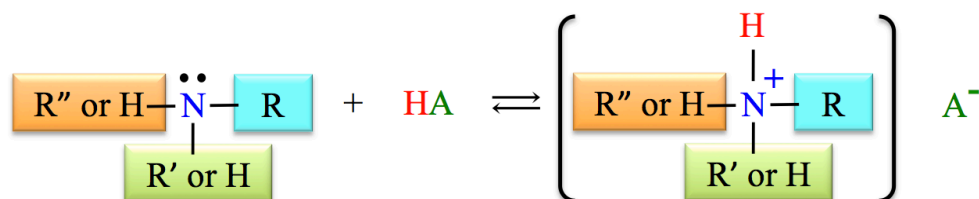
3) Formation of Amides: The Reaction of Carboxylic Acids with Amines

- An **amide** is produced when a *carboxylic acid* reacts with an *amine* or *ammonia* (NH_3).

a carboxylic acid   an amine   an amide   water
(or NH_3)
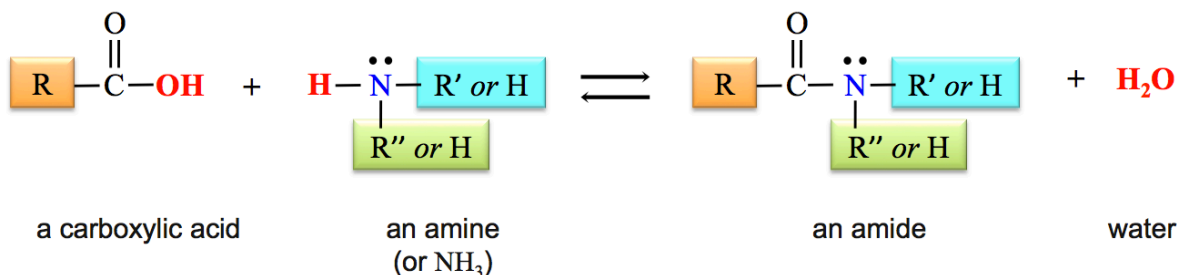
4) Hydrolysis of Amides

- The reverse of the *amide formation* reaction is the **hydrolysis of amides**.
- With heat and an acid catalyst, an amide can be hydrolyzed to produce a **carboxylic acid** and an **amine** (or ammonia).

an amide   water   a carboxylic acid   an amine

2
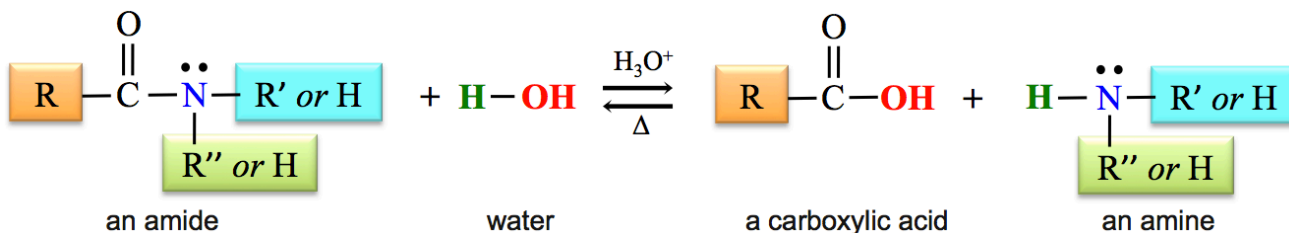
1) Write the chemical equation for the reaction of propanoic acid with 1-butanol (an alcohol). The formula of 1-butanol is CH_3-CH_2-CH_2-CH_2-OH.

2) Write the chemical equation for the reaction of ethanoic acid with N-methylethanamine.
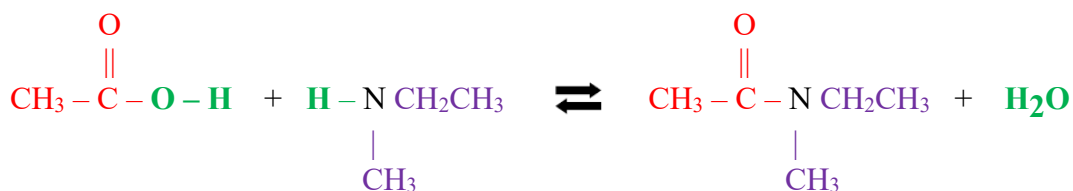
3) Write the chemical equation for a pentanoate ion **acting as base** when it reacts with hydrochloric acid (HCl).

4) Write the chemical equation for the **decarboxylation** of 2-methyl-propanoic acid.

5) Write the chemical equation for the reaction of propanoic acid with water.

6) Write the chemical equation for the reaction of *N,N*-diethyl-1-propanamine with water. (Hint: the amine is a base):

7) Complete the following reactions:

a)

$$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 - \overset{\displaystyle\overset{\text{O}}{\|}}{\text{C}} - \text{OH (aq)} + \text{H}_2\text{O (l)} \quad \rightleftharpoons$$

b)

$$\text{CH}_3 - \underset{\underset{\text{CH}_2\text{CH}_3}{|}}{\text{N}} - \text{H (aq)} + \text{H}_2\text{O (l)} \quad \rightleftharpoons$$

c)

$$\text{CH}_3\text{CH}_2 - \overset{\displaystyle\overset{\text{O}}{\|}}{\text{C}} - \text{OH (aq)} + \text{NaOH (aq)} \quad \rightleftharpoons$$

d)

$$\text{CH}_3 - \overset{\displaystyle\overset{\text{O}}{\|}}{\text{C}} - \text{O} - \text{H} + \text{CH}_3\text{CH}_2\,\underset{\underset{\text{CH}_2\text{CH}_3}{|}}{\text{CHCH}_2\text{OH}} \quad \rightleftharpoons$$

e) decarboxylation

$$CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H \quad \rightleftharpoons \quad ? \quad + \quad CO_2$$

f)

$$CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H \quad + \quad NH_3 \quad \rightleftharpoons$$

g)

$$CH_3CH_2\ \underset{\underset{\displaystyle CH_3}{|}}{CH}CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H \quad + \quad CH_3OH \quad \rightleftharpoons$$

h)

$$CH_3\ CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H \quad + \quad \underset{\underset{\displaystyle CH_2CH_3}{|}}{H}NCH_2CH_3 \quad \rightleftharpoons$$

i)

$$CH_3CH_2\ \overset{\overset{\displaystyle O}{\|}}{C} - OH \quad + \quad H_2O \quad \rightleftharpoons$$

8) Fill in the missing reactant(s):

a)

$\rightleftarrows$ $CH_3\ CH_2CH_2CH_3$ + CO_2 (decarboxylation reaction)

b)

$$O$$
$$\|$$
$\rightleftarrows$ $CH_3CH_2CH_2 - C - N{-}CH_3$ +   H-O-H
$$|$$
$$H$$

c)

$$O$$
$$\|$$
+ CH_3OH $\rightleftarrows$ $CH_3CH_2\ CHCH_2 - C - O - CH_3$ + H_2O
$$|$$
$$CH_3$$

d)

$$O$$
$$\|$$
+ H_2O (l) $\rightleftarrows$ $CH_3CH_2CH_2CH_2{-}\ C - O^-$ (aq) + H_3O^+ (aq)

e)

$$H$$
$$|\ +$$
+ H_2O (l) $\rightleftarrows$ $CH_3CH_2CH_2 -\ N - H$ (aq) + OH^- (aq)
$$|$$
$$CH_2CH_3$$

6

f)

$$CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH \ (aq) \ + \qquad \rightleftarrows \qquad CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O^- \ Na+ \ (aq) \quad + \quad H_2O \ (l)$$

g)

$$CH_3 \ CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH \ + \qquad \rightleftarrows \qquad CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - CH_2CHCH_2CH_3 + H_2O$$
$$\overset{\displaystyle |}{CH_2CH_3}$$

h)

$$+ \quad \underset{\underset{\displaystyle CH_2CH_3}{|}}{HNCH_2CH_3} \quad \rightleftarrows \quad CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - \underset{\underset{\displaystyle CH_2CH_3}{|}}{NCH_2CH_3} \quad + \quad H_2O$$

Key

1) Write the chemical equation for the reaction of propanoic acid with 1-butanol (an alcohol). The formula of 1-butanol is CH_3-CH_2-CH_2-CH_2-OH.

$$CH_3CH_2 - \overset{\displaystyle O}{\overset{\|}{C}} - O - H \ + \ CH_3CH_2\,CH_2\,CH_2{-}OH \ \rightleftharpoons \ CH_3CH_2 - \overset{\displaystyle O}{\overset{\|}{C}} - O - CH_2CH_2\,CH_2\,CH_3 + H_2O$$

2) Write the chemical equation for the reaction of ethanoic acid with *N*-methylethanamine.

$$CH_3 - \overset{\displaystyle O}{\overset{\|}{C}} - O - H \ + \ \underset{\underset{\displaystyle CH_3}{\textstyle |}}{H - N\,CH_2CH_3} \ \rightleftharpoons \ CH_3 - \overset{\displaystyle O}{\overset{\|}{C}} - \underset{\underset{\displaystyle CH_3}{\textstyle |}}{N\,CH_2CH_3} \ + \ H_2O$$

3) Write the chemical equation for a pentanoate ion **acting as base** when it reacts with hydrochloric acid (HCl).

$$CH_3\,CH_2\,CH_2CH_2\overset{\displaystyle O}{\overset{\|}{C}} - O^- \ + \ HCl \ \rightleftharpoons \ CH_3\,CH_2\,CH_2CH_2\overset{\displaystyle O}{\overset{\|}{C}} - OH \ + \ Cl^-$$

4) Write the chemical equation for the **decarboxylation** of 2-methyl-propanoic acid.

$$\underset{\underset{\displaystyle CH_3}{\textstyle |}}{CH_3CH} - \overset{\displaystyle O}{\overset{\|}{C}} - O - H \ \rightleftharpoons \ CH_3CH_2\,CH_3 \ + \ CO_2$$

5) Write the chemical equation for the reaction of propanoic acid with water.

$$CH_3CH_2 - \overset{\displaystyle O}{\overset{\|}{C}} - OH \ (aq) \ + \ H_2O \ (l) \ \rightleftharpoons \ CH_3CH_2 - \overset{\displaystyle O}{\overset{\|}{C}} - O^- \ (aq) \ + \ H_3O^+ \ (aq)$$

8

6) Write the chemical equation for the reaction of *N,N*-diethyl-1-propanamine with water. (Hint: the amine is a base):

$$CH_3CH_2 - N - CH_2CH_3 \ (aq) + H_2O \ (l) \rightleftharpoons CH_3CH_2 - \overset{H}{\underset{|}{N}}{}^+ - CH_2CH_3 \ (aq) + OH^- \ (aq)$$

with $CH_2CH_2CH_3$ substituent on N (left) and $CH_2CH_2CH_3$ (right)

7) Complete the following reactions:

a)

$$CH_3CH_2CH_2CH_2 - \overset{O}{\overset{||}{C}} - OH \ (aq) + H_2O \ (l) \rightleftharpoons CH_3CH_2CH_2CH_2 - \overset{O}{\overset{||}{C}} - O^- \ (aq) + H_3O^+ \ (aq)$$

b)

$$CH_3 - \underset{\underset{CH_2CH_3}{|}}{N} - H \ (aq) + H_2O \ (l) \rightleftharpoons CH_3 - \overset{H}{\underset{\underset{CH_2CH_3}{|}}{\overset{|}{N}}}{}^+ - H \ (aq) + OH^- \ (aq)$$

c)

$$CH_3CH_2 - \overset{O}{\overset{||}{C}} - OH \ (aq) + NaOH \ (aq) \rightleftharpoons CH_3CH_2 - \overset{O}{\overset{||}{C}} - O^- \ Na^+ \ (aq) + H_2O \ (l)$$

d)

$$CH_3 - \overset{O}{\overset{||}{C}} - O - H + CH_3CH_2 \underset{\underset{CH_2CH_3}{|}}{CH}CH_2OH \rightleftharpoons CH_3 - \overset{O}{\overset{||}{C}} - O - CH_2\underset{\underset{CH_2CH_3}{|}}{CH}CH_2CH_3 + H_2O$$

e)

$$CH_3CH_2 - \overset{O}{\overset{||}{C}} - O - H \rightleftharpoons CH_3CH_3 + CO_2$$

9

f)

$$CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H + NH_3 \rightleftharpoons CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - NH_2 + H\text{-}O\text{-}H$$

g)

$$CH_3CH_2\,CHCH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH + CH_3OH \rightleftharpoons CH_3CH_2\,CHCH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - CH_3 + H_2O$$
$$\underset{CH_3}{\vert} \qquad\qquad\qquad\qquad \underset{CH_3}{\vert}$$

h)

$$CH_3\,CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH + \underset{\underset{CH_2CH_3}{\vert}}{HNCH_2CH_3} \rightleftharpoons CH_3CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - \underset{\underset{CH_2CH_3}{\vert}}{NCH_2CH_3} + H_2O$$

i)

$$CH_3CH_2\,\overset{\overset{\displaystyle O}{\|}}{C} - OH + H_2O \rightleftharpoons CH_3CH_2\overset{\overset{\displaystyle O}{\|}}{C} - O^- + H_3O^+$$

---

8. Fill in the missing reactant(s):

a)

$$CH_3\,CH_2CH_2\,CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - O - H \rightleftharpoons CH_3\,CH_2CH_2CH_3 + CO_2$$

b)

$$CH_3CH_2\,CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH + CH_3NH_2 \rightleftharpoons CH_3CH_2\,CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - \underset{\underset{H}{\vert}}{NCH_3} + H\text{-}O\text{-}H$$

c)

$$CH_3CH_2\ CHCH_2-\overset{\displaystyle O}{\overset{\|}{C}}-\mathbf{OH}\ +\ CH_3OH \rightleftharpoons CH_3CH_2\ CHCH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O-CH_3\ +\ \mathbf{H_2O}$$

$$\underset{\ \ \ \ \ \ \ \ \ \ \ \ CH_3}{|}\qquad\qquad\qquad\qquad\qquad\qquad\underset{\ \ \ \ \ \ \ \ \ \ \ \ CH_3}{|}$$

d)

$$CH_3CH_2CH_2CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O\mathbf{H}\ (aq)\ +\ \mathbf{H_2O}\ (l) \rightleftharpoons CH_3CH_2CH_2CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O^-\ (aq)\ +\ \mathbf{H_3O^+}\ (aq)$$

e)

$$CH_3CH_2CH_2\ -N-\mathbf{H}\ (aq)+\ \mathbf{H_2O}\ (l) \rightleftharpoons CH_3CH_2CH_2\ -\overset{\mathbf{H}}{\overset{|\ +}{N}}-H\ (aq)\ +\mathbf{OH^-}\ (aq)$$

$$\underset{CH_2CH_3}{|}\qquad\qquad\qquad\qquad\qquad\qquad\underset{CH_2CH_3}{|}$$

f)

$$CH_3CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O\mathbf{H}\ (aq)\ +\ \mathbf{NaOH}\ (aq) \rightleftharpoons CH_3CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O^-\ Na^+\ (aq)\ +\ \mathbf{H_2O}\ (l)$$

g)

$$CH_3\ CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-\mathbf{OH}\ +\ CH_3CH_2\ CHCH_2O\mathbf{H} \rightleftharpoons CH_3CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-O-CH_2CHCH_2CH_3+\mathbf{H_2O}$$

$$\underset{\ \ \ \ \ \ \ \ \ \ \ \ CH_2CH_3}{|}\qquad\qquad\qquad\qquad\qquad\underset{\ \ \ \ \ \ \ \ \ \ \ \ CH_2CH_3}{|}$$

h)

$$CH_3\ CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-\mathbf{OH}\ +\ \mathbf{H}NCH_2CH_3 \rightleftharpoons CH_3CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-NCH_2CH_3\ +\ \mathbf{H_2O}$$

$$\underset{\ \ \ \ \ \ CH_2CH_3}{|}\qquad\qquad\qquad\qquad\qquad\underset{\ \ \ \ \ \ CH_2CH_3}{|}$$

Chapter 10 Lecture Notes: Alcohols, Ethers, Aldehydes, and Ketones

Educational Goals

1. Given the structure of an **alcohol**, **ether**, **thiol**, **sulfide**, **aldehyde**, **or ketone** molecule, be able to give the systemic names and vice versa.

2. Know and understand the intermolecular forces that attract alcohol, ether, thiol, sulfide, disulfide, aldehyde, and ketone molecules to one another, and how these forces affect boiling points and melting points.

3. Identify **alcohols** as primary (1°), secondary (2°), or tertiary (3°).

4. Predict the products of the reactions in chapter 10 that involve alcohols, thiols, aldehydes, and/or ketones:
   - oxidation of thiols to produce disulfides
   - nucleophilic substitution reaction of alkyl halides and hydroxide
   - hydration of alkenes
   - dehydration of alcohols
   - oxidation of alcohols
   - oxidation of aldehydes
   - reduction of aldehydes and ketones
   - hemiacetal and acetal formation

5. Predict the **major** and **minor products** for the **hydration of an alkene**.

6. Predict the **major** and **minor products** for the **dehydration of an alcohol**.

Alcohols

The Structure of Alcohols

Alcohols contain one or more _____ *functional groups* **(-OH)** attached to a hydrocarbon (alkyl group) part. The general form of an alcohol is shown below.

$$R \quad \ddot{O}-H$$
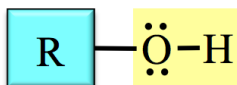
A specific example of an alcohol is *ethanol*. Condensed structural formulas and a ball-and-stick model for *ethanol* are shown below.
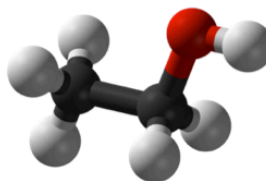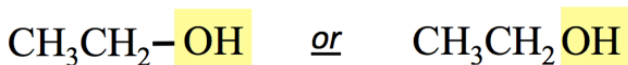
$$CH_3CH_2-OH \quad \underline{or} \quad CH_3CH_2 OH$$

black sphere = carbon
red sphere = oxygen
white sphere = hydrogen

The skeletal structure of *ethanol* is shown below. I have added large dots to indicate the carbon atom positions.

OH

Alcohols are classified as primary (1°), secondary (2°), or tertiary (3°) based on the number of **R** groups *attached to the carbon that is "_____" (bonded to) the hydroxyl group*.
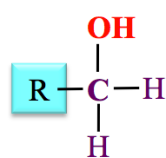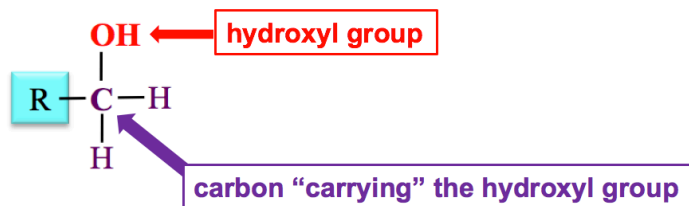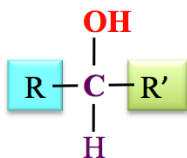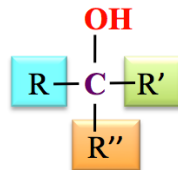
In **primary (1°) alcohols**, *the carbon that is "carrying" the hydroxyl group* is bonded to *one* **R** group. An example of a primary alcohol is 1-propanol.
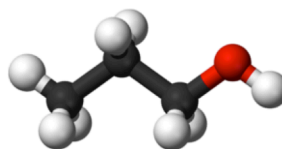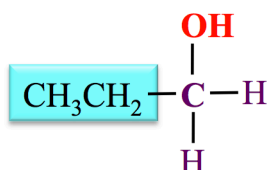
1-propanol (a 1° alcohol)

In **secondary (2°) alcohols**, *the carbon "carrying" the hydroxyl group* is bonded to *two* **R** groups. An example of a secondary alcohol is 2-butanol:
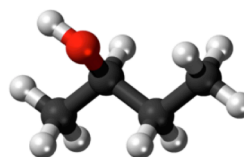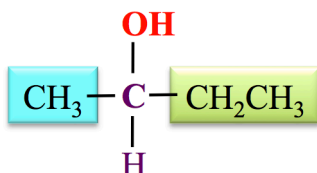
2-butanol (a 2° alcohol)

In **tertiary (3°) alcohols**, *the carbon "carrying" the hydroxyl group* is bonded to *three* **R** groups. An example of a tertiary alcohol is 2-methyl-2-propanol:
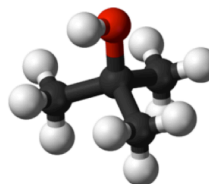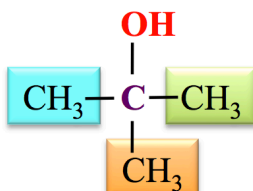
2-methyl-2-propanol (a 3° alcohol)

2

Identify each of the alcohols shown below as either primary (1°), secondary (2°), or tertiary (3°).

a.
$$\begin{array}{c} OH \\ | \\ CH_3CH_2-C-H \\ | \\ H \end{array}$$

b.
$$\begin{array}{c} OH \\ | \\ CH_3CH_2CH_2-C-CH_2CH_3 \\ | \\ CH_3 \end{array}$$

c.
$$\begin{array}{c} OH \\ | \\ H-C-CH_2CH_3 \\ | \\ CH_3 \end{array}$$

d.
$$\begin{array}{c} OH \\ | \\ CH_3CHCHCH_2CH_2CH_3 \\ | \\ CH_3 \end{array}$$

e.
$$\begin{array}{c} CH_3CHCH_3 \\ | \\ OH \end{array}$$

f.
$$\begin{array}{c} CH_2CH_3 \qquad OH \\ | \qquad\qquad | \\ CH_3CH_2CCH_2CH_2CH_2CH_2CH_2 \\ | \\ CH_3 \end{array}$$
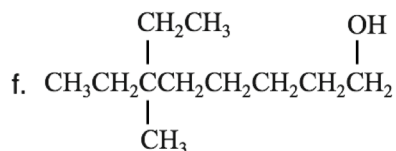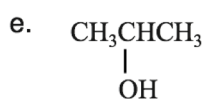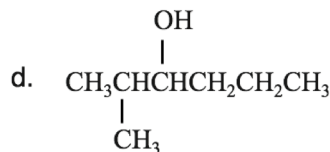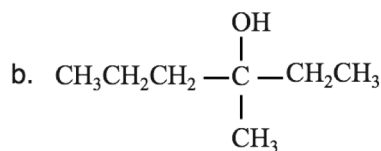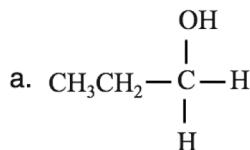
Naming Alcohols

The *systematic method* for naming alcohols is based on the hydrocarbon naming method.

Step 1: Find and name the *parent chain*.

The *parent chain is the longest, continuous chain of carbon atoms that **contains the** _____ *of* _____ *to the* _____ *group* (OH)*.

- Count the number of carbon atoms in the parent chain. Starting with the alkane name that corresponds to the number of carbon atoms in the parent chain, replace the "**e**" at the end of the alkane name with "**ol**."

    - For example, if the parent chain of an alcohol contains *two carbons*, it would be called ethan**ol**.

        ethan**e** ⟹ ethan**ol**

- For alcohols with *more than two carbons*, the position of *the point of attachment to the **hydroxyl group*** must be indicated by adding a number before the parent chain.

    - Assign *position numbers* to the carbons in the parent chain. Position number **1** is assigned to the carbon at the _____ *of the parent chain* that is _____ **to the *hydroxyl group.***

        - If the hydroxyl group is bonded to carbon number **1** of the parent chain, then "**1-**" is used as a prefix to the parent chain name. For example, in the molecule below, the parent chain is called **1**-pentanol.
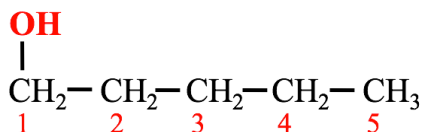
$$\begin{array}{c} \textbf{OH} \\ | \\ \underset{1}{CH_2}-\underset{2}{CH_2}-\underset{3}{CH_2}-\underset{4}{CH_2}-\underset{5}{CH_3} \end{array}$$

3

- If the hydroxyl group is bonded to carbon number **2** of the parent chain, then "**2-**" is used as a prefix to the parent chain name. For example, in the molecule below, the parent chain is called **2**-pentanol.

$$\overset{\displaystyle \overset{\textbf{OH}}{|}}{CH_3-\underset{2}{CH}-\underset{3}{CH_2}-\underset{4}{CH_2}-\underset{5}{CH_3}}$$
$$\underset{1}{}$$
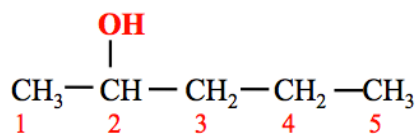
Steps 2, **3**, and **4** are done the **same way** as you did when naming other organic molecules.

Step 2: Name any alkyl group substituents.

Step 3: Determine the *point of attachments* of alkyl groups to the parent chain.

Step 4: Construct the name of the alcohol by placing the alkyl groups in alphabetical order and specifying their position number, followed by the name of the parent chain.

Example: Name the molecule that is shown below.

$$\overset{\overset{\textstyle CH_3}{|}}{CH_3CH_2CHCH_2CH_2CH_2-OH}$$
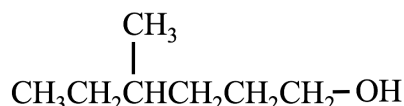
Solution:

Step 1: Find and name the parent chain.

- The *parent chain is the longest, continuous chain of carbon atoms that contains the point of attachment to the hydroxyl group* (OH).

$$\overset{\overset{\textstyle CH_3}{|}}{\underset{6\quad5\quad4\quad3\quad2\quad1}{CH_3CH_2CHCH_2CH_2CH_2}}-OH$$
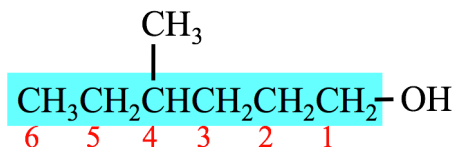
The hydroxyl group is bonded to carbon number **1** of the parent chain, so "**1-**" is used as a prefix to the parent chain name. **The parent chain is called 1-hexanol.**

Step 2: Name any alkyl group substituents. methyl

Step 3: Determine the *point of attachments* of alkyl groups to the parent chain. 4-methyl

Step 4: Construct the name of the alcohol by placing the alkyl groups in alphabetical order and specifying their position number, followed by the name of the parent chain.

The name of the molecule is **4-methyl-1-hexanol**.

Understanding Check

Write the *systematic name* for each of alcohol molecules that are shown here.

$$CH_3-OH$$

$$\overset{\overset{\textstyle OH}{|}}{CH_3CH_2CH_2-\underset{\underset{\textstyle CH_3}{|}}{C}-CH_2CH_3}$$

$$\overset{\overset{\textstyle CH_2CH_3}{|}}{CH_3CH_2\underset{\underset{\textstyle CH_3}{|}}{C}CH_2CH_2CH_2CH_2CH_2}\overset{\overset{\textstyle OH}{|}}{}$$

4

Let's do a problem where we are given the name of an alcohol, and wish to draw its structural formula.

Example: Draw the *line bond structure* of **3-methyl-2-butanol**.

Solution:

First draw the **carbons** of the *parent chain*. The parent chain is **2-butanol**, therefore it contains *four* carbons.

$$C \underline{\qquad} C \underline{\qquad} C \underline{\qquad} C$$

The "**2-**" prefix in **2-butanol** indicates that the *hydroxyl group* is bonded to carbon number **2** of the parent chain. Since we are drawing a line bond structure, we must include the bonds to all atoms **and** all lone pairs. Remember to add the lone pairs to the *oxygens* on the *hydroxyl group*.
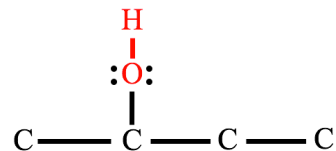
Next, add the *carbon* of the methyl substituent.

- Since we are drawing the structure of **3-methyl**-2-butanol, the methyl group's carbon is attached to carbon number **3** of the parent chain.
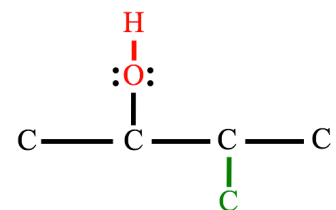
To finish, add enough hydrogens to each carbon in order to satisfy the octet rule.
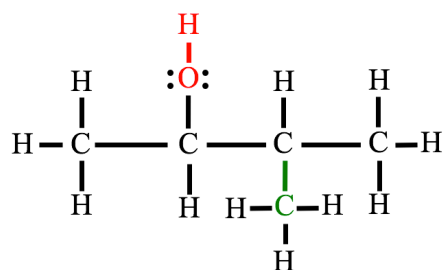
Understanding Check: We just drew the **line bond structure** of **3-methyl-2-butanol**. Draw the *condensed* ***and*** the *skeletal* structural formula of **3-methyl-2-butanol**.

Understanding Check: Draw the ***line bond structure*** of 4-methyl-3-heptanol.

5

Polyhydroxy Alcohols

Molecules with more than one hydroxyl group are called _____ *alcohols*.

- An example of a polyhydroxy alcohol is *glycerol* (also known as glycerin).

    - Glycerol is an important biomolecule because it is one of the precursors to triglycerides (fats and vegetable oils) and some of the compounds found in cell membranes (glycerophospholipids and glycerooglycolipids).

- The condensed structure and the ball-and-stick model of glycerol are shown below.

$$\underset{CH_2}{\overset{OH}{|}} - \underset{CH}{\overset{OH}{|}} - \underset{CH_2}{\overset{OH}{|}}$$
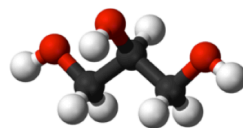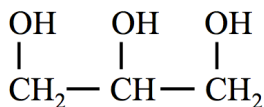
glycerol (a polyhydroxy alcohol)

Cyclic Alcohols

When the *hydroxyl group* of an alcohol is bound to a _____ *structure* it is called a **cyclic alcohol**.

Cyclic alcohols can be *secondary* (2°) or *tertiary* (3°).

Cyclic alcohols are named in a manner similar to that for *cycloalkanes*.

- Starting with the *cycloalkane* name that corresponds to the number of carbon atoms in the *ring structure*, cyclic alcohols are named by replacing the "**e**" at the end of the *cyclo*alkane name with "**ol**."

- The ring-carbon that is carrying the **OH** is always designated as position number **1**. Note the names of the cyclic alcohols that are shown above.
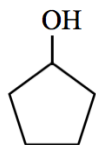
cyclopentanol
(2° alcohol)
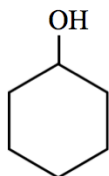
cyclohexanol
(2° alcohol)
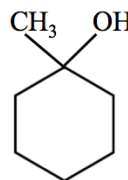
1-methylcylohexanol
(3° alcohol)

Understanding Check

Draw a skeletal structural formula for cyclopropanol and for cyclobutanol.

Properties of Alcohols

Water Solubility of Alcohols

Smaller alcohol molecules have significant water solubility because of their ability to interact with water through _____ *bonding* and _____-_____ *interactions*.

As their nonpolar (hydrocarbon) parts get larger, the water solubilities of alcohols decrease.

Melting and Boiling Points of Alcohols

Alcohol molecules have higher melting and boiling points than alkanes of similar size because of their ability to interact with each other through **hydrogen bonding** and **dipole-dipole interactions**.

As their nonpolar (hydrocarbon) parts get larger, the melting and boiling points of alcohols **increase** because of increasing _____ *forces*.

Water Solubility and Melting Points of Some Alcohols

Molecule Name	Condensed Structure	Water Solubility (g/100 mL)	Boiling Point (°C)
methanol	CH_3OH	miscible*	65.0
ethanol	CH_3CH_2OH	miscible	78.5
1-propanol	$CH_3CH_2CH_2OH$	miscible	97.4
1-butanol	$CH_3CH_2CH_2CH_2OH$	8.0	117
1-pentanol	$CH_3CH_2CH_2CH_2CH_2OH$	2.2	138

*miscible indicates that the substance will mix/dissolve at any alcohol to water ratio.

Alcohols have biological, industrial, and medical applications.

Alcohols are used as fuels, medications, recreational drugs, antiseptic agents, industrial solvents, antifreeze, detergents, and preservatives. Humans have consumed ethanol as a recreational drug since the Neolithic age (stone age).

Annual Per Capita Ethanol Consumption (liters) by Country
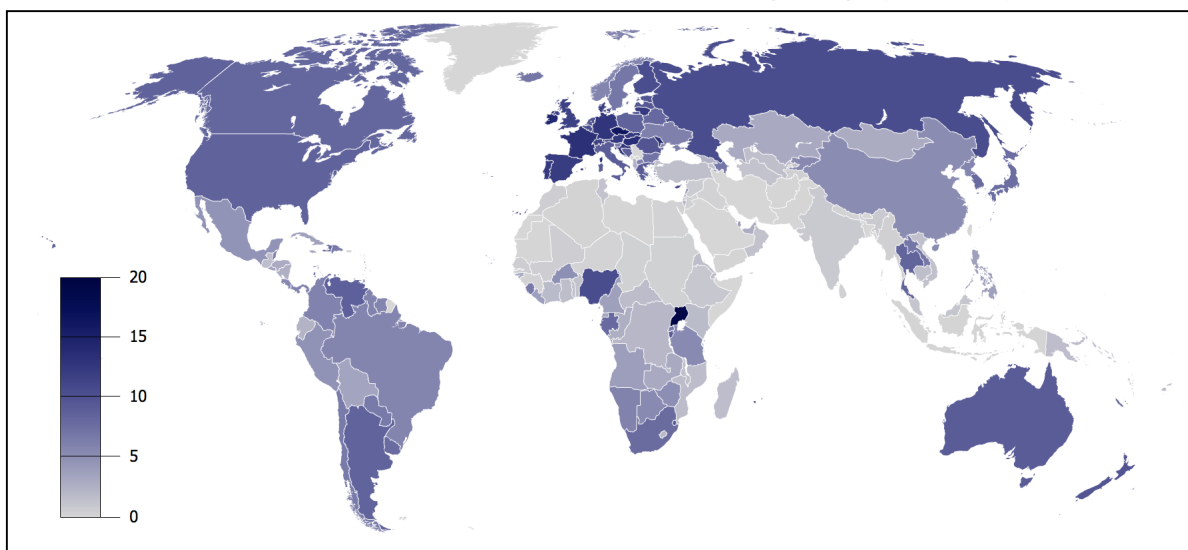
Annual per capita recorded ethanol consumption (liters) by country in 2004. Based on the data of WHO Global Status Report on Alcohol 2004 and Statistical Information System.

Ethanol, 1-propanol, and 2-propanol are used, with about 10-30% water, as antiseptic (surface antimicrobial) agents. One or more of these three alcohols serve as the active ingredients in many hand sanitizers, such as Purell.

Methanol is added to automotive windshield washer fluid, de-icers, and gasoline additive products as an antifreeze agent. Antifreeze agents lower the melting points of liquids.

$$\begin{array}{cc} OH & OH \\ | & | \\ CH_2 & \!\!\!\!\!-\!\!\!\!\! & CH_2 \end{array}$$
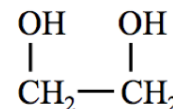
ethylene glycol

Aqueous ethylene glycol (50% v/v), a polyhydroxy alcohol, is used as engine antifreeze. It is quite effective as an antifreeze because of its ability to disrupt water-water hydrogen bonding (because of its own ability to hydrogen bond with water). A trace of fluorescent color is added to antifreeze to facilitate in leak detection.

Methanol, ethanol, and some other small alcohol molecules are used as fuel. This includes use in internal combustion engine automobiles. Since alcohol can be produced by renewable resources and lowers pollutant emissions, many countries require the addition of alcohol to gasoline. In the United States, many states mandate that alcohol be added to gasoline.

Alcohols are used as preservatives for specimens in biological sciences, and as solvents for medical drugs, perfumes, and the preparation of plant extracts, such as vanilla.

Formation of Alcohols

1) Alcohol Fermentation

Ethanol is produced in nature in a process called ***alcohol* _____.**

In the 1850s and 1860s, Louis Pasteur discovered that fermentation involved living organisms.

It was not until 1897 that Eduard Buchner found that ground fragments of dead yeast could produce ethanol and CO_2.

Louis Pasteur (1822-1895)
French microbiologist and chemist.

- As a result of Buchner's work, the term "enzyme" was applied to materials that enabled fermentation, and the understanding that fermentation was a result of enzymatic processes gained acceptance.

Eduard Buchner (1860-1917)
German chemist and zymologist.

- Buchner's results are often regarded as the birth of *biochemistry*, and he was awarded the Nobel Prize in chemistry for this work in 1907.

Alcohol fermentation is a series of chemical reactions that convert sugar molecules, such as glucose, into ethanol and CO_2.

- The final step in this reaction series involves an enzyme which is only present in yeast and some bacteria.

The overall reaction of ethanol formation from a sugar molecule (glucose) is shown below.

$$C_6H_{12}O_6 \longrightarrow 2\,CH_3CH_2OH + 2\,CO_2$$

glucose   **ethanol**   **carbon dioxide**
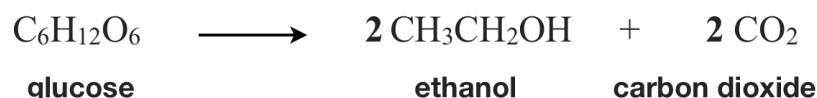
2) Alcohol Formation in Nucleophilic Substitution Reactions

If you were a chemistry major, you would take a year-long organic chemistry class in which you would study the mechanisms of all of the reactions that we cover in this course.

A reaction mechanism is a description of the sequence of bond-breaking and bond-formation that occurs in a chemical reaction.

Since the intention of this course is to cover general, organic, and biochemistry *in just one semester*, we don't have the time - or need - to study the reaction mechanisms for all of the chemical reactions that I present. However, I do wish to introduce you to one very commonly observed reaction mechanism - the "nucleophilic substitution II" (S_N2) reaction mechanism.

In the nucleophilic substitution (S_N2) reaction for the formation of an alcohol, a hydroxide ion reacts with an _____ _____ molecule.

- An **alkyl halide** is a hydrocarbon that had one of its hydrogens replaced with a halogen (group VII element: F, Cl, Br, or I).

$$R - X \quad + \quad OH^- \quad \rightleftharpoons \quad R - OH \quad + \quad X^-$$

alkyl halide   hydroxide ion   alcohol   halogen ion
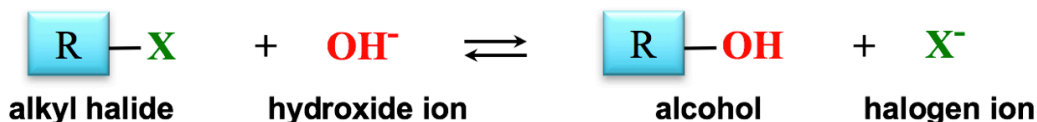
X represents
F, Cl, Br, or I

- Specific examples of nucleophilic substitution reactions for the formation of alcohols are shown below.

$$CH_3 - Cl \quad + \quad OH^- \quad \rightleftharpoons \quad CH_3 - OH \quad + \quad Cl^-$$

$$CH_3 - Br \quad + \quad OH^- \quad \rightleftharpoons \quad CH_3 - OH \quad + \quad Br^-$$

$$CH_3CH_2CH_2 - I \quad + \quad OH^- \quad \rightleftharpoons \quad CH_3CH_2CH_2 - OH \quad + \quad I^-$$

The negative charge of the hydroxide ion is quite attracted to the *partial* positive charge of ***the carbon that is bonded to the halogen atom***.

The reaction mechanism is called ***nucleophilic substitution*** because the nucleophile (**OH⁻**) is attracted to the *nucleus* of the partially positive carbon, and then ***substitutes*** *for* (*replaces*) the halogen (**X**).

The S$_N$2 chemical reaction involves ***making one new bond and breaking one old bond***. First, a lone pair from the hydroxide nucleophile forms a bond to the carbon that is carrying the halogen.

| hydroxide ion | bromomethane (an alkyl halide) | | transition state |
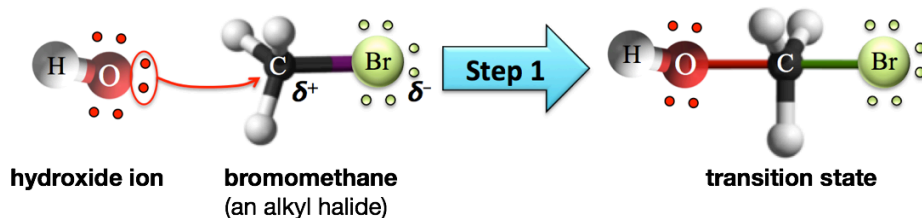
The species which is formed by the newly-made bond is called a _____ _____. The transition state is a ***high-energy molecule*** because there are *ten* electrons (five single bonds) around a carbon atom instead of the lower-energy octet.

The *transition state* has a ***high energy***, which means that it is _____. The weakest of the five bonds (the bond to the halogen) will quickly break. When this bond breaks, the halogen takes with it the two electrons that were in its bond to the carbon, and an alcohol is produced.

| transition state | methanol (an alcohol) | bromide ion |

Let's consider the energy reaction diagram for this S$_N$2 reaction:

S$_N$2 Reaction Energy Diagram

In S$_N$2 reactions, ***the transition state*** is the highest energy configuration of all the particles involved the chemical reaction.

Understanding Check: Predict the products of the following nucleophilic substitution reaction.

$$CH_3CH_2\!-\!Br \quad + \quad OH^- \quad \rightleftharpoons$$
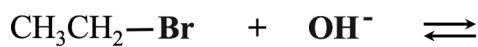
3) Hydration of Alkenes

In chapter 6, you learned that an _____ can react with **water** to produce an **alcohol**.

- A hydrogen from H_2O is added to one of the double-bonded carbon atoms and **OH** from the H_2O is added to the **other** double-bonded carbon atom in the **alkene,** to produce the corresponding **alcohol.**

General Form of the Chemical Equation for the Hydration of an Alkene:
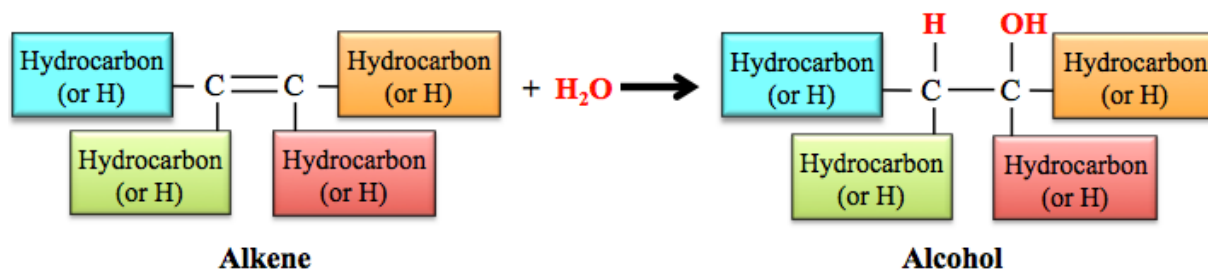
Alkene   Alcohol

In chapter 6, I showed you a *bond flipping method* to help you predict the structure of the alcohol that is produced when you add H_2O *"across a double bond."*

Step 1: Draw the H_2O to be added *across the double bond* and the alkene as shown below.
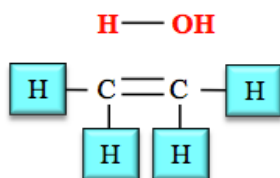
Step #1:
Draw the **H - OH** directly
above the double bond.

Steps 2 and 3: *Flip* the bonds, as shown below, to get the alcohol product of the reaction.

Step #2: Flip one of the
double bonds **up** to the **H**

Step #3: Flip the **H-OH**
single bond **down** to the **C**

Alcohol Product

In chapter 6, we always began with **symmetric** alkenes when doing hydration reactions.

An alkene is _____ when a **line** drawn perpendicular to, and through, the middle of the double bond of its structural formula results in _____ *parts on each side of the line.*
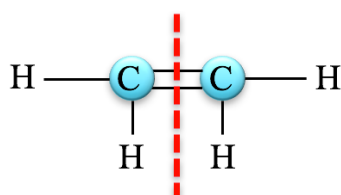
ethene (a symmetric alkene)

11

Another example of a *symmetric alkene* is *2-butene*.

Note that parts of the molecule on each side of the **dashed line** bisecting the carbon-carbon double bond are *identical*.
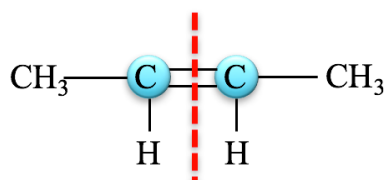
2-butene (a symmetric alkene)

When a **symmetric alkene** undergoes a hydration reaction, there is only _____ *possible product*.

Example: The hydration of 2-butene. $CH_3CH \Longrightarrow CHCH_3 + H_2O$
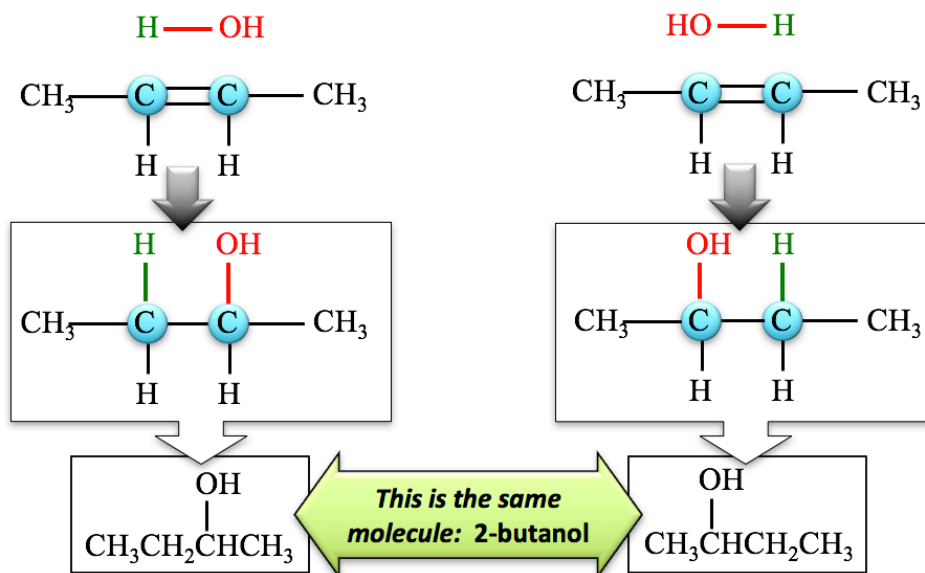
The _____ alcohol molecule is produced regardless of which of 2-butene's double-bonded carbons gets the added **OH** group.

The reason that the addition of the **OH** to *either* double-bonded carbon results in the same alcohol (2-butanol) is that the 2-butene is *symmetric*.

An example of an _____*alkene* is *propene*.

Note that the dashed line bisecting the carbon-carbon double bond results in _____*identical parts* on each side of the line.
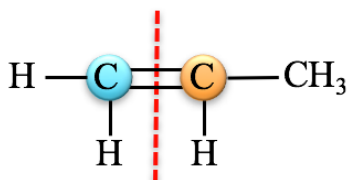
propene (an <u>a</u>symmetric alkene)

When an **asymmetric alkene** undergoes a hydration reaction, there are _____ *different alcohol molecules produced*.

Example: The hydration of propene.
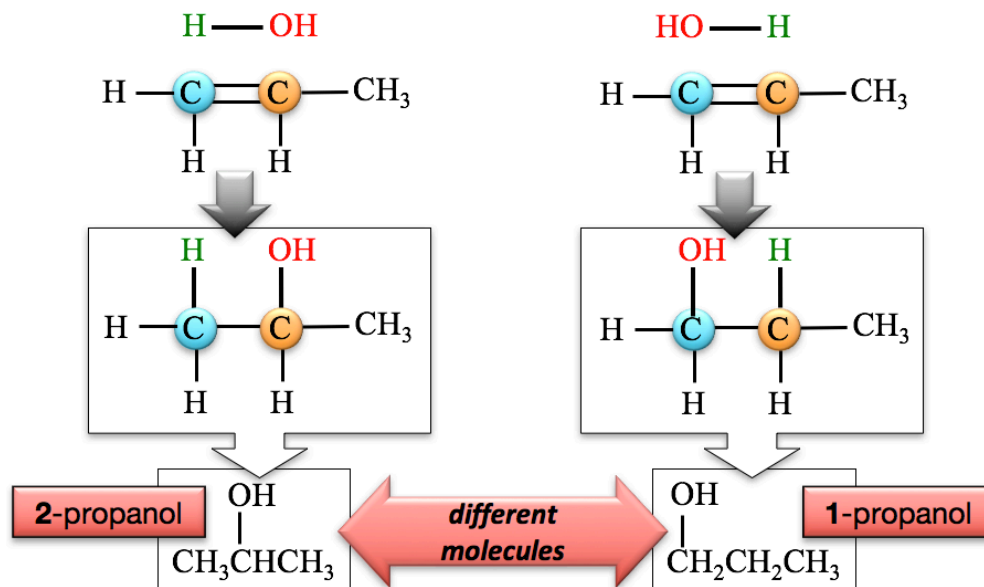
The addition of the **OH** group to propene's *right-most* double-bonded carbon produces **2**-propanol.

The addition of the **OH** group to the *left-most* double-bonded carbon produces **1**-propanol.

The hydration of an asymmetric alkene *does ____ produce an _____ amount of each alcohol product*.

- For example, in the hydration of propene, there is **more 2**-propanol than **1**-propanol produced.
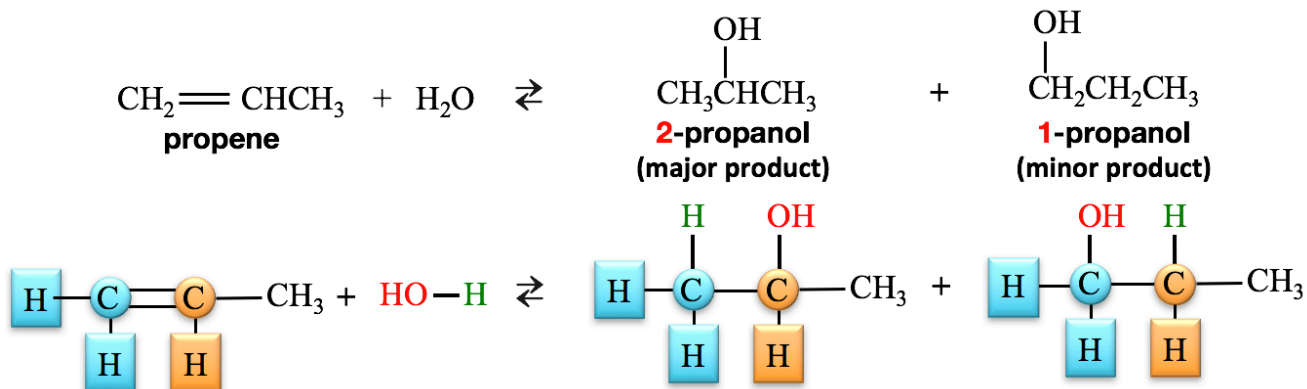
The product made in **greater** quantity is called the "_____ *product*."

The product made in **lesser** quantity is called the "_____ *product*."

It is possible to predict the **major** and **minor products** for the hydration of an *asymmetric alkene* using **Markovnikov's Rule**.

- This rule says that, the **major product** is formed by adding the **H** - from water - to the alkene's double-bonded carbon that **originally carried the most hydrogens**, and adding the **OH** to the **other** double-bonded carbon.
  - An easy way to remember this rule is by using the old saying, "**the rich get richer**," where the **H**'s represent money.

2-propanol
(major product)

1-propanol
(minor product)

$$H-C=C-CH_3 \;+\; HO-H \;\rightleftarrows\; H-C-C-CH_3 \;+\; H-C-C-CH_3$$
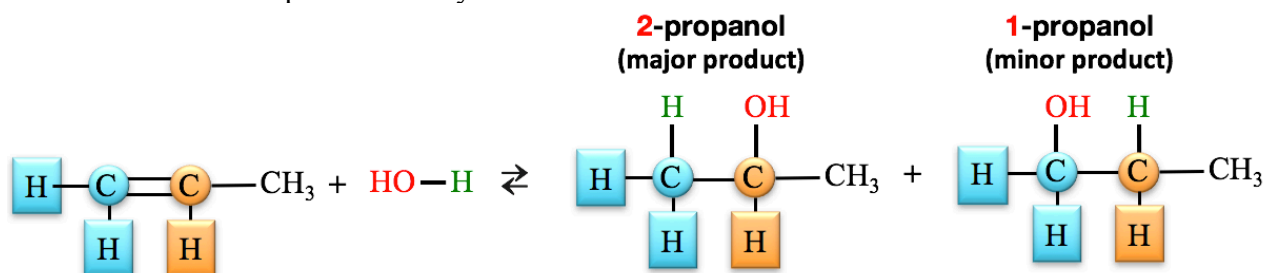
The **minor product** is formed by adding the **H** and **OH** in a manner **opposite** to that described for the *major product*.

Understanding Check

Draw **and** name the major and minor products for the hydration of 2-methyl-2-butene.

$$CH_3CH = CCH_3 \;+\; H_2O \;\rightleftarrows$$
$$\quad\quad\quad |$$
$$\quad\quad\quad CH_3$$
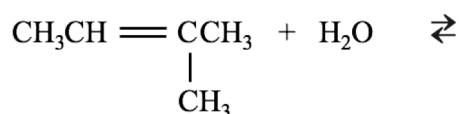
Compounds that are Related to Alcohols

Water and **alcohols** are said to be "**structurally** _____" because of their bonding patterns. If one of the hydrogens from water is **replaced** by an alkyl group (**R**), then an **alcohol** is obtained.

$$H-\ddot{\underset{..}{O}}-H \qquad\qquad R-\ddot{\underset{..}{O}}-H$$
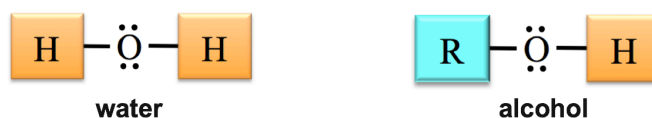
water   **alcohol**

Ethers and **alcohols** are *structurally related* compounds. If the hydrogen from an alcohol is replaced by an alkyl group (**R'**), then an _____ is obtained.

$$R-\ddot{\underset{..}{O}}-H \qquad\qquad R-\ddot{\underset{..}{O}}-R'$$

alcohol   **ether**

Peroxides are *structurally related* to **water, ethers,** and **alcohols**. If a _____ oxygen is added to water, ethers, or alcohols, as in the arrangement shown below, then a _____ is obtained.

$$R \text{ or } H-\ddot{\underset{..}{O}}-\ddot{\underset{..}{O}}-R' \text{ or } H$$

general form of a peroxide
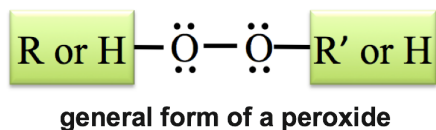
Ethers

The Structure of Ethers

Ethers contain an _____ *atom* that is attached to _____ alkyl (**R**) groups.

A specific example of an ether is *diethyl ether*.

- Diethyl ether was introduced as a surgical anesthetic in the 1840s. It is rarely used as an anesthetic currently because of the availability of more desirable substances.

Both of the alkyl (**R**) groups in diethyl ether are ethyl groups ($-CH_2CH_3$).

$CH_3CH_2-O-CH_2CH_3$ *or* $CH_3CH_2OCH_2CH_3$
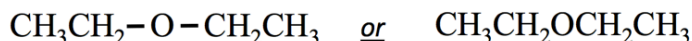
condensed structures of diethyl ether

ball-and-stick model of diethyl ether
black sphere = carbon
red sphere = oxygen white
sphere = hydrogen

skeletal structure of diethyl ether

Cyclic Ethers

A cyclic compound that has an oxygen atom in one of the ring positions is called a _____ *ether*.

Cyclic ethers are **hetero*cyclic*** compounds because their rings contain more than one type of element.

- Examples of cyclic ethers:
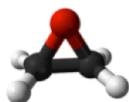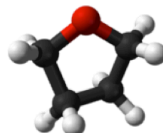
ethylene oxide   **tetrahydrofuran (THF)**   **dioxane**
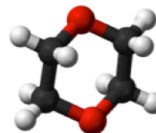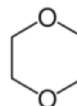
Naming Ethers

We will use what is referred to as the "_____ *names*" for ethers.

- This *trivial* method for naming ethers **is *not*** based on the IUPAC hydrocarbon naming method.

Step 1. Identify the alkyl group names for the two alkyl (R) groups.

- If the two **R** groups are *identical* use the "di" prefix before alkyl group name.

Step 2. Construct the name of the ether by placing the alkyl groups in alphabetical order followed by the word "ether."

- Use a space between the alkyl group names and before the word "ether."

Examples:
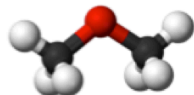
CH_3-O-CH_3 $CH_3-O-CH_2CH_3$ $CH_3CH_2-O-CH_2CH_3$
dimethyl ether   **ethyl methyl ether**   **diethyl ether**
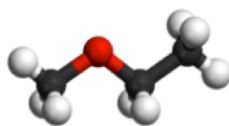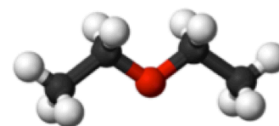
15

Understanding Check: Name the molecule that is shown here.

$$CH_3CH_2-O-CH_2CH_2CH_3$$
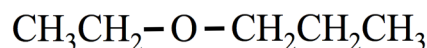
Water Solubility of Ethers

Smaller ethers have significant water solubility because of their ability to interact with **water** through **hydrogen bonding** and **dipole-dipole interactions**.

As their nonpolar (hydrocarbon) parts get *larger*, the water solubilities of ethers *decrease*.

Melting and Boiling Points of Ethers

Ethers have higher melting and boiling points than *hydrocarbons* of **similar size** because they can interact with each other through dipole-dipole interactions - they are polar molecules.

As their nonpolar (hydrocarbon) parts get larger, the melting and boiling points of ethers increase because of increasing London forces.

Ethers are **unable** to **hydrogen bond** *with each other*, and therefore, they have lower melting and boiling points than *alcohols* and *carboxylic acids* of **similar size**.

Ethers in Nature and Industry

Ethers have natural, industrial, and biochemical applications.

Dimethyl ether and ethyl methyl ether are used as aerosol spray propellants.

Dimethyl ether is used as an industrial solvent and in the perfume industry for the extraction of fragrant compounds from their natural sources.

Ethylene oxide, a cyclic ether, is used in the medical industry and hospitals as a disinfectant or sterilization agent for heat sensitive equipment.

- For example, disposable plastic syringes are sterilized using pure ethylene oxide.

Peroxides

Peroxides contain two oxygen atoms that are single-bonded to each other and situated between hydrogens, alkyl groups, or any other organic groups.
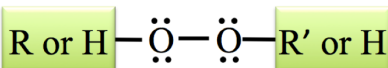
general form of a peroxide

Peroxides are quite reactive because of the two oxygen atoms that are single-bonded to each other. A much more stable configuration (lower energy) results when the oxygen-oxygen single bond breaks, and the oxygen atoms acquire more electrons by oxidizing another molecule. It is for this reason that peroxides are very effective oxidizing agents, and are frequently used as disinfectants and bleaching agents.

A specific example of a peroxide is *hydrogen peroxide*.

$$H - \ddot{O} - \ddot{O} - H$$
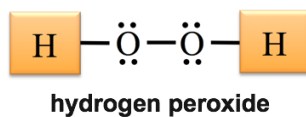
hydrogen peroxide

Hydrogen peroxide is important in human and animal metabolism. An extremely toxic byproduct of the production of ATP in the mitochondria is the superoxide ion (O_2^-) ion. This is not the *monoatomic* oxide ion (O^{2-}); it is an unstable *diatomic* ion with a 1⁻ charge. The superoxide ion is extremely toxic to cells because it can react with and damage (oxidize) DNA, proteins, and membrane component compounds. Almost all organisms have evolved enzymes called superoxide dismutases (SOD) to quickly remove superoxide ions. These enzymes are *antioxidant agents*. SOD enzymes catalyze the reaction of superoxide ions and water to produce hydrogen peroxide, oxygen, and hydroxide ions.

$$2\,O_2^- \;+\; 2\,H_2O \;\xrightarrow{\text{SOD}}\; H_2O_2 \;+\; O_2 \;+\; 2\,OH^-$$
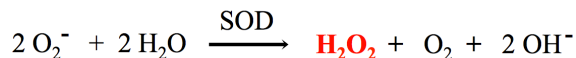
Though not quite as strong an oxidizer as superoxide, hydrogen peroxide is also an oxidizing agent, and is therefore quite toxic to cells. However, the hydrogen peroxide produced from superoxide is quickly converted to oxygen and water by an enzyme called catalase.

$$2\,H_2O_2 \;\xrightarrow{\text{catalase}}\; 2\,H_2O \;+\; O_2$$
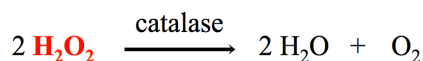
Sulfur Analogs

When the oxygen atom(s) of water, alcohol, ether, or peroxide is replaced by _____, the resulting compound is called a **sulfur analog**.

- For example, the ***sulfur analog of water,*** dihydrogen sulfide, is obtained if the oxygen in a water molecule is replaced by sulfur.

$$H - \ddot{O} - H \qquad\qquad H - \ddot{\underset{..}{S}} - H$$

H₂O   **H₂S**
dihydrogen sulfide
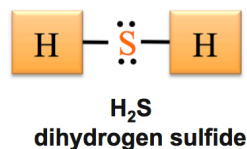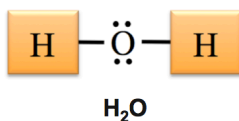
Dihydrogen sulfide (H_2S) is often called hydrogen sulfide. Although H_2S is heavier than H_2O, it is a gas at room temperature. The reason for this difference is that, unlike water, H_2S molecules are unable to hydrogen bond with each other. H_2S has the foul odor of rotten eggs. It is toxic and very reactive (explosive, flammable, and corrosive). H_2S occurs in nature when bacteria metabolize organic matter in the absence of oxygen. This often happens in sewers and swamps. It is also found in natural gas, some water wells, and volcanic gases. It is found in very low concentration in humans, where it acts as a chemical signaling molecule.

Thiols

The ***sulfur analog of an alcohol*** is obtained if the oxygen in an alcohol is replaced by sulfur.

The resulting molecule is called a _____.

$$R - \ddot{O} - H \qquad\qquad R - \ddot{\underset{..}{S}} - H$$

alcohol   **thiol**
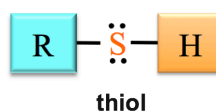
Thiols are often referred to as *mercaptans*. Many thiols have the aroma of garlic. Thiol aromas can be pungent and annoying. There are several thiols in the spray of skunks.

A specific example of a **thiol** is *2-methyl-2-propanethiol*.

SH
|
CH₃CCH₃
|
CH₃

2-methyl-2-propanethiol

black sphere = carbon
yellow sphere = sulfur
white sphere = hydrogen

2-methyl-2-propanethiol is added, in very small amounts, to natural gas as an odorant in order to help detect gas leaks or mistakenly-opened valves.

The **-SH** functional group, which defines the thiol family of organic compounds, is referred to as a ***thiol group*** or a ***sulfhydryl group***.

Naming Thiols

Thiols are systematically named in the same way as *alcohols **with only one exception***:

- The term "**thiol**" is added to the end the alkane name that indicates the number of carbons in the parent chain (***instead of*** replacing the "e" from the alkane name with "ol," as we did for alcohols).

- **Examples:**

CH₃CH₂−SH
ethanethiol

CH₃
|
CH₃CHCH₂CH₂−SH
3-methyl-1-butanethiol
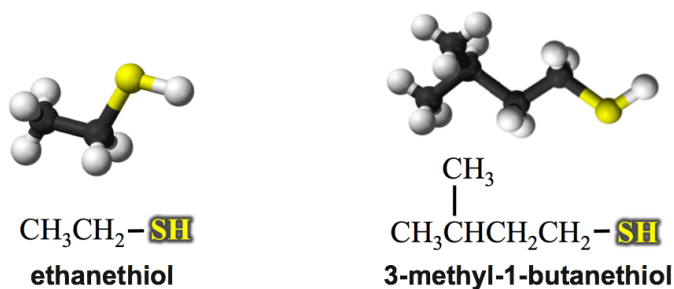
As was the case for alcohols, the point of attachment of the ***thiol group*** (-SH) must be indicated for thiols with more than two carbons in their parent chain. The point of attachment to the thiol group is indicated by writing the position number *in front of* the parent chain name.

Understanding Check: Name the molecule that is shown here.

$$CH_3CH_2CH_2CH_2CH_2SH$$
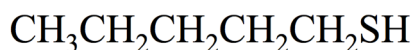
Sulfides

The ***sulfur analog of an ether*** is obtained if the oxygen in an ether molecule is replaced by sulfur.

The resulting molecule is called a _____. Sulfides are also referred to as **thioethers**.

R — Ö — R′
ether

R — S̈ — R′
sulfide

A specific example of a sulfide is *dimethyl sulfide* (DMS).

$$CH_3 - \boxed{S} - CH_3$$

dimethyl sulfide (DMS)
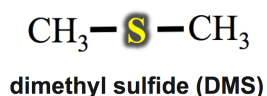
DMS is found in the atmosphere in greater concentration than any other organic sulfur-containing compound because it is produced by phytoplankton. It is also produced by bacteria in sewers. DMS has a characteristic cabbage-like odor. It is produced from cooking certain vegetables - corn, cabbage, beetroot - and seafood.

Naming Sulfides

We will use *common* names for sulfides, as we did for ethers.

Step 1. Identify the alkyl group names for each of the R groups.

- If the two **R** groups are *identical* use the "**di**" prefix before the alkyl group name.

Step 2. Name the sulfide by placing the alkyl groups in alphabetical order followed by the word "sulfide."

- Use a space between the alkyl group names and before the word "**sulfide**."

Examples:

$$CH_3 - \boxed{S} - CH_3 \qquad CH_3 - \boxed{S} - CH_2CH_3 \qquad CH_3CH_2 - \boxed{S} - CH_2CH_3$$
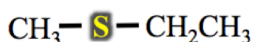
dimethyl sulfide   **ethyl methyl sulfide**   **diethyl sulfide**

Understanding Check: Name the molecule that is shown here.

$$CH_3CH_2 - S - CH_2CH_2CH_3$$
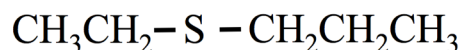
Disulfides

The **sulfur analog of a peroxide** is obtained if the two oxygens in a peroxide molecule are replaced by two sulfurs.

The resulting molecule is called a _____.
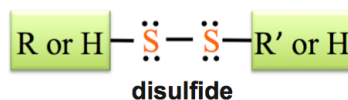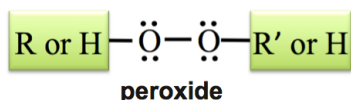
The **S-S** bond is called a **disulfide bond**.

Disulfides can be made from the reaction of *two* thiols. In this reaction, the thiols are **oxidized** to form a disulfide.
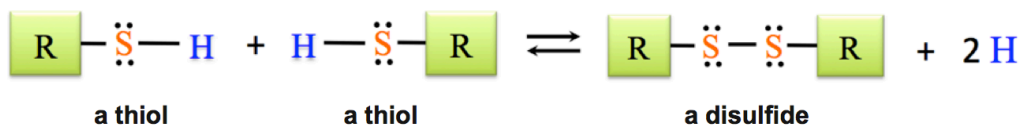
You can recognize that the thiol reactants were _____ because they _____ *hydrogen* in the reaction.

The disulfide bond is important in protein biochemistry.

$$\overset{O}{\underset{\underset{\underset{SH}{CH_2}}{|}}{^+NH_3CH}}\overset{||}{C} - O^-$$
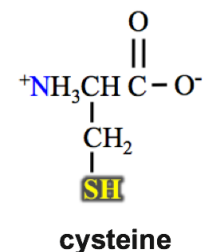
cysteine

Cysteine **is one of the twenty common amino acid molecules that make up proteins.** **Cysteine**, shown on the right, contains a thiol group that is capable of forming *disulfide bonds* with other cysteine-thiols.

Two **thiol (SH) groups** *on the same protein molecule* **or** two thiol groups on two *different protein molecules* can react to form disulfide bonds. The disulfide bonds in protein play an important role in how many proteins maintain their shape, which is critical in their biological function. This concept is illustrated (on the right) in **a large protein molecule - represented as a thick orange ribbon** - that is held into a particular shape with the help of some disulfide bonds. You will learn more details of protein structure and function in chapter 15.
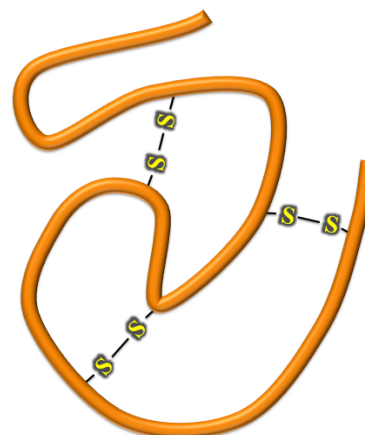
Understanding Check

Draw the condensed structure of the disulfide that is formed by the reaction of two methanethiol molecules.

Aldehydes and Ketones

The Structure of Aldehydes and Ketones

The general forms of **aldehydes** and **ketones** are shown below.

carbonyl carbon
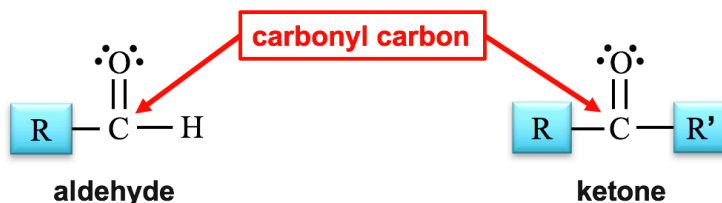
aldehyde

ketone

In *aldehydes*, **the carbonyl carbon is bonded to** _____ **R group and** _____ **hydrogen (H).**

- **Exception:** the simplest aldehyde, *formaldehyde,* which has the carbonyl carbon bonded to *two* hydrogens.

formaldehyde
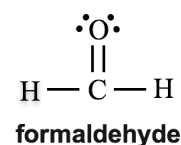
In *ketones*, **the carbonyl carbon is bonded to** _____ **R groups.**

An example of an aldehyde and a ketone:

$$\text{O}$$
$$\|$$
$$\text{CH}_3\text{CH}_2\text{CH}$$

propanal
(an aldehyde)

$$\text{O}$$
$$\|$$
$$\text{CH}_3\text{C}\,\text{CH}_3$$

propanone
(a ketone)
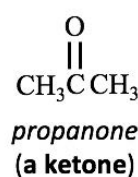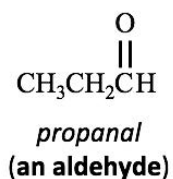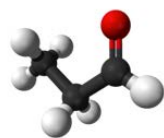
Sometimes a shorthand notation "**CHO**" is used for the carbonyl group *and* the hydrogen that is bonded to the carbonyl carbon when drawing *aldehydes*, as shown below.

$$\text{O}$$
$$\|$$
$$\text{CH}_3\text{CH}_2\,\text{CH}$$
$$\longrightarrow$$
$$\text{CH}_3\text{CH}_2\,\text{CHO}$$

two *equivalent* ways to draw an aldehyde

Any molecule that contains a **carbonyl group (C=O)** is called a _____ _____.

So far, you have been introduced to several *carbonyl compounds*: aldehydes, ketones, carboxylic acids, esters, and amides.

As a review, and for comparison, the general form for each of these families is shown below.

aldehyde

ketone

carboxylic acid

ester

amide
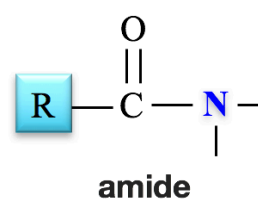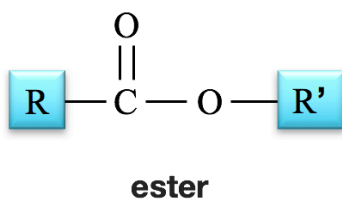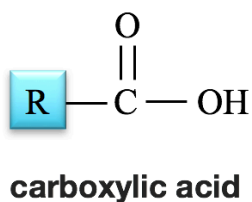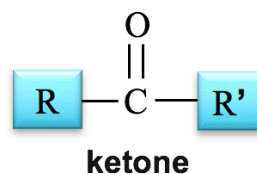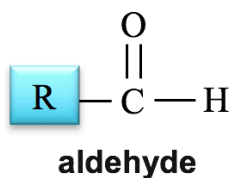
Understanding Check: Classify each of the following molecules as either an **aldehyde** or a **ketone**.

a.

$$\text{O}$$
$$\|$$
$$\text{CH}_3\text{CH}_2\text{CH}_2-\text{C}-\text{H}$$

b.

$$\text{O}$$
$$\|$$
$$\text{CH}_3\text{CH}_2\text{CH}_2-\text{C}-\text{CH}_2\text{CH}_3$$

c.

$$\text{O}$$
$$\|$$
$$-\text{C}-\text{H}$$
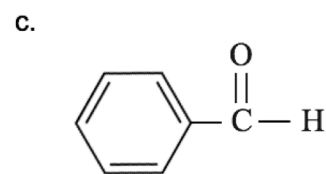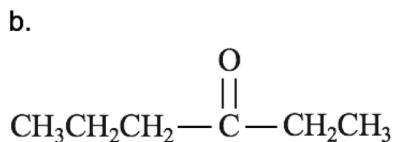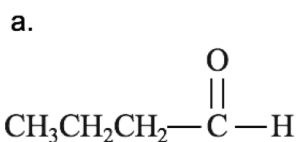
Naming Aldehydes and Ketones

Common Names for Aldehydes and Ketones

Small aldehydes and ketones, those with a relatively few number of carbon atoms, are often identified by *common names*.

- Examples of *common names* used for aldehydes:

$$H-\overset{\overset{\displaystyle O}{\|}}{C}-H \qquad CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-H$$

formaldehyde   **acetaldehyde**   **benzaldehyde**
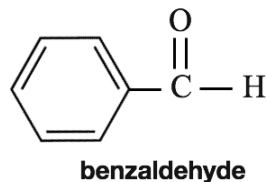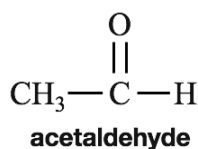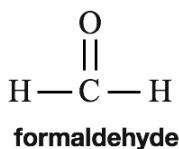
Sometimes, *common names* for **ketones** list the names of the alkyl groups bonded to the *carbonyl group* followed by the word **ketone**.

- Examples:

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-CH_3 \qquad CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-CH_2CH_3$$

dimethyl ketone (or acetone)   **ethyl methyl ketone**
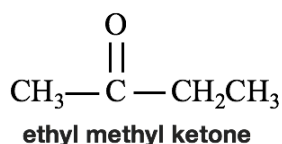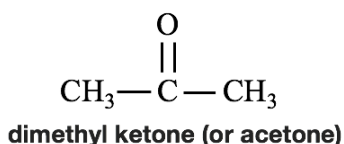
Systematic Names for Aldehydes and Ketones

The **systematic method** for naming aldehydes and ketones is based on the hydrocarbon naming method.

Step 1: Find and name the *parent chain*.

The *parent chain is the longest, continuous chain of carbon atoms that **contains the** _____ carbon*.

- **For aldehydes**, starting with the alkane name that corresponds to the number of carbon atoms in the parent chain, replace the "**e**" at the end of the alkane name with "**al**." For example, if the parent chain of an aldehyde contains two carbons, it would be called ethan<u>al</u>.

    ethan**e** ⟶ ethan**al**

- **For aldehydes**, the carbonyl carbon will *always* be at the _____of the parent chain and is assigned position number **1**.

- **For ketones**, starting with the alkane name that corresponds to the number of carbon atoms in the parent chain, replace the "**e**" at the end of the alkane name with "**one**." For example, if the parent chain of a ketone contains three carbons, it would be called propanone.

    propan**e** ⟶ propan**one**
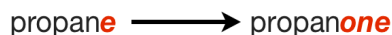
- **For ketones** with *more than four carbons*, the position of the *carbonyl carbon* must be indicated by adding a number as a prefix to the parent chain name.

    - Position number **1** is assigned to the carbon at the *end of the parent chain* that is

        _____ **to the *carbonyl carbon*.**

    - For example, if the carbonyl carbon is in position number **2** of a parent chain that contains five carbon atoms, then the parent chain is called **2**-pentanone.

$$\underset{1}{CH_3}\overset{\overset{\displaystyle O}{\|}}{\underset{2}{C}}\underset{3}{CH_2}\underset{4}{CH_2}\underset{5}{CH_3}$$
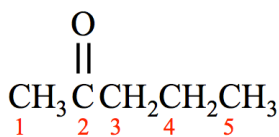
Steps 2, **3**, and **4** are done the **same way** as you did when systematically naming other organic molecules.

Step 2: Name any alkyl group substituents.

Step 3: Determine the *point of attachments* **of alkyl groups to the parent chain.**

Step 4: Construct the name of the molecule by placing the alkyl groups in alphabetical order and specifying their position number, followed by the name of the parent chain.

Aldehyde *Systematic Name* **Examples:**

$$
\underset{\textbf{methanal}}{H-\overset{\overset{\textstyle O}{\|}}{C}-H}
\qquad\qquad
\underset{\textbf{ethanal}}{CH_3\overset{\overset{\textstyle O}{\|}}{C}-H}
\qquad\qquad
\underset{\textbf{2-methylpropanal}}{CH_3\underset{\underset{\textstyle CH_3}{|}}{C}H\overset{\overset{\textstyle O}{\|}}{C}-H}
$$
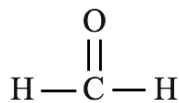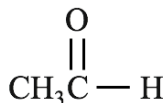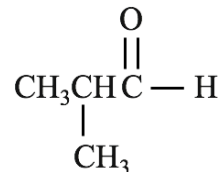
Ketone *Systematic Name* **Examples:**
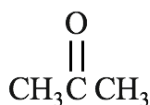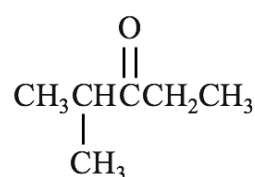
$$
\underset{\textbf{propanone}}{CH_3\overset{\overset{\textstyle O}{\|}}{C}CH_3}
\qquad
\underset{\textbf{2-pentanone}}{CH_3\overset{\overset{\textstyle O}{\|}}{C}CH_2CH_2CH_3}
\qquad
\underset{\textbf{2-methyl-3-pentanone}}{CH_3\underset{\underset{\textstyle CH_3}{|}}{C}H\overset{\overset{\textstyle O}{\|}}{C}CH_2CH_3}
$$

Understanding Check: Write the *systematic names* for each of the molecules shown here.

a.
$$CH_3\,\underset{\underset{\textstyle CH_3}{|}}{C}HCH_2\overset{\overset{\textstyle O}{\|}}{C}-H$$

b.
$$CH_3\underset{\underset{\textstyle CH_3}{|}}{\overset{\overset{\textstyle CH_3}{|}}{C}}CH_2CH_2CH_2\overset{\overset{\textstyle O}{\|}}{C}CH_3$$

c.
$$CH_3\underset{\underset{\textstyle CH_3}{|}}{C}H\overset{\overset{\textstyle O}{\|}}{C}CH_2CH_2CH_3$$
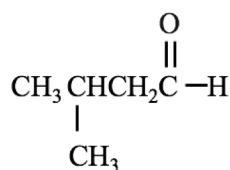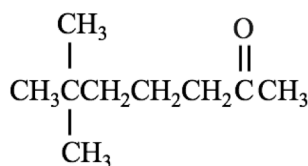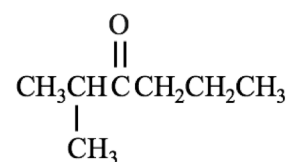
Understanding Check: Draw the *condensed* **and** *skeletal* structure for each of these molecules.

a. **4-methyl-2-pentanone**   b. **5,5-dimethylhexanal**   c. **3-ethyl-4-octanone**

Cyclic Ketones

A **cyclic ketone** is a molecule in which a *carbonyl carbon* occupies a position *between two other carbons* in a ring structure.

- Examples:
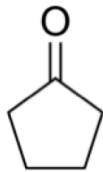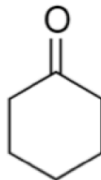
cyclopentanone   cyclohexanone

Cyclic ketones are named in a manner similar to that for *cyclic alcohols*.

- Starting with the cycloalkane name that corresponds to the number of carbon atoms in the ring structure chain, replace the "**e**" at the end of the *cyclo*alkane name with "**one**."

Frequently Encountered Aldehydes and Ketones
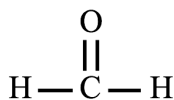
methanal (*or* formaldehyde)

Methanal, (common name *formaldehyde*) is quite toxic; however, it is frequently used because of its ability to kill viruses, fungi, and bacteria. It is used to disinfect and sterilize equipment. Formaldehyde will react with other compounds, and chemically bond multiple molecules together into "polymers." Polymers are molecules *composed of multiple repeated subunits*. The polymers that are formed using formaldehyde as linking agents are used to make plastics and adhesives, and for binding plywood. Formaldehyde-linked polymers may "out-gas" formaldehyde in the curing process, therefore it is important to use safety precautions when handling these materials. In 2011, the US National Toxicology Program categorized formaldehyde as "known to be a human carcinogen".
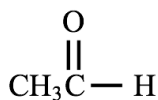
ethanal (*or* acetaldehyde)

Ethanal (common name *acetaldehyde*) has a sweet aroma. It is narcotic if taken in large enough amounts. It occurs in smaller quantities, naturally, in coffee, bread, and ripe fruit, especially in apples. Its use is widespread in industry, notably in the formation of polymer adhesives such as carpenter's glue (also known as white glue or Elmer's glue). I will discuss acetaldehyde's biological significance later in this chapter.
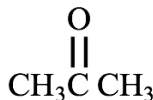
propanone (*or* acetone)

Propanone (common name *acetone*) is often used as a solvent and cleaning agent. It has the ability to dissolve many organic compounds and is also miscible with water. It is used as household nail-polish remover. Acetone has a high vapor pressure, and is highly flammable. It is not significantly toxic and is not currently regarded as a carcinogen, a mutagenic chemical, or a concern for chronic neurotoxicity issues.

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Properties of Aldehydes and Ketones

Water Solubility and Boiling Points of Some Aldehydes and Ketones

Aldehyde Name	Condensed Structure	Water Solubility (g/100 mL)	Boiling Point (°C)
ethanal	CH_3CHO	miscible	21
propanal	CH_3CH_2CHO	16	49
butanal	$CH_3CH_2CH_2CHO$	7	76
pentanal	$CH_3CH_2CH_2CH_2CHO$	1	103

Ketone Name	Condensed Structure	Water Solubility (g/100 mL)	Boiling Point (°C)
propanone	CH_3COCH_3	miscible	56
2-butanone	$CH_3COCH_2CH_3$	26	80
2-pentanone	$CH_3COCH_2CH_2CH_3$	6	102

Water Solubility of Aldehydes and Ketones

Smaller aldehyde and ketone molecules have significant water solubility because of their ability to interact with water through hydrogen bonding and dipole-dipole interactions.

As their nonpolar parts get larger, the solubilities of aldehydes and ketones decrease.

Boiling Points of Aldehydes and Ketones

As their nonpolar parts get larger, the boiling points of aldehydes and ketones increase because of increasing London forces.

$CH_3CH_2CH_2CH_3$
butane
boiling point = 0 °C

$CH_3CH_2\overset{\overset{\displaystyle O}{||}}{C}H$
propanal
boiling point = 50 °C

$CH_3\overset{\overset{\displaystyle O}{||}}{C}CH_3$
propanone
boiling point = 56 °C

$CH_3CH_2CH_2OH$
propanol
boiling point = 97 °C

Aldehydes and ketones have **higher** boiling points than **hydrocarbons** of similar size because of their ability to interact with each other through *dipole-dipole interactions*.

Aldehydes and ketones have **lower** boiling points than **alcohols** or **carboxylic acids** of similar size because aldehydes and ketones *are **not** capable* of interacting with each other through *hydrogen bonding*.

- Although aldehydes and ketones do have lone pairs of electrons on their oxygen atoms, they do not contain a hydrogen bonded to an N, O, or F that would be needed for hydrogen bonding with each other.

Reactions Involving Alcohols, Aldehydes, and Ketones

Reactions of Alcohols

1.   **The *Dehydration* of Alcohols**

I introduced you to the *dehydration of alcohols* reaction in chapter 6. Dehydration of alcohols is the *reverse* of the hydration of alkenes. H_2O is _____ from an alcohol to form an alkene.

- In the dehydration of an alcohol, a hydroxyl group (**OH**) is removed from one carbon, and an **H** is removed from *another carbon* that is _____ to the carbon from which the hydroxyl group was removed. A _____ ***bond*** forms between these two carbons.

- This reaction is catalyzed by a strong acid (H_3O^+) or an enzyme.

The *general form* of the equation for the de*hydration of an alcohol reaction*.

alcohol   alkene
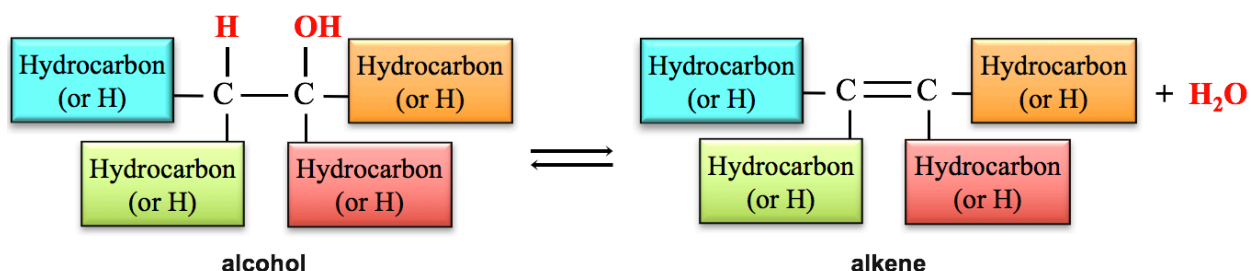
In chapter 6, I showed you a *bond flipping method* to help you predict the structure of the alkene that is produced when you "remove **H_2O**" to form a double bond." Let's review that method now by removing **H_2O** from 1-propanol (dehydration of 1-propanol). Beginning with the structure of the alcohol, perform the following steps:

Step #1: Flip the bond between the C and **OH** **up** to an **H** on *an adjacent* carbon.

Step #2: Flip the C-**H** bond from the *adjacent* carbon **down** to make a double bond to the C that originally carried the OH

Alkene and **H_2O** Products
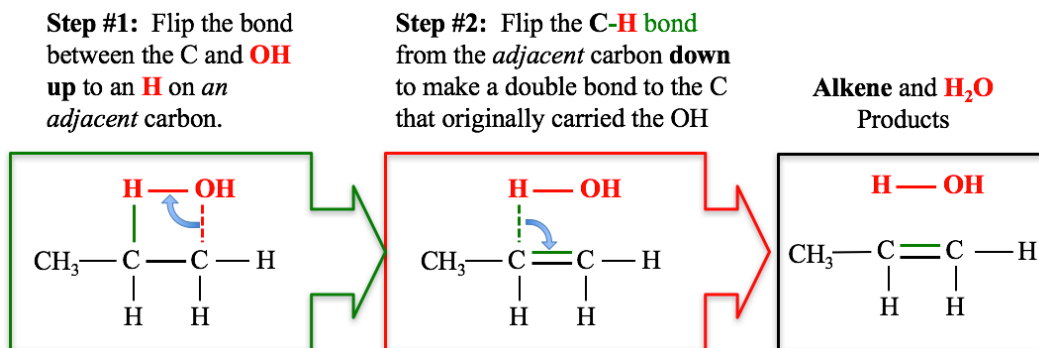
For the dehydration of a ***primary* (1°) *alcohol*** there is only one carbon that is **adjacent** to the *carbon carrying the* **OH**, therefore there is only _____ possible alkene product.

1-propanol
a primary (1°) alcohol

propene
(an alkene)
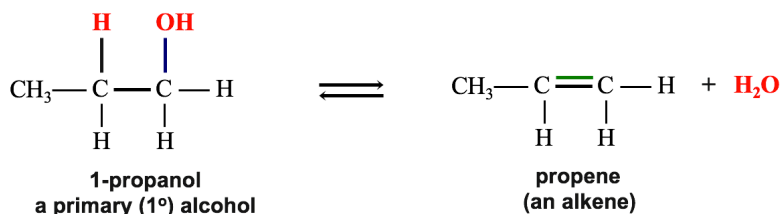
The dehydration of a _____ *secondary (2⁰)* or a *symmetric tertiary (3⁰) alcohol* only produces a **single** alkene product.

- A *2⁰ or 3⁰ alcohol* is *symmetric* if the *alkyl groups* bonded to the *carbon carrying the* **OH** are *identical*.

    - For example, **2-propanol**, shown below, is *symmetric*. Note that the *alkyl groups* bonded to the *carbon carrying the* **OH** are *identical*; they are both methyl groups.

2-propanol
a symmetric secondary (2°) alcohol
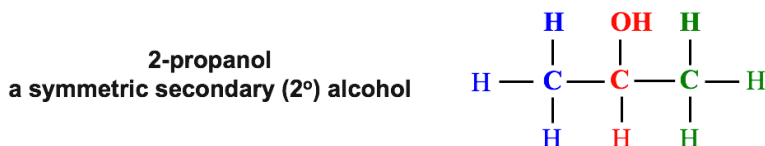
When a *symmetric alcohol* is dehydrated, it makes no difference from which **adjacent carbon** a hydrogen is removed to form the double bond; the alkene product is the same.

2-propanol

2-propanol

propene and H_2O

propene and H_2O

$CH_2{=}CH{-}CH_3$

$CH_3{-}CH{=}CH_2$

This is the **same** molecule!
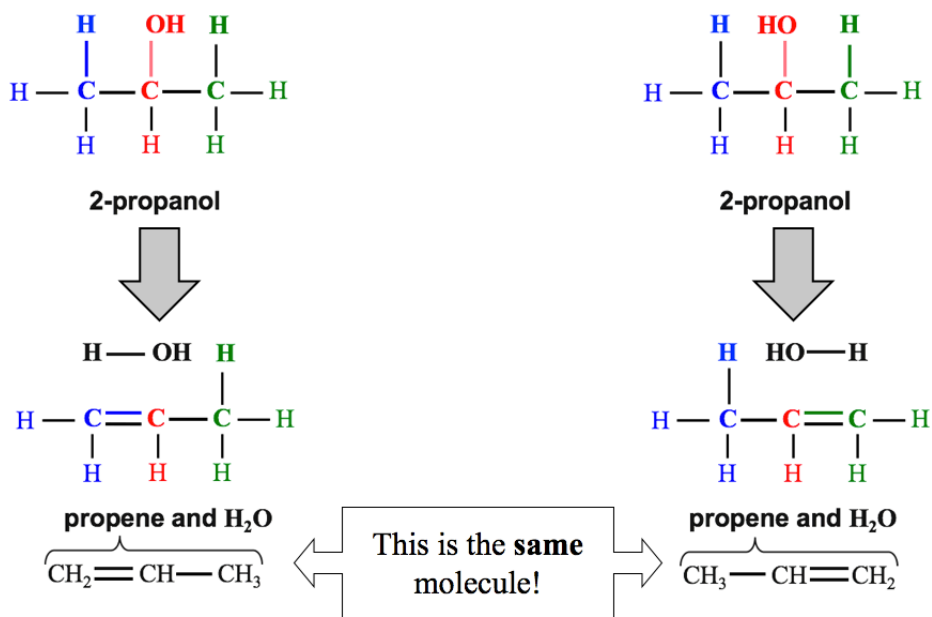
When an _____ *2⁰ or 3⁰* **alcohol** undergoes a dehydration reaction, there are _____ *different alkene molecules produced*.

- *2⁰ and 3⁰ alcohols* are **asymmetric** when the *alkyl groups* bonded to the *carbon carrying the* **OH** are _____ *identical*.

    - An example of an **asymmetric alcohol** is **2-butanol**, shown here.

2-butanol (an **a**symmetric alcohol)

OH

$CH_3CH_2CHCH_3$
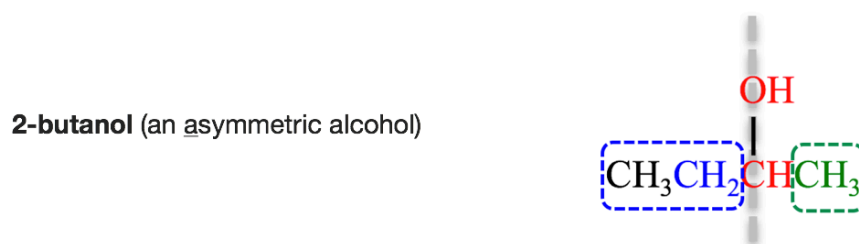
- Note that the alkyl groups that are bonded to the *carbon carrying the* **OH**, *are not identical*; one is a methyl group and the other is an ethyl group.

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Let's have a look at the **two *different alkenes that are produced*** when **2-butanol** undergoes a dehydration reaction.

CASE 1: remove an **H** from the *adjacent carbon* on the ***left***-hand side of the carbon carrying the **OH**.

CASE 2: remove an **H** from the *adjacent carbon* on the ***right***-hand side of the carbon carrying the **OH**.
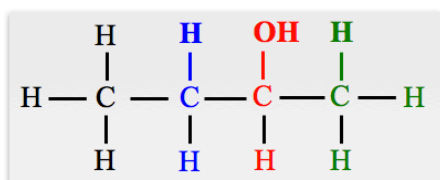
2-butanol

2-butene and H₂O

$$CH_3CH = CHCH_3$$
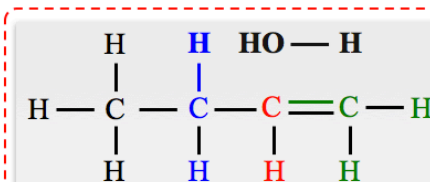
Two *different* alkenes are produced.

2-butanol

1-butene and H₂O

$$CH_3CH_2CH = CH_2$$

You have previously learned that the *hydration* of an asymmetric *alkene **does not produce equal amounts of both alcohol products***. A similar situation occurs for the *dehydration* of alcohols.

For example, in the dehydration of 2-butanol, about *four times* as much **2**-butene (*major product*) as **1**-butene (*minor product*) is produced.

It is possible to predict the major and minor products for the dehydration of an alcohol; in the ***major product***, the double bond is formed between the *carbon that was carrying the* **OH** and the adjacent carbon that ***originally carried fewer hydrogens***.

The ***minor product*** is formed between the *carbon that was carrying the* **OH** and the adjacent carbon that ***originally carried more hydrogens***.

Minor Product: 1-butene.
The double bond is formed *less often* between the **carbon (C)** that is "carrying" the **OH** and the adjacent carbon (C) that originally carried *more* hydrogen atoms.

$$CH_3CH_2CHCH_3 \; \overset{H_3O^+}{\rightleftharpoons} \; CH_3CH = CHCH_3 \; + \; CH_3CH_2CH = CH_2 \; + \; H_2O$$

Major Product: 2-butene.
The double bond is formed *more often* between the **carbon (C)** that is "carrying" the **OH** and the adjacent carbon (C) that originally carried *fewer* hydrogen atoms.

$$\underset{CH_3CH_2CHCH_3}{\overset{\overset{\displaystyle OH}{|}}{}} \rightleftharpoons CH_3CH = CHCH_3 + CH_3CH_2CH = CH_2 + H_2O$$

Minor Product: 1-butene

Major Product: 2-butene

In the formation of the _____ *alkene product,* the adjacent carbon that originally contained _____ hydrogens will _____ *another* hydrogen when the double bond is formed.

- An easy way to remember the alcohol dehydration rule for the ***major product*** is with the old saying, "*the **poor** get **poorer**,*" where hydrogen atoms (**H**) represent money.

Understanding Check

Draw *and* name the **major** *and* **minor products** for the dehydration of 3-ethyl-4-octanol.

$$\underset{\overset{|}{CH_2CH_3}}{CH_3CH_2\overset{\overset{\displaystyle OH}{|}}{C}HCHCH_2CH_2CH_2CH_3} \rightleftharpoons H_2O +$$
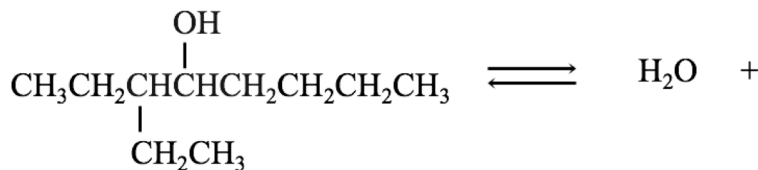
Major Product	**Minor Product**

---

2) The *Oxidation* of Alcohols

An *oxidation can* only occur when it is accompanied by a *reduction*.

- The reactant that is **oxidized** *loses* one or more electrons and the reactant that is **reduced** *gains* those electrons.

You learned that the *oxidation* of an organic compound in a reaction can be identified by ***the addition of oxygen and/or loss of hydrogen***.

For the *reduction* of an organic compound, the opposite occurs; ***the addition of hydrogen and/or loss of oxygen***.

When an alcohol is oxidized, the hydrogen from the hydroxyl group (**OH**) and a hydrogen (**H**) attached to *the carbon that is carrying the hydroxyl group* are both removed, *and* the C-O **single bond** is changed to a _____ **bond**.

General form of the equation for the *oxidation of an alcohol*:

$$R - \underset{\underset{\textbf{H}}{|}}{\overset{\overset{\text{O}\textbf{H}}{|}}{C}} - \text{R' or H} \quad \overset{[O]}{\rightleftharpoons} \quad R - \overset{\overset{O}{||}}{C} - \text{R' or H}$$
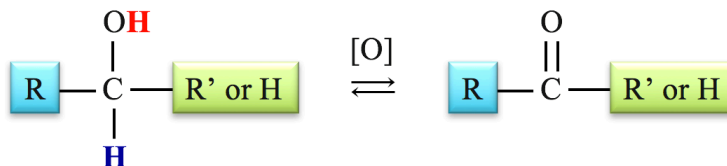
The reason that this reaction is classified as an *oxidation* (loss of electrons) is that the hydrogen that is bonded to the hydroxyl-carrying carbon, leaves the alcohol and takes _____ *of the electrons* from the bond with it.

A hydrogen with *two electrons* is called a _____ *ion* (**H:⁻**).

The "**[O]**," drawn above (or below) the arrows in a chemical equation, is often used to indicate that the reactant is being *oxidized,* and should not be confused with the presence of a catalyst.

When oxidation is indicated by using "**[O]**," then the identity of the oxidizing agent - which is actually a reactant - and the destination of the hydrogens are often omitted from the chemical equation.

- When doing so, it is acceptable - and expected - that the equation is not balanced.

The **structure** of the alcohol determines the identity of its oxidation product.

a) **Oxidation of Primary (1°) Alcohols**

Oxidation of a primary (1°) alcohol produces an _____.

$$R - \underset{\underset{\textbf{H}}{|}}{\overset{\overset{\text{OH}}{|}}{C}} - \text{H} \quad \overset{[O]}{\rightleftharpoons} \quad R - \overset{\overset{O}{||}}{C} - \text{H}$$

a primary (1°) alcohol   **an aldehyde**
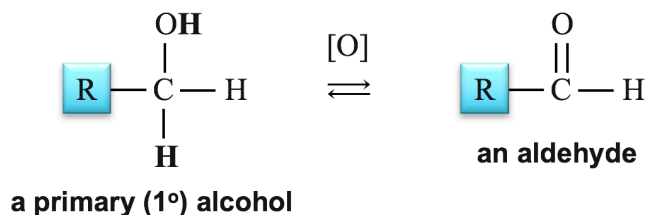
The oxidation of a primary alcohol produces an aldehyde because the hydroxyl group of a primary alcohol is attached to a carbon *at an end of the parent chain*, and therefore the carbonyl group in the product is *at the end of the chain*.

A specific example of the oxidation of a primary alcohol is the oxidation of *ethanol*:

$$CH_3 - \underset{\underset{\textbf{H}}{|}}{\overset{\overset{\text{O}\textbf{H}}{|}}{C}} - \text{H} \; + \; NAD^+ \quad \xrightarrow[\text{[O]}]{\substack{\text{alcohol} \\ \text{dehydrogenase}}} \quad CH_3 - \overset{\overset{O}{||}}{C} - \text{H} \; + \; NAD\textbf{H} \; + \; \textbf{H}^+$$

ethanol   **ethanal**
(a primary (1°) alcohol)   **an aldehyde**
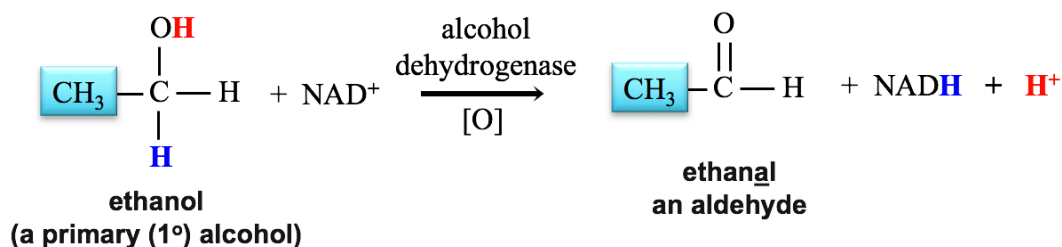
The **H⁺** that is produced will quickly react with water to form a hydronium ion (**H₃O⁺**). The evolution of the alcohol dehydrogenase enzyme for this reaction was important in order to remove naturally-occurring ethanol that we consume in some foods. Ethanol is toxic to cells. Although not an evolutionary requirement, the existence of this enzyme allows for the consumption of alcoholic beverages. The drug **disulfiram** (sold as *Antabuse*), is designed to deter individuals from drinking. It works by inhibiting the alcohol dehydrogenase enzyme, and thereby produces very undesirable effects when alcohol is consumed.

Certain organic molecules and inorganic oxidizing agents, such as MnO_4^-, can _____ oxidize aldehydes to produce _____ _____ .

$$\underset{\substack{\text{primary (1°) alcohol}}}{R-\underset{\underset{H}{|}}{\overset{\overset{OH}{|}}{C}}-H} \quad\underset{\rightleftarrows}{\overset{[O]}{}}\quad \underset{\text{aldehyde}}{R-\overset{\overset{O}{||}}{C}-H} \quad\underset{\rightleftarrows}{\overset{[O]}{}}\quad \underset{\text{carboxylic acid}}{R-\overset{\overset{O}{||}}{C}-OH}$$
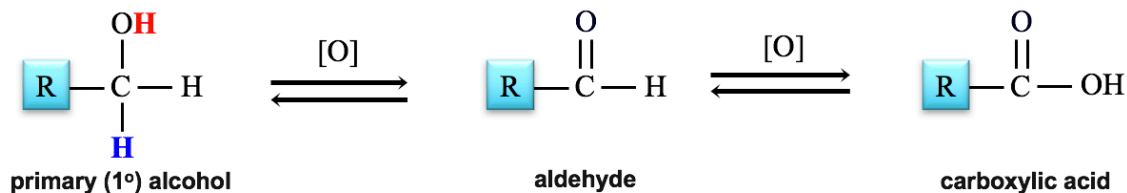
Example: For humans (and many animals) the conversion of the ethanal (an aldehyde) to acetic acid (a carboxylic acid) in the second step of the alcohol oxidation reaction, shown below, is catalyzed by an enzyme called *acetaldehyde dehydrogenase*.

$$\underset{\text{ethanol}}{CH_3-\underset{\underset{H}{|}}{\overset{\overset{OH}{|}}{C}}-H} \quad\xrightarrow[{[O]}]{\substack{\text{alcohol}\\\text{dehydrogenase}}}\quad \underset{\text{ethanal}}{CH_3-\overset{\overset{O}{||}}{C}-H} \quad\xrightarrow[{[O]}]{\substack{\text{acetaldehyde}\\\text{dehydrogenase}}}\quad \underset{\substack{\text{ethanoic acid}\\\text{(acetic acid)}}}{CH_3-\overset{\overset{O}{||}}{C}-OH}$$
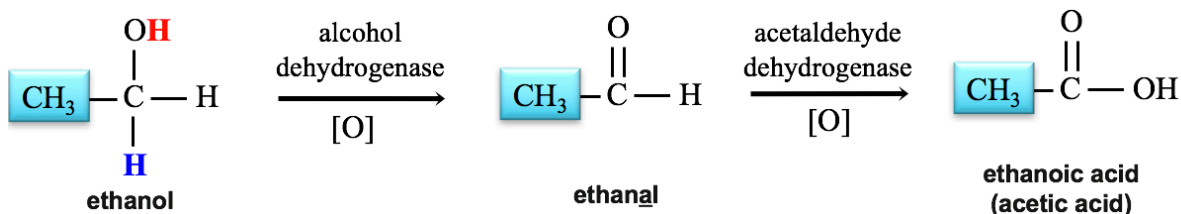
Most individuals of Asian descent have one of two variations in their DNA that each result in an ***especially efficient*** form of the *alcohol dehydrogenase* enzyme that catalyzes the *first* reaction (ethanol to ethanal). These individuals convert ethanol to ethanal very quickly. About half of the Asian individuals who have one of those DNA variants, also have ***a second DNA variation*** that results in a ***less*** *functional* acetaldehyde dehydrogenase enzyme to catalyze the *second reaction* above. For individuals with both of these DNA variants, *high* ethanal levels occur when consuming alcoholic beverages, which cause the red blotches/flushes (erythema) on the face, neck, shoulders, and, sometimes, the entire body. This condition is known as ***alcohol flush***. A*lcohol flush* has been correlated with a greatly-increased risk of esophageal cancer ***for those who drink***. The DNA variants leading to alcohol flush are most common among individuals of Asian descent, but do also occur, though much less frequently, in individuals of other geographical descents.

b) **Oxidation of Secondary (2⁰) Alcohols**

The oxidation of a secondary alcohol produces a _____ .

$$\underset{\substack{\text{a secondary (2°) alcohol}}}{R-\underset{\underset{H}{|}}{\overset{\overset{OH}{|}}{C}}-R'} \quad\underset{\rightleftarrows}{\overset{[O]}{}}\quad \underset{\text{a ketone}}{R-\overset{\overset{O}{||}}{C}-R'}$$
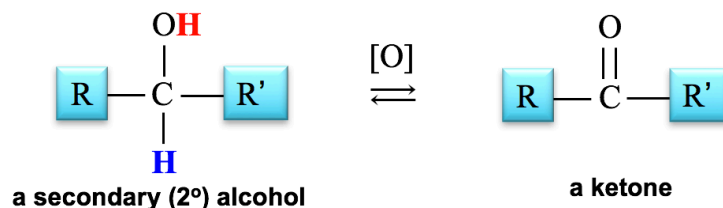
A **ketone** is produced because the hydroxyl group of a secondary alcohol is attached to a carbon *that is **not** at the end of the parent chain*, and therefore the carbonyl group in the product is ***not*** *at the end of the parent chain.*

A specific example of the oxidation of a secondary alcohol is the oxidation of 2-propanol.

$$\underset{\text{2-propanol}}{CH_3\underset{\underset{H}{|}}{\overset{\overset{OH}{|}}{C}}CH_3} \quad\underset{\rightleftarrows}{\overset{[O]}{}}\quad \underset{\text{propanone}}{CH_3\overset{\overset{O}{||}}{C}CH_3}$$
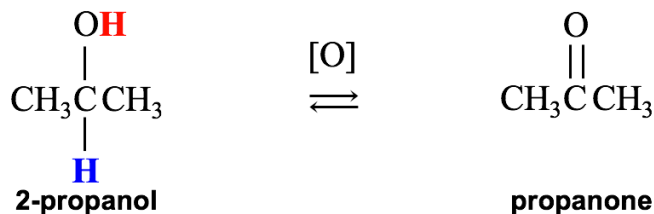
c) Oxidation of Tertiary (3⁰) Alcohols

A tertiary alcohol _____ be oxidized to an aldehyde or a ketone because tertiary alcohols do not have a hydrogen attached to the *carbon that is carrying the hydroxyl group*.

$$R - \underset{\underset{R''}{|}}{\overset{\overset{OH}{|}}{C}} - R' \quad \overset{[O]}{\rightleftarrows} \quad \text{no reaction}$$
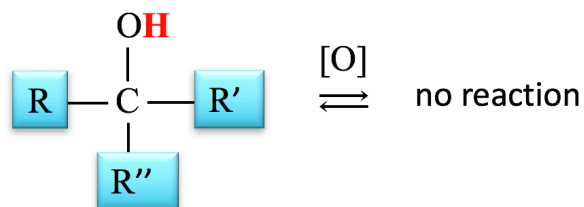
Understanding Check

MnO$_4^-$ will first oxidize a primary alcohol to an aldehyde, and then it will oxidize the aldehyde to produce a carboxylic acid.

$$\underset{\text{butanol}}{CH_3CH_2CH_2CH_2OH} \quad \overset{[O]}{\rightleftarrows} \quad \text{an aldehyde} \quad \overset{[O]}{\rightleftarrows} \quad \text{a carboxylic acid}$$
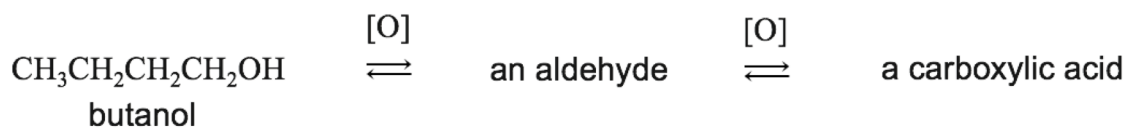
Draw *and* name the **aldehyde** that is initially formed, and then the **carboxylic acid** that is subsequently formed in the oxidation of butanol when MnO$_4^-$ is used as the oxidizing agent.

Understanding Check

Draw *and* name the organic molecule that is formed in the reaction shown here.

$$\underset{CH_3CH_2CHCH_2CH_3}{\overset{\overset{OH}{|}}{}} \quad \overset{[O]}{\rightleftarrows}$$
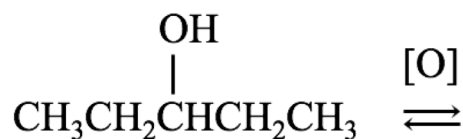
Reactions of Aldehydes and Ketones

1.   The Oxidation of Aldehydes

Aldehydes can be oxidized to *carboxylic acids*.

- I told you about the oxidation of aldehydes when I discussed the oxidation of *primary alcohols* to form *aldehydes*, which, under certain conditions are further oxidized to *carboxylic acids*.

$$R - \overset{\overset{\displaystyle O}{\|}}{C} - H \quad \underset{\rightleftharpoons}{[O]} \quad R - \overset{\overset{\displaystyle O}{\|}}{C} - OH$$

an aldehyde   a carboxylic acid

> This oxygen comes from the oxidizing agent.
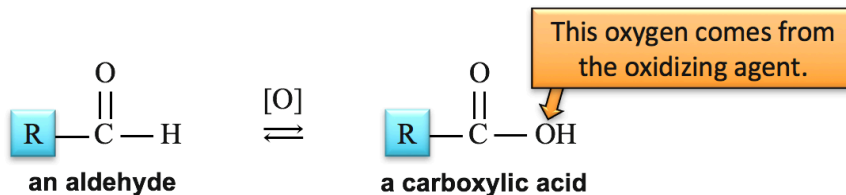
A specific example of the *oxidation of an aldehyde* is a reaction that my students do in a laboratory activity. They use the permanganate ion (MnO_4^-) to oxidize *benzaldehyde*.
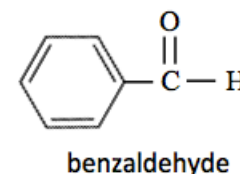
In the following review problem, I would like you to draw the carboxylic acid that is produced when this reaction occurs.

benzaldehyde

Understanding Check

Draw the structure of the *carboxylic acid* that is formed in the *oxidation* of benzaldehyde.

- The **R** group in benzaldehyde is a *benzene ring*.

$$\text{benzaldehyde} \quad \underset{\rightleftharpoons}{[O]}$$

benzaldehyde

---
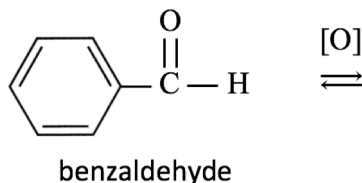
2) The Reduction of Aldehydes and Ketones

Reduction of an aldehyde **or** a ketone produces an _____.

- This is the _____ of the *oxidation* of alcohols reaction.

> **The general form of the equation for the *reduction* of an aldehyde or ketone:**
>
> $$R - \overset{\overset{\displaystyle O}{\|}}{C} - R' \text{ or } H \quad \underset{\rightleftharpoons}{[R]} \quad R - \overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - R' \text{ or } H$$
>
> an aldehyde or ketone   an alcohol
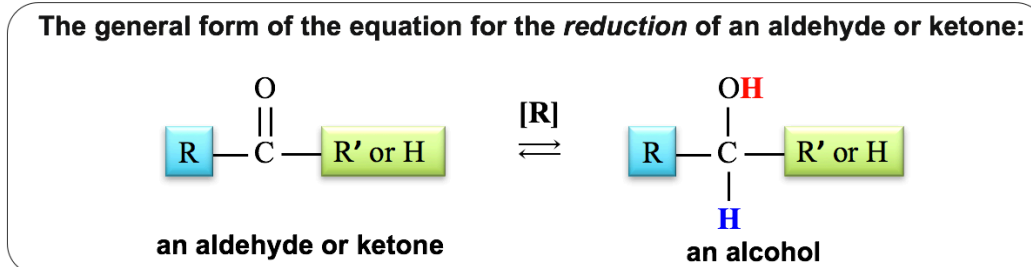
As was the case for "**[O]**," an "**[R]**" is often written above the arrows in a chemical equation to indicate that the reactant is being *reduced*.

- When reduction is indicated by using "**[R]**," then the identity of the reducing agent reactant and the source of the hydrogens (or destination of oxygens) are often omitted from the chemical equation. In this case, the equation need not be balanced.

Reduction of aldehydes or ketones involves the formation of a bond to the *carbonyl carbon* by a
_____ _____ (**H:⁻**), accompanied by the bonding of an **H⁺** ion to the carbonyl-oxygen atom,
and the conversion of the carbon-oxygen *double* bond into a *single* bond.
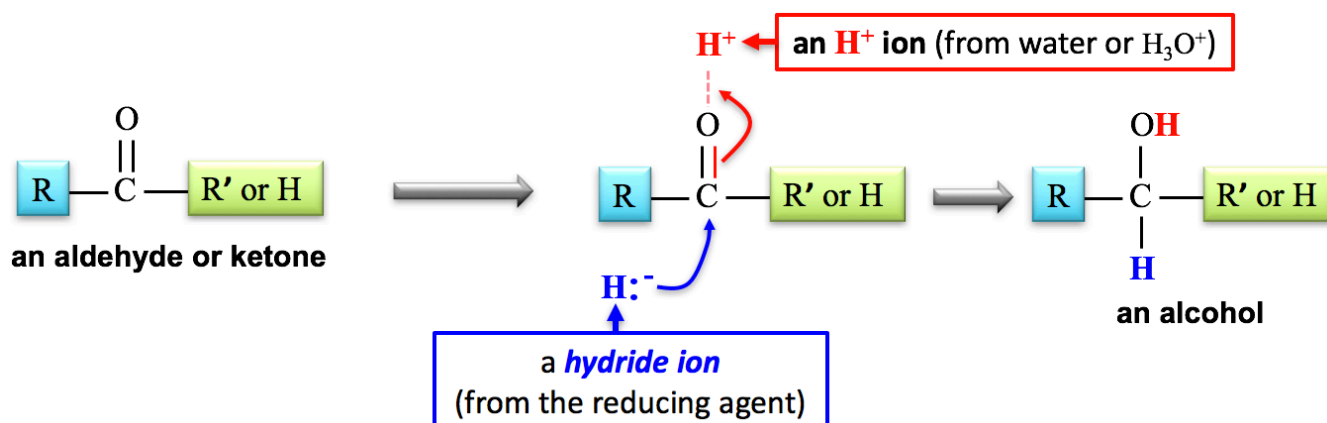
Aldehydes are reduced to _____ (1°) *alcohols*.

an aldehyde
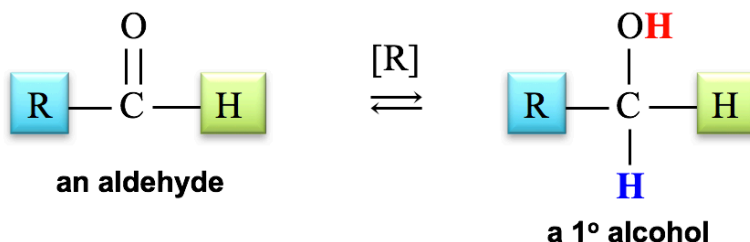
a 1° alcohol

Ketones are reduced to _____ (2°) *alcohols.*
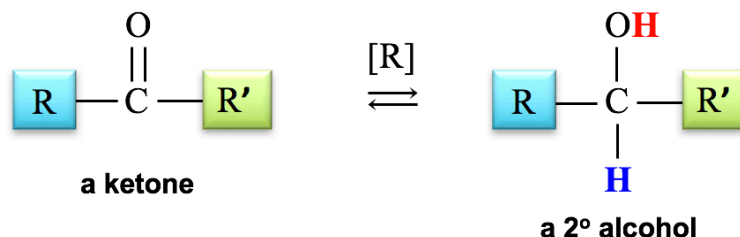
a ketone

a 2° alcohol

In **biological systems**, the *hydride ion* (**H:⁻**) used in the reduction of aldehydes or ketones is supplied by
nicotinamide adenine dinucleotide hydride (NAD**H**) or other organic hydride ion sources.

- For example, the final reaction in yeast's alcohol fermentation process is the reaction of ethanal
  with NAD**H** and an **H⁺** to form ethanol and NAD⁺.

$CH_3 - \overset{\overset{\textstyle O}{\textstyle ||}}{C} - H$ + NAD**H** + **H⁺** $\xrightarrow[\text{[R]}]{\text{enzyme}}$ $CH_3 - \overset{\overset{\textstyle O\mathbf{H}}{|}}{C\mathbf{H}} - H$ + NAD⁺

ethanal
(an aldehyde)

ethanol
(a 1° alcohol)
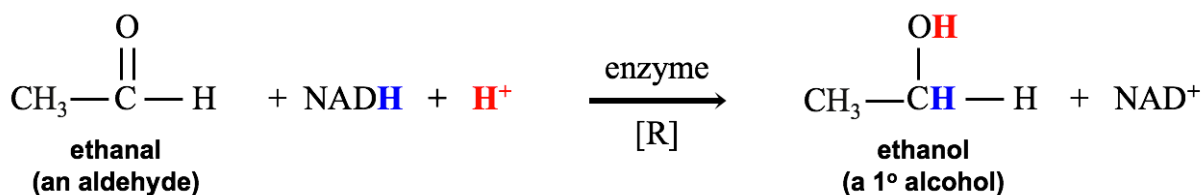
In the laboratory, hydride ions from aluminum hydride (AlH_4^-), or borohydride (BH_4^-) are used as reducing agents.

Hydrogen gas (H_2) is used as a reducing agent in laboratory and industrial applications.

- Reductions that use hydrogen gas (H_2) are called _____ *reactions*.

They occur at high temperatures and in the presence of metal catalysts - often platinum (Pt) metal surfaces. Hydrogenation reactions do not use the mechanism of the addition of *hydride* ($H:^-$) and H^+ ions that I previously described. A discussion of the mechanism for catalytic hydrogenation is beyond the scope of this book; however, you can predict the products for the reduction/hydrogenation of aldehydes or ketones by adding H_2 "across" the carbon-oxygen double bond (the carbonyl group), as we did for adding H_2 and H_2O "across" a C=C double bond.

To more easily visualize the addition of H_2 across the carbonyl group, it is convenient to redraw the aldehyde or ketone reactant with the **R'** or **H** group flipped downward, as shown below.
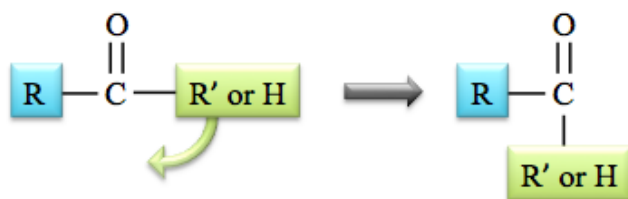
Next, draw the H_2 molecule to the side of the carbonyl group, and then flip the bond between the hydrogens downward to make a new bond to the carbonyl carbon:
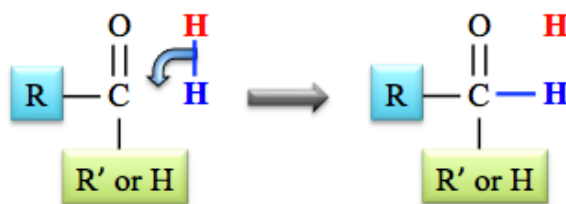
Finally, flip one pair of electrons from the carbonyl group's double bond upward to form a bond with the remaining *unbound* hydrogen (**H**).
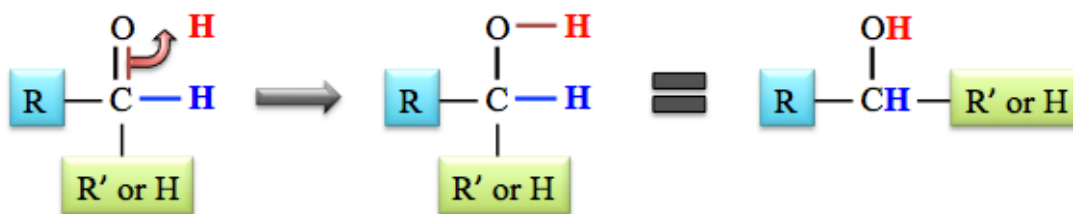
- A specific example of the hydrogenation of a ketone is the reaction of propanone with H_2.

propanone H_2 2-propanol
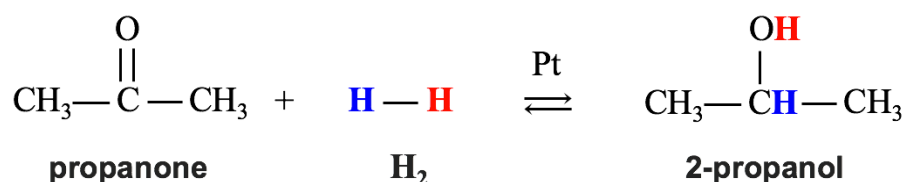
Draw the condensed structure ***and*** name the alcohol produced in the **reduction** of each of the following aldehydes or ketones.

- **NOTE:** When reduction reactions are indicated by "**[R]**," you do not need to include the source of hydrogens, and the equation will therefore *not be balanced*.

a.
$$\text{CH}_3\text{CHCH}_2\overset{\displaystyle O}{\overset{\displaystyle \|}{\text{C}}}\text{—H} \quad \overset{[R]}{\rightleftharpoons}$$
$$\underset{\displaystyle \text{CH}_3}{|}$$

b.
$$\text{CH}_3\underset{\displaystyle \underset{\displaystyle \text{CH}_3}{|}}{\overset{\displaystyle \overset{\displaystyle \text{CH}_3}{|}}{\text{C}}}\text{CH}_2\text{CH}_2\text{CH}_2\overset{\displaystyle O}{\overset{\displaystyle \|}{\text{C}}}\text{CH}_3 \quad \overset{[R]}{\rightleftharpoons}$$

c.
$$\text{CH}_3\text{CH}\overset{\displaystyle O}{\overset{\displaystyle \|}{\text{C}}}\text{CH}_2\text{CH}_2\text{CH}_3 \quad \overset{[R]}{\rightleftharpoons}$$
$$\underset{\displaystyle \text{CH}_3}{|}$$

3) The Reaction of Aldehydes or Ketones with Alcohols: Hemiacetal and Acetal Production

A _____ is a molecule that contains ***both*** an **OR** group *and* **OH** group that are bonded to the _____ carbon.

$$\text{R} - \overset{\displaystyle \text{OH}}{\underset{\displaystyle \text{R' or H}}{\text{C}}} - \text{OR}$$
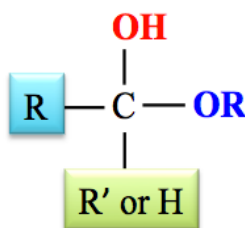
general form of a hemiacetal

An _____ is a molecule that contains _____ **OR** groups, where *both* **OR** groups are bonded to the *same* carbon.

$$\text{R} - \overset{\displaystyle \text{OR}}{\underset{\displaystyle \text{R' or H}}{\text{C}}} - \text{OR}$$
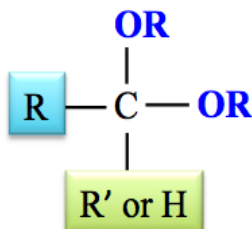
general form of an acetal

An *aldehyde or a ketone* will react with an *alcohol* to form a **hemiacetal**.

The **OR"** from the *alcohol* forms a bond to the *carbonyl-carbon* of the aldehyde or ketone, the **H** from the *alcohol* bonds to the *carbonyl-oxygen*, and the carbonyl group's double bond is changed to a single bond.

| **aldehyde or ketone** | **alcohol** | **hemiacetal** |
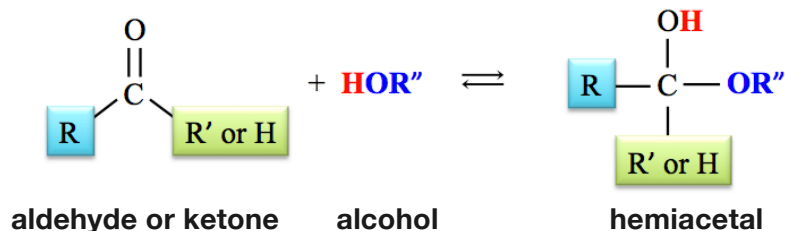
The *hemiacetal* that is formed can react with a _____ *alcohol molecule* to form an **acetal** and an H_2O molecule. The structure of the *acetal* that is produced is drawn by *exchanging* the **R"** group *of the alcohol* and the **H** from the *hemiacetal's* hydroxyl group (**OH**), as shown below.

| **hemiacetal** | **alcohol** | **acetal** | H_2O |
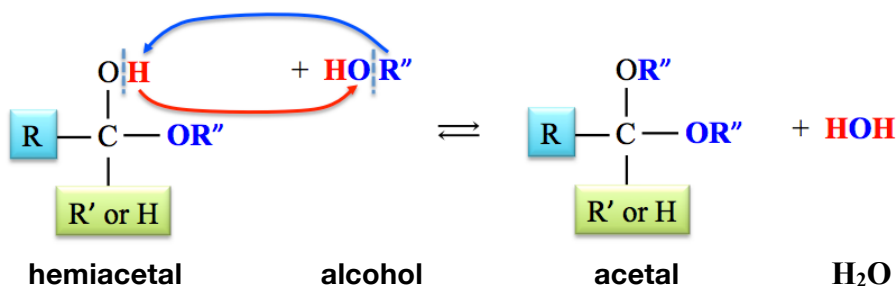
Example: Draw the structure of the hemiacetal - and then the acetal - that is formed by the reaction of ethanal with ethanol.
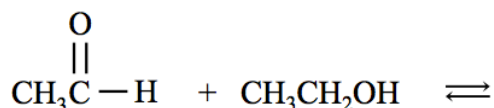
Solution: To form the *hemiacetal*, the **OR** from the *alcohol* forms a bond to the carbonyl carbon of the aldehyde or ketone, the **H** from the alcohol bonds to the carbonyl *oxygen*, and the carbonyl group's double bond is changed to a single bond. A simple way to do this is to add the alcohol "across" the carbonyl double bond.

To add the alcohol (CH_3CH_2OH) across the carbonyl group, it is convenient to redraw the aldehyde as shown below.
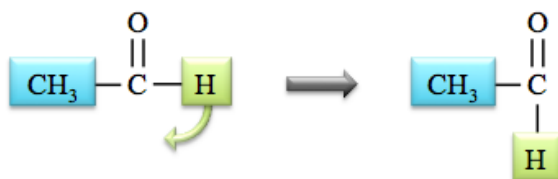
Next, draw the *alcohol molecule* to the side of the carbonyl group, as shown below, and then flip the bond from the *alcohol's hydroxyl group* downward to make a new bond to the carbonyl carbon.

37
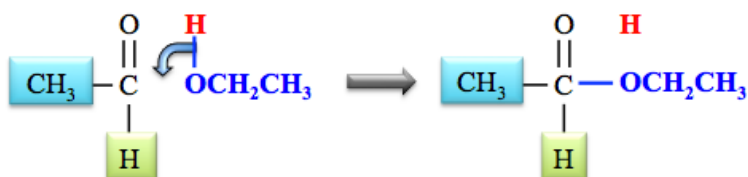
Finally, flip one pair of electrons from the carbonyl group upward to form a bond to the remaining *unbound* hydrogen (**H**).

$$CH_3-\overset{\overset{\displaystyle O \,\curvearrowright\, H}{\|}}{\underset{\underset{\displaystyle H}{|}}{C}}-OCH_2CH_3 \quad\longrightarrow\quad CH_3-\overset{\overset{\displaystyle O-H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-OCH_2CH_3 \;\equiv\; CH_3\,\overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-OCH_2CH_3$$
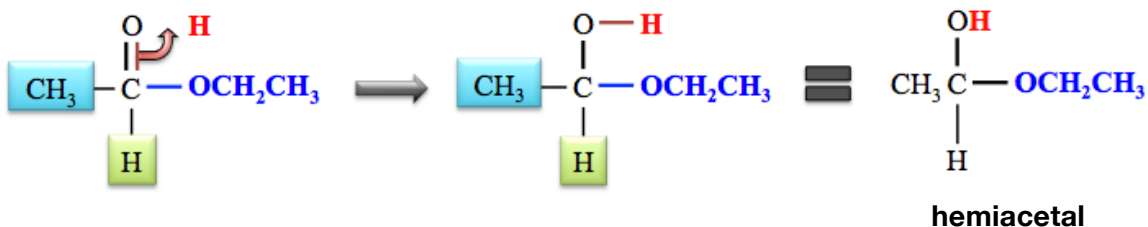
hemiacetal

The **hemiacetal** that is formed can react with a *second ethanol molecule* to form an **acetal** and an H_2O molecule. The structure of the **acetal** can be drawn by **exchanging** the **R** group *of the alcohol* (CH_3CH_2) and the **H** from the *hemiacetal's* hydroxyl group:
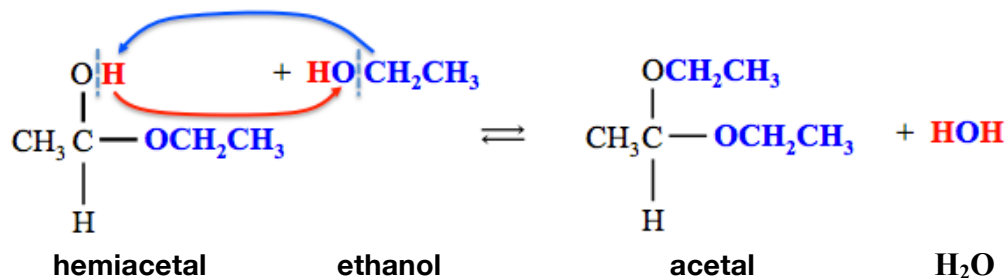
$$CH_3\,\overset{\overset{\displaystyle O{\mid}H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-OCH_2CH_3 \;+\; HO{\mid}CH_2CH_3 \;\rightleftharpoons\; CH_3\,\overset{\overset{\displaystyle OCH_2CH_3}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-OCH_2CH_3 \;+\; HOH$$

hemiacetal　　　　**ethanol**　　　　　　**acetal**　　　　　H_2O

Understanding Check

Draw the hemiacetal, and then the acetal, that are formed in the reaction shown below.

$$CH_3CH_2\overset{\overset{\displaystyle O}{\|}}{C}-H \;\;+\; CH_3OH \;\;\rightleftharpoons$$

Understanding Check

Draw the hemiacetal, and then the acetal, that are formed in the reaction shown below.

$$CH_3CH_2\overset{\overset{\displaystyle O}{\|}}{C}\,CH_2CH_3 \;\;+\; CH_3OH \;\;\rightleftharpoons$$

38
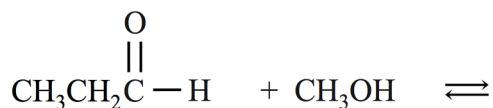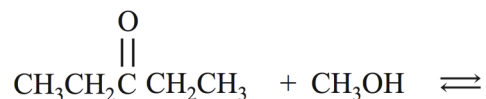
Naming the Molecules in Chapter 10 Worksheet and Key

1) Write the names of the following organic molecules.

NOTE: If you are having a hard time with these, try drawing the line bond structures first.

$CH_3CH_2\ CH_2\ CH_2$—OH

_____

$CH_3CH_2\ CHCH_2OH$
       |
      CH_2CH_3

_____

$$\overset{\displaystyle O}{\underset{\displaystyle CH_3-C-H}{\|}}$$

_____

$$\overset{\displaystyle O}{\underset{\displaystyle CH_3CH_2-C-CH_2CH_3}{\|}}$$

_____

_____

_____

$$\overset{\displaystyle O}{\underset{\displaystyle CH_3\ CH_2\ CH_2-C-\mathbf{H}}{\|}}$$

_____

_____

1
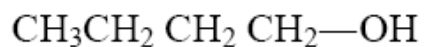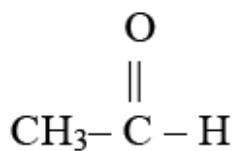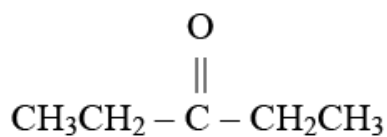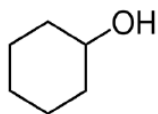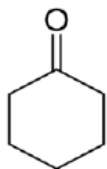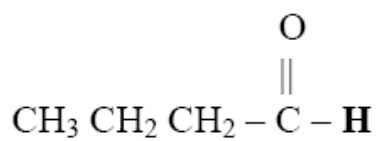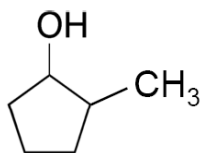
2) Draw the **condensed structural formula** for the following compounds.

    a) methanol

    b) 2-butanol
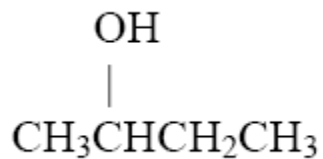
    c) 2-methyl-2-butanol
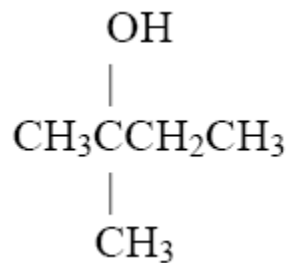
    d) propanone
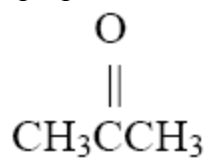
    e) 3-methylpentanal
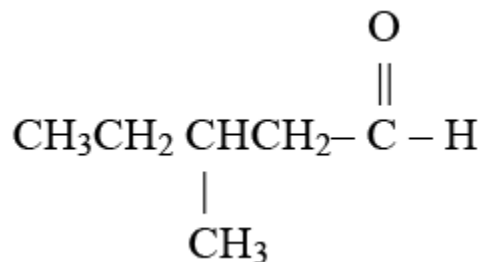
    f) cyclopentanol
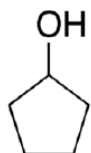
    g) 3-methylcyclopentanone
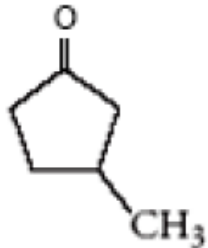
    h) butanone

    i) 3-methyl-1-butanol

1) Write the names of the following organic molecules:

$CH_3CH_2\ CH_2\ CH_2—OH$

.... 1-butanol

$CH_3CH_2\ CHCH_2OH$
       |
     CH_2CH_3 .... 2-ethyl-1-butanol

$$\underset{\textstyle CH_3-\overset{\textstyle O}{\overset{\textstyle ||}{C}}-H}{}$$

.... ethanal

$$\underset{\textstyle CH_3CH_2-\overset{\textstyle O}{\overset{\textstyle ||}{C}}-CH_2CH_3}{}$$

.... 3-pentanone

.... cyclohexanol

.........cyclohexanone

$$\underset{\textstyle CH_3\ CH_2\ CH_2-\overset{\textstyle O}{\overset{\textstyle ||}{C}}-\textbf{H}}{}$$ .... butanal

..............2-methylcyclopentanol

2) Draw the **condensed structural formula** for the following compounds

a) methanol

$$CH_3OH$$

b) 2-butanol

$$\underset{\underset{\displaystyle CH_3CHCH_2CH_3}{|}}{OH}$$

c) 2-methyl-2-butanol

$$\underset{\underset{\displaystyle \underset{\underset{\displaystyle CH_3}{|}}{CH_3CCH_2CH_3}}{|}}{OH}$$

d) propanone

$$\underset{\underset{\displaystyle CH_3CCH_3}{||}}{O}$$

e) 3-methylpentanal

$$CH_3CH_2\,\underset{\underset{\displaystyle CH_3}{|}}{CHCH_2-}\overset{\overset{\displaystyle O}{||}}{C}-H$$

f) cyclopentanol

g) 3-methylcyclopentanone

h) butanone

$$\begin{array}{c} O \\ \| \\ CH_3\ CH_2CCH_3 \end{array}$$

i) 3-methyl-1-butanol

$$CH_3\ CHCH_2CH_2-\mathbf{OH}$$
$$\qquad |$$
$$\qquad CH_3$$

Reactions of Chapter 10 Worksheet and Key

1) Alcohol Fermentation

Alcohol fermentation is a series of chemical reaction that convert sugar molecules, such a glucose, into ethanol and CO_2. The overall reaction of ethanol formation from a sugar molecule called glucose is shown below:

$$C_6H_{12}O_6 \longrightarrow 2\,CH_3CH_2OH \quad + \quad 2\,CO_2$$

$$\text{glucose} \qquad\qquad \text{ethanol} \qquad\qquad \text{carbon dioxide}$$

2) Nucleophilic Substitution

The general form of the equation for an S_N2 reaction for the production of alcohol is shown below (**X** represents F, Cl, Br, or I).

$$\text{R—X} \quad + \quad \text{OH}^- \quad \rightleftharpoons \quad \text{R—OH} \quad + \quad \text{X}^-$$

alkyl halide   **hydroxide ion**   **alcohol**   **halogen ion**
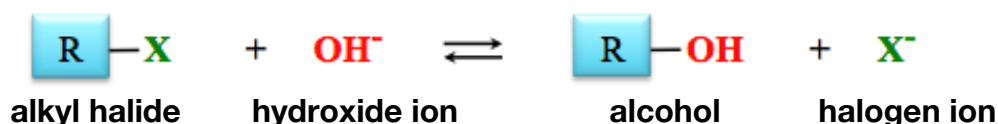
3) Hydration of Alkenes

A hydrogen atom from **H_2O** is added to one of the double bonded carbon atoms and the **-OH** from the **H_2O** is added to the **_other_** double bonded carbon atom in the **_alkene_** to produce the corresponding **_alcohol._** The **_general form_** of the chemical equation for the hydration of an alkene reaction is shown below:
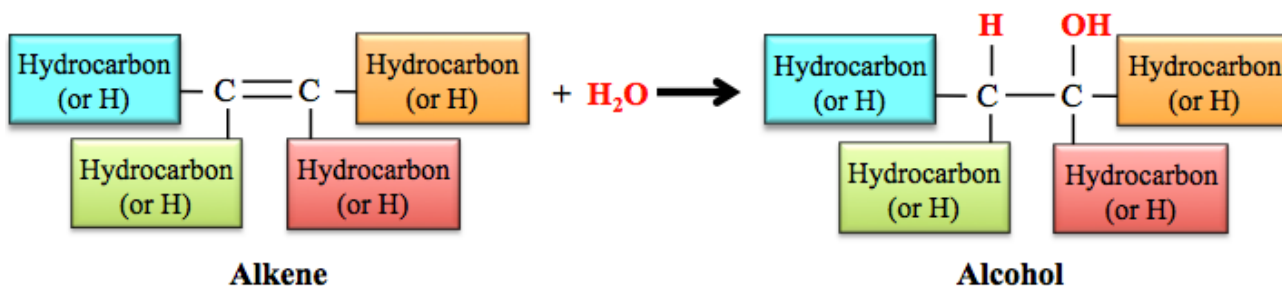
When an **_asymmetric alkene_** undergoes a hydration reaction, there are **_two different alcohol molecules produced_** - the product that is produced in greater quantity is called the **major product**, the product made in lesser quantity is called the **minor product**. It is possible to predict the major and minor products for the hydration of an asymmetric alkene using **Markovnikov's Rule**.

4) The *Dehydration* of Alcohols

A hydroxyl group (**OH**) is removed from a carbon atom and an **H** is removed from a carbon that is *adjacent* to the carbon that was bonded to the hydroxyl group. A double bond forms between these two carbons. The **general form** of the chemical equation for the *hydration of an alcohol reaction* is shown below:
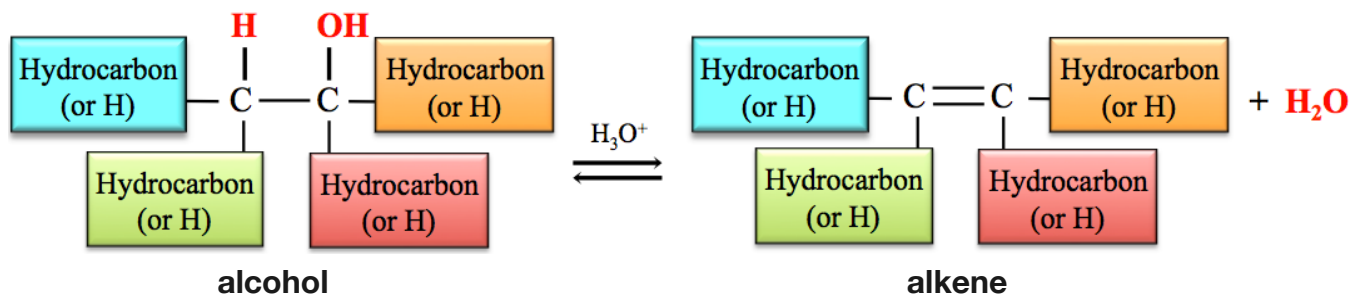
alcohol   **alkene**

When an **asymmetric 2° or 3° alcohol** undergoes a dehydration reaction, there are **two different alkene molecules produced** (*major* and *minor* products).

5) The *Oxidation* of Alcohols

When an alcohol is oxidized, the hydrogen from the hydroxy group (**OH**) and a hydrogen attached to *the carbon that is carrying the hydroxy group* are both removed, *and* the C-O *single* bond is changed to *double* bond. The general form of the equation for the **oxidation of an alcohol** is shown below.
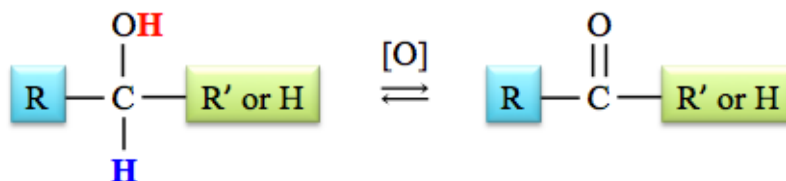
Oxidation of Primary (1°) Alcohols

Oxidation of a *primary (1°) alcohol* produces an *aldehyde*:

a primary alcohol   **an aldehyde**
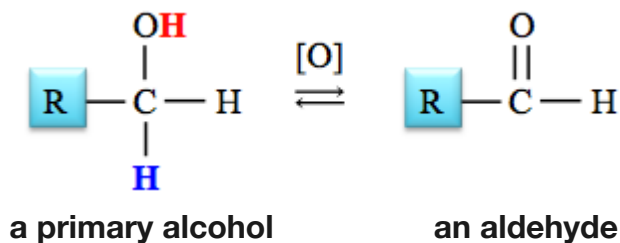
Certain oxidizing agents, such as CrO_3 or MnO_4^-, and/or enzymes can further oxidized aldehydes to produce carboxylic acids.

| 1° alcohol | aldehyde | carboxylic acid |
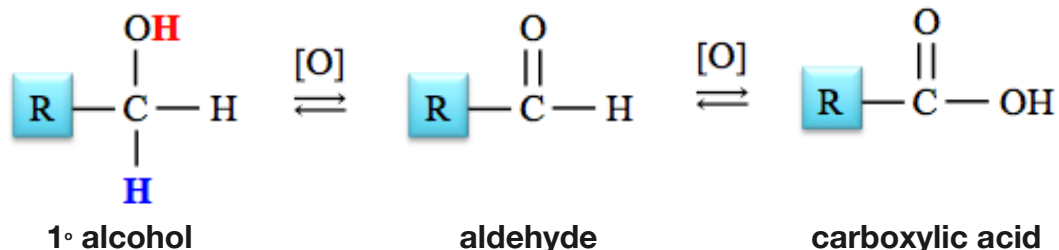
Oxidation of Secondary (2°) Alcohols

The oxidation of a secondary alcohol produces a **ketone** as shown below.
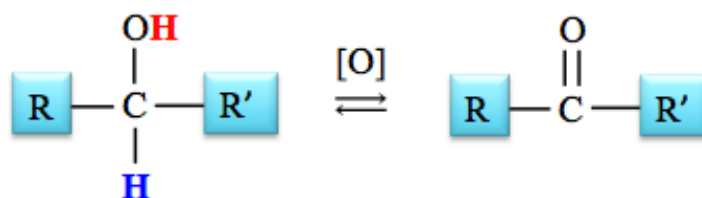
Tertiary (3°) alcohols cannot be converted to aldehydes or ketones by oxidation.

6) The Oxidation of Aldehydes

Aldehydes can be oxidized to **carboxylic acids**. The general form of the chemical equation for the oxidation of an aldehyde is shown below.

This oxygen comes from the oxidizing agent.

| aldehyde | carboxylic acid |
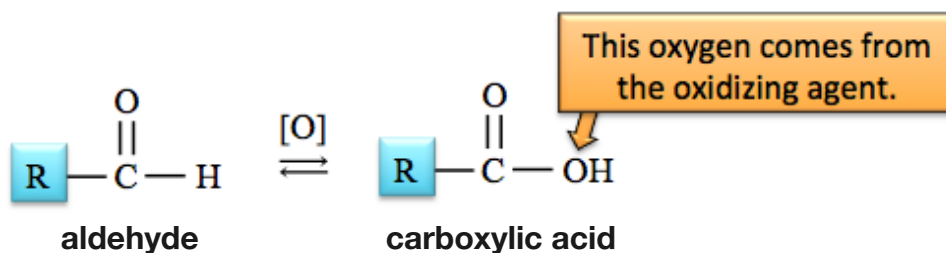
7) The Reduction of Aldehydes and Ketones

Reduction of aldehydes and ketones is the reverse of the oxidation of alcohol reactions. The general form of the equation for the **reduction of an aldehyde or ketone** is shown below.

| aldehyde or ketone | alcohol |

3
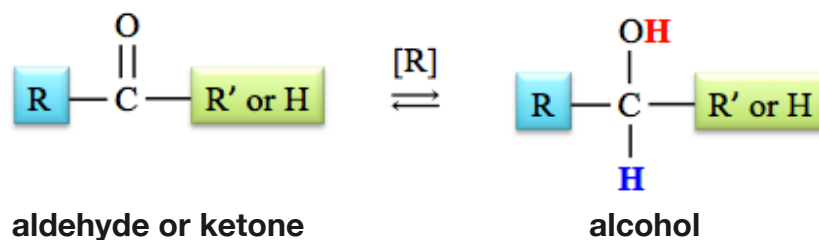
Aldehydes are reduced to *primary alcohols*.

aldehyde   a primary (1°) alcohol
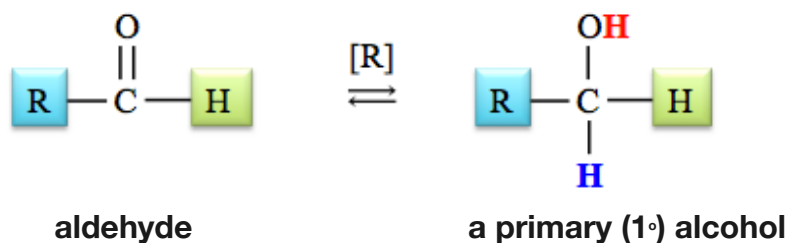
Ketones are reduced to *secondary alcohols*.

ketone   a secondary (2°) alcohol
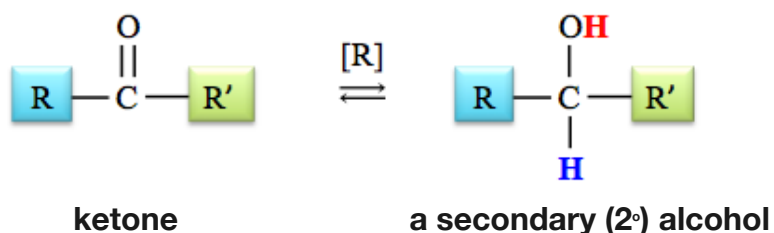
8) The Reaction of Aldehydes or Ketones with Alcohols: Hemiacetal and Acetal Production

An *aldehyde <u>or a ketone</u>* will react with an *alcohol* to form a **hemiacetal**.

aldehyde or ketone   alcohol   hemiacetal
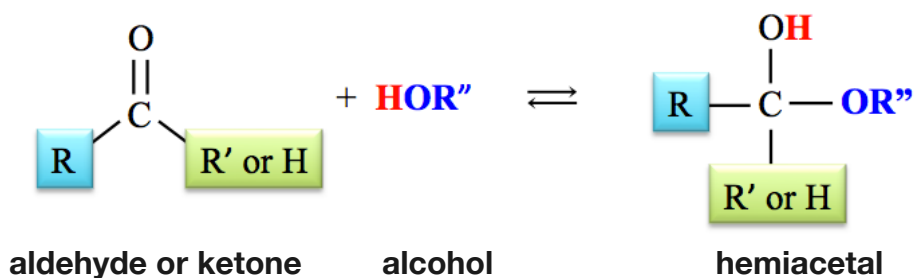
The **hemiacetal** that is formed can react with a *second alcohol molecule* to form an **acetal** and an H_2O molecule.

hemiacetal   alcohol   acetal H_2O

4
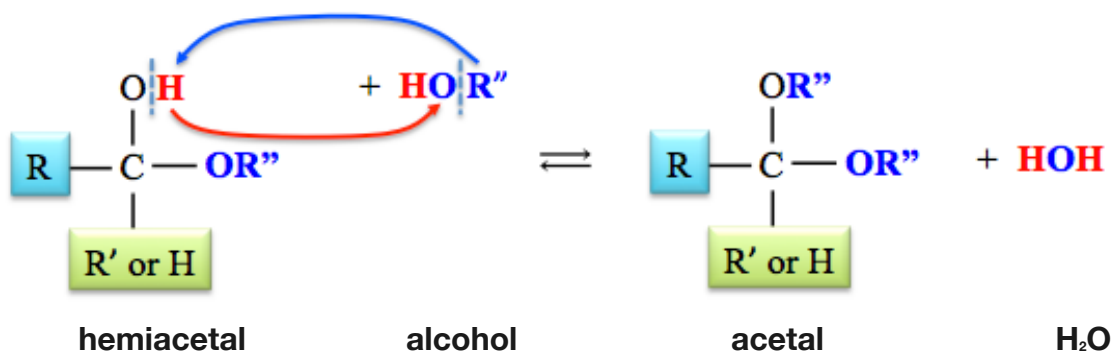
Questions:

1) Draw the condensed structure for the organic molecule that is produced when **butanal** is **oxidized**.

2) Draw the condensed structure for the **aldehyde** that is produced when **ethanol** is oxidized**.**

3) Draw the condensed structure for the organic molecule that is produced when **2-butanol** is oxidized.

4) Write the chemical equation for the formation of (a) the **hemiacetal**, and, (b) the **acetal** when **2-methyl-propanal** reacts with **methanol**.

5) Draw the condensed structure for the organic molecule that is produced when **propanone** is **reduced**.

6) Write the chemical equation for the *hydration* of **cis-3-hexene** *and* explain why there is only one possible product (no major or minor product) for this particular reactant.

7) Draw the condensed structure of the major **and** minor products for the ***dehydration*** reaction of **2-pentanol**.

8) Write the chemical equation for the ***hydration*** of **cyclopentene.**

9) Complete the following reactions. If there is more than one possible product, draw both products and label the major and minor product. If no reaction is possible, write "NO REACTION".

a)

$CH_3CHCH_2CH_2Br$ + OH⁻   ⇌
    |
    CH_3

b) write the product formed using excess oxidizing agent

                      [O]
$CH_3CHCH_2CH_2OH$ ⇌
    |
    CH_3

c)
   OH
   | [O]
$CH_3CCH_2CH_3$ ⇌
   |
   CH_3

d) Draw the hemiacetal product.

$$\underset{\qquad\qquad}{CH_3 - \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - H} + \underset{\underset{\displaystyle CH_2CH_3}{|}}{CH_3CH_2\ CHCH_2OH} \quad \rightleftharpoons$$

e)

$$\underset{\underset{\displaystyle H \quad CH_3}{|\quad\ |}}{CH_3CH_2 - C = C - CH_2CH_3} + H_2O \quad \rightleftharpoons$$

f)

$$\underset{CH_3CHCH_2CH_3}{\overset{\displaystyle OH}{\overset{\displaystyle |}{}}} \quad \overset{[O]}{\rightleftharpoons}$$

g) Draw the **acetal** product.

$$\underset{\underset{\displaystyle CH_3}{|}}{CH_3CH_2\ CHCH_2 - \overset{\displaystyle O}{\overset{\displaystyle \|}{C}} - H} + 2\ CH_3CH_2OH \quad \rightleftharpoons$$

7

h)

$$OH$$
$$CH_3 - CH - CHCH_2CH_3 \rightleftharpoons$$
$$CH_3$$

i)

$$O$$
$$\|$$
$$CH_3CH_2 - C - CH_2CH_3 \quad + \quad H_2 \quad \overset{[R]}{\rightleftharpoons}$$

j)

$$O$$
$$\|$$
$$CH_3 - C - H \quad \overset{[R]}{\rightleftharpoons}$$

k)

$$O$$
$$\|$$
$$CH_3CH_2 - C - CH_2CH_3 + 2\ CH_3CH_2OH \rightleftharpoons$$
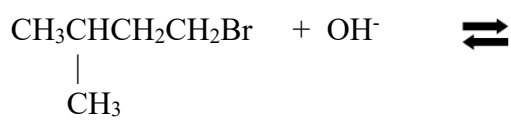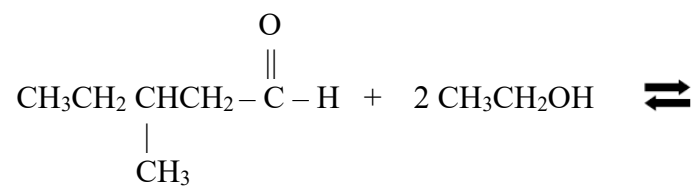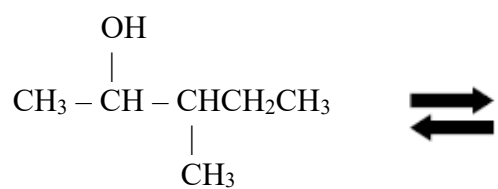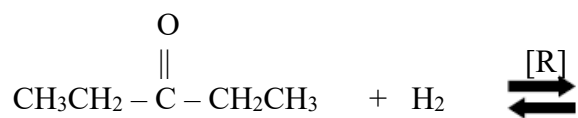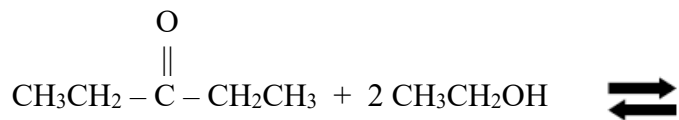
l) Dehydration

$$\rightleftharpoons$$

m) Reduction

$$\rightleftharpoons$$

8

10) Fill in the missing reactant(s):

a)

       +   ⇌ $CH_3CH_2CH_2-OH$ + Br⁻

b)

   + H_2O ⇌

$$CH_3CH_2 - \overset{\displaystyle H}{\underset{\displaystyle H}{C}} - \overset{\displaystyle OH}{\underset{\displaystyle CH_3}{C}} - CH_2CH_3 \quad \text{Major Product}$$

c)

[O]

⇌

$$CH_3CH_2\overset{\displaystyle O}{\overset{\displaystyle \|}{C}}CH_2CH_3$$

d)

  +   2 CH_3CH_2OH ⇌

$$CH_3CH_2\,CH_2CH_2 - \overset{\displaystyle O-CH_2CH_3}{\underset{\displaystyle H}{C}} - O - CH_2CH_3 + H_2O$$

e)

⇌

$$CH_3CH_2CH_2CH = \underset{\displaystyle CH_3}{C} - CH_3 + \text{ H-O-H}$$

Major Product

9

f) Draw the **alcohol** that is *oxidized* when excess MnO_4^- is used as an oxidizing agent.

$$\xrightarrow{[O]} \rightleftharpoons \quad CH_3CH\,CH_2CH_2CH_2\overset{\overset{\displaystyle O}{\|}}{C}-OH$$
$$\underset{\underset{\displaystyle CH_3}{|}}{}$$

g)

$$\rightleftharpoons \quad CH_3CH=CHCH_3 \;+\; H_2O$$

h)

$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-H \quad + \qquad \rightleftharpoons \quad CH_3-\overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-O-CH_2\underset{\underset{\displaystyle CH_3}{|}}{CHCH_3}$$

i)

$$+ \; H_2 \quad \xrightarrow{[R]} \rightleftharpoons \quad CH_3CH_2\overset{\overset{\displaystyle OH}{|}}{CH}CH_2CH_2CH_3$$

10

j)

Major Product

$\rightleftharpoons$

Minor Product

+ H_2O

k)

[O]

$\rightleftharpoons$

l)

[R]

$\rightleftharpoons$

CH_3CH_2OH

m)

$\rightleftharpoons$

$$CH_3CH_2 - \overset{\displaystyle OCH_2CH_3}{\underset{\displaystyle OCH_2CH_3}{\overset{|}{\underset{|}{C}}}} - CH_2CH_3 \quad + \quad H_2O$$

Key

1) Draw the condensed structure for the organic molecule that is produced when **butanal** is **oxidized**.

$$CH_3\ CH_2\ CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - H \qquad \underset{\rightleftarrows}{[O]} \qquad CH_3\ CH_2CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - OH$$

2) Draw the condensed structure for the **aldehyde** that is produced when **ethanol** is **oxidized.**

$$CH_3\ CH_2 - OH \qquad \underset{\rightleftarrows}{[O]} \qquad CH_3 - \overset{\overset{\displaystyle O}{\|}}{C} - H$$

3) Draw the condensed structure for the organic molecule that is produced when **2-butanol** is **oxidized**.

$$\overset{\overset{\displaystyle OH}{|}}{CH_3CH_2CHCH_3} \qquad \underset{\rightleftarrows}{[O]} \qquad CH_3\ \overset{\overset{\displaystyle O}{\|}}{CH_2CCH_3}$$

4) Write the chemical equation for the formation of (a) the **hemiacetal** and, (b) the **acetal** when **2-methyl-propanal** reacts with **methanol**.

$$CH_3CH - \overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle CH_3}{|}}{C}} - H + CH_3OH \rightleftarrows CH_3CH - \overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle CH_3\ \ H}{|\ \ |}}{C}} - OCH_3 + CH_3OH \rightleftarrows CH_3CH - \overset{\overset{\displaystyle OCH_3}{|}}{\underset{\underset{\displaystyle CH_3\ \ H}{|\ \ |}}{C}} - OCH_3 + H_2O$$

5) Draw the condensed structure for the organic molecule that is produced when **propanone** is **reduced**.

$$\overset{\overset{\displaystyle O}{\|}}{CH_3CCH_3} \ + \ H_2 \qquad \underset{\rightleftarrows}{[R]} \qquad \overset{\overset{\displaystyle OH}{|}}{CH_3CHCH_3}$$

12

6) Write the chemical equation for the hydration of **cis-3-hexene** _**and**_ explain why there is only one possible product (no major or minor product) for this particular reactant.

$$CH_3CH_2 - C = C - CH_2CH_3 \;+\; H_2O \;\rightleftharpoons\; CH_3CH_2 - \overset{OH}{\underset{H}{C}} - \overset{H}{\underset{H}{C}} - CH_2CH_3$$

with H, H below the double bond carbons on the left.

- There is only one product because the alkene is symmetric. No matter what carbon receives the **OH**, the product is 3-hexanol.

7) Draw the condensed structure of the major _**and**_ minor product for the _**dehydration**_ reaction of **2-pentanol**.
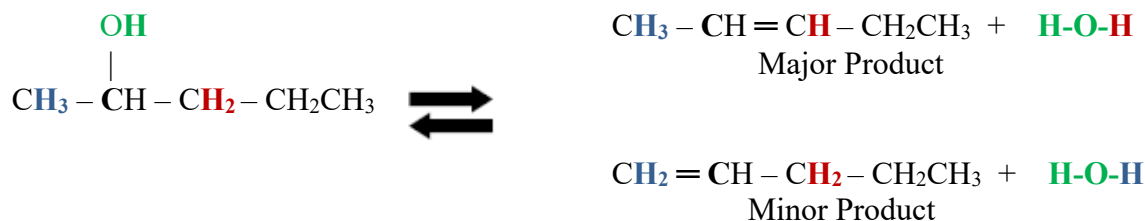
$$CH_3 - \overset{OH}{\underset{|}{CH}} - CH_2 - CH_2CH_3 \;\rightleftharpoons\;$$

$$CH_3 - CH = CH - CH_2CH_3 \;+\; H\text{-}O\text{-}H$$
Major Product

$$CH_2 = CH - CH_2 - CH_2CH_3 \;+\; H\text{-}O\text{-}H$$
Minor Product

8) Write the chemical equation for the _**hydration**_ of **cyclopentene.**
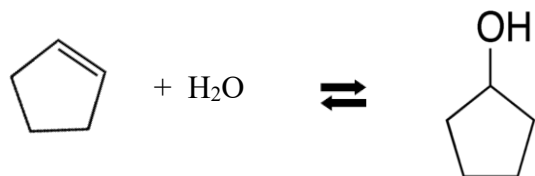
9) Complete the following reactions. If there is more than one possible product, then draw both products and label the major and minor product. If no reaction is possible, write "NO REACTION".

a)

$$CH_3CHCH_2CH_2Br \;+\; OH^- \;\rightleftharpoons\; CH_3\,CHCH_2CH_2\text{–}OH \;+\; Br^-$$
with CH_3 branches below each structure.

b) write the product formed using excess oxidizing agent

$$CH_3CHCH_2CH_2OH \;\overset{[O]}{\rightleftharpoons}\; CH_3\,CH\,CH_2\overset{O}{\overset{\|}{C}}\text{–}OH$$
with CH_3 branches below each structure.

13

c)

$$\underset{\underset{CH_3}{|}}{\overset{\overset{OH}{|}}{CH_3CCH_2CH_3}}$$ $\overset{[O]}{\rightleftharpoons}$ NO REACTION, 3° ALCOHOLS CAN NOT BE OXIDIZED

d) draw the hemiacetal product

$$\overset{\overset{O}{||}}{CH_3-C-}\ H\ +\ \underset{\underset{CH_2CH_3}{|}}{CH_3CH_2\ CHCH_2OH}$$ $\rightleftharpoons$ $$\underset{\underset{H}{|}}{\overset{\overset{OH}{|}}{CH_3-C}}-O-\underset{\underset{CH_2CH_3}{|}}{CH_2CH}\ CH_2CH_3$$

e)

$$\underset{\underset{H\quad CH_3}{|\quad\ |}}{CH_3CH_2-C=C-CH_2CH_3}\ +\ H_2O$$ $\rightleftharpoons$ $$\underset{\underset{H\quad CH_3}{|\quad\ |}}{\overset{\overset{H\quad OH}{|\quad\ |}}{CH_3CH_2-C-C-CH_2CH_3}}\quad\text{Major Product}$$

$$\underset{\underset{H\quad CH_3}{|\quad\ |}}{\overset{\overset{OH\ H}{|\quad|}}{CH_3CH_2-C-C-CH_2CH_3}}\quad\text{Minor Product}$$

f)

$$\underset{\underset{CH_3CHCH_2CH_3}{}}{\overset{\overset{OH}{|}}{CH_3CHCH_2CH_3}}$$ $\overset{[O]}{\rightleftharpoons}$ $$\overset{\overset{O}{||}}{CH_3CCH_2CH_3}$$

g) Draw the **acetal** product.

$$\underset{\underset{CH_3}{|}}{CH_3CH_2\ CHCH_2}-\overset{\overset{O}{||}}{C}-H\ +\ 2\ CH_3CH_2OH$$ $\rightleftharpoons$ $$\underset{\underset{CH_3\quad\ H}{|\qquad|}}{CH_3CH_2\ CHCH_2}-\overset{\overset{O-CH_2CH_3}{|}}{C}-O-CH_2CH_3\ +\ H_2O$$

h)

$$CH_3 - CH = C - CH_2CH_3 \ + \ \text{H-O-H}$$
$$|$$
$$CH_3$$

Major Product

OH
|
$$CH_3 - CH - CHCH_2CH_3$$ ⇌
|
$$CH_3$$

$$CH_2 = CH - CH - CH_2CH_3 \ + \ \text{H-O-H}$$
$$|$$
$$CH_3$$

Minor Product

i)

O
‖
$$CH_3CH_2 - C - CH_2CH_3 \ + \ H_2$$ ⇌ [R]

OH
|
$$CH_3CH_2 - C - CH_2CH_3$$
|
H

j)

O
‖
$$CH_3 - C - H$$ ⇌ [R]

OH
|
$$CH_3 - C - H$$
|
H

k)

O
‖
$$CH_3CH_2 - C - CH_2CH_3 \ + \ 2\ CH_3CH_2OH$$ ⇌

$$OCH_2CH_3$$
|
$$CH_3CH_2 - C - CH_2CH_3 \ + H_2O$$
|
$$OCH_2CH_3$$

l) Dehydration

 ⇌ + H₂O

m) Reduction

 ⇌

15

10) Fill in the missing reactant(s):

a)

$CH_3CH_2CH_2Br$ + OH^- ⇌ $CH_3CH_2CH_2$–OH + Br^-

b)

$CH_3CH_2 - C = C - CH_2CH_3$ + H_2O ⇌ $CH_3CH_2 - \overset{H}{\underset{H}{C}} - \overset{OH}{\underset{CH_3}{C}} - CH_2CH_3$ Major Product
$\quad\quad\quad\quad \underset{H}{|} \quad \underset{CH_3}{|}$

c)

$CH_3 CH_2\overset{OH}{\overset{|}{C}}HCH_2CH_3$ $\overset{[O]}{⇌}$ $CH_3CH_2\overset{O}{\overset{||}{C}}CH_2CH_3$

d)

$CH_3CH_2CH_2CH_2-\overset{O}{\overset{||}{C}}-H$ + 2 CH_3CH_2OH ⇌ $CH_3CH_2\ CH_2CH_2 - \overset{O-CH_2CH_3}{\underset{H}{\overset{|}{C}}} - O - CH_2CH_3$ + H_2O

e) Two possible answers:

OH
|
$CH_3CH_2CH_2 - CH - CHCH_3$ ⇌ $CH_3CH_2CH_2CH = C - CH_3$ + H-O-H
|
CH_3

CH_3
Major Product

OR

OH
|
$CH_3CH_2CH_2CH_2 - C - CH_3$ ⇌ $CH_3CH_2CH_2CH = C - CH_3$ + H-O-H
|
CH_3

CH_3
Major Product

f) Draw the alcohol that is oxidized when excess MnO_4^- is used as an oxidizing agent.

$CH_3CHCH_2CH_2 CH_2CH_2OH$ $\xrightarrow{[O]}$ $CH_3CH CH_2CH_2CH_2C - OH$
| ||
CH_3 O
                                                            |
                                                          CH_3

g)

OH
|
$CH_3CHCH_2CH_3$ ⇌ $CH_3CH=CHCH_3$ + H_2O

h)

O
||
$CH_3 - C - H$ + CH_3CHCH_2OH ⇌ $CH_3 - C - O - CH_2CHCH_3$
| | |
CH_3 H CH_3

OH
|

i)

O
||
$CH_3CH_2 CCH_2CH_2CH_3$ + H_2 $\xrightarrow{[R]}$ $CH_3CH_2CHCH_2CH_2CH_3$
|
OH

17

j)

OH

CH₃

⇌

CH₃

Major Product

+ H₂O

CH₃

Minor Product

k)

OH

[O]

⇌

O

l)

O
‖
CH₃– C – H

[R]
⇌

CH₃CH₂OH

m)

O
‖
CH₃CH₂ – C – CH₂CH₃ + **2** CH₃CH₂**OH**

⇌

OCH₂CH₃
|
CH₃CH₂ – C – CH₂CH₃   +   H₂O
|
OCH₂CH₃

Chapter 11 Lecture Notes: Carbohydrates

Educational Goals

1. Given a *Fischer projection* of a monosaccharide, classify it as either **aldoses** or **ketoses**.

2. Given a *Fischer projection* of a monosaccharide, classify it by the number of carbons it contains.

3. Given a *Fischer projection* of a monosaccharide, identify it as a **D-sugar** or **L-sugar**.

4. Given a *Fischer projection* of a monosaccharide, identify **chiral carbons** and determine the *number of stereoisomers* that are possible.

5. Identify *four* common types of **monosaccharide derivatives**.

6. Predict the products when a monosaccharide reacts with **a reducing agent** or with *Benedict's reagent*.

7. Define the term **anomer** and explain the difference between α and β *anomers*.

8. Understand and describe **mutarotation**.

9. Given its *Haworth projection*, identify a monosaccharide either a **pyranose** or a **furanose**.

10. Identify the **anomeric carbon** in *Haworth structures.*

11. Compare and contrast **monosaccharides**, **disaccharides**, **oligosaccharides**, and **polysaccharides.**

12. Given the structure of an oligosaccharide or polysaccharide, identify the **glycosidic bond**(s) and characterize the glycosidic linkage by the bonding pattern [for example: β(1⟶4)].

13. Given the *Haworth structures* of two monosaccharides, be able to draw the **disaccharide** that is formed when they are connected by a **glycosidic bond**.

14. Understand the difference between **homopolysaccharides** and **heteropolysaccharides**.

15. Compare and contrast the *two components* of **starch**.

16. Compare and contrast **amylopectin** and **glycogen**.

17. Identify **acetal** and **hemiacetal** bonding patterns in carbohydrates.

An Introduction to Carbohydrates

Carbohydrates are quite abundant in nature. More than *half of the carbon* found in living organisms is contained in carbohydrate molecules, most of which are contained in plants.

The primary reason for such an abundance is that a carbohydrate is produced by a series of chemical reactions that we call *photosynthesis*.

Energy from sunlight is used by plants to provide energy to drive the photosynthesis process. In the photosynthesis process, carbon dioxide and water are converted to oxygen gas and a *carbohydrate* called *glucose*.

Plants can use *glucose* to produce the ATP molecules that are needed to do the work necessary for life.

Plants store excess glucose as *starch*, for later use.

Animals obtain energy that is stored in *starch* by eating plants, or by eating animals that ate plants or had herbivores in their food-chain.

Carbohydrates are also referred to as _____ or _____.

Monosaccharides

_____ are the smallest carbohydrates and serve as the building blocks of larger carbohydrates.

- They are also referred to as _____ *sugars*.

Monosaccharides have the general chemical formula of $C_n(H_2O)_n$; where **n** (the number of carbon atoms) can be *three* to *seven*.

They are *polyhydroxyl* **aldehydes** or **ketones**:

- Monosaccharides contain either an _____ group *or* a _____ bonding pattern.

- Monosaccharides contain *more than one* _____ (OH) *group*.

A monosaccharide that contains an *aldehyde group* is called an _____.

A monosaccharide that contains the *ketone bonding pattern* is called a _____.
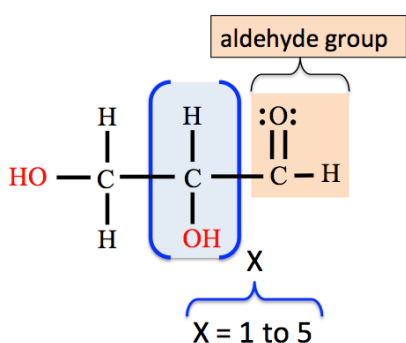
general form of an aldose
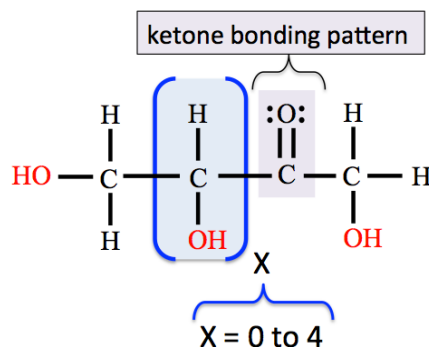
general form of a ketose

Note that the group in the parenthesis can repeat.
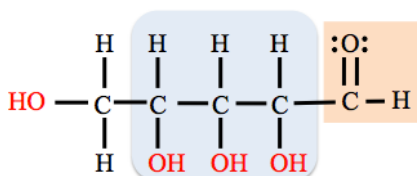
an aldose structure where X = 3
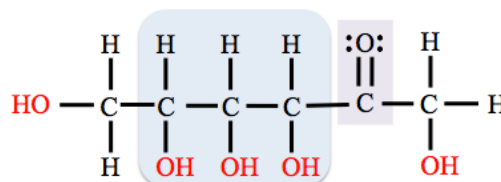
a ketose structure where X = 3

Understanding Check:

Classify each of the following monosaccharides as either an *aldose* or a *ketose*

a.

b.

c.

2
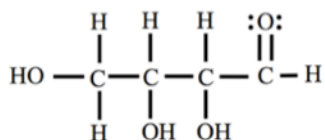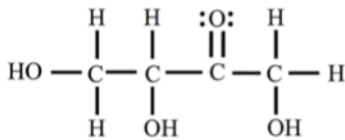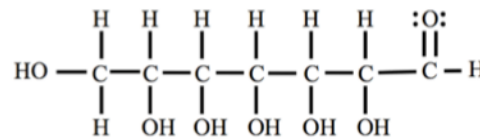
Monosaccharides can be classified according to the **number of** _____ they contain.

Number of Carbons	Classification
3	triose
4	tetrose
5	pentose
6	hexose
7	heptose

A monosaccharide may also be classified by _____ the number of carbons _____ whether it is an **aldose** or a **ketose**.

- This is done by using the prefix "_____" for aldoses, or "_____" for ketoses, in front of "triose," "tetrose," "pentose," "hexose," or "heptose."

  - For example, an **aldose** that contains **five** carbons is an **aldopentose**.

an aldopentose
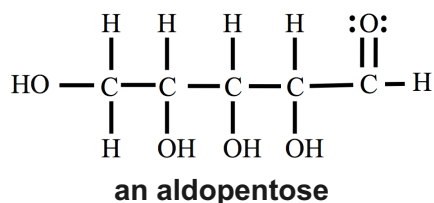
Understanding Check:

Classify each of the following monosaccharides using the prefix "aldo" for aldoses, or "keto" for ketose, in front of " triose," "tetrose," "pentose," "hexose," or "heptose."

a.
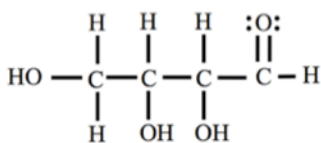
b.
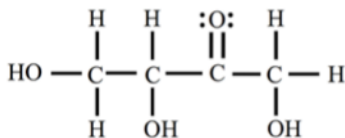
c.
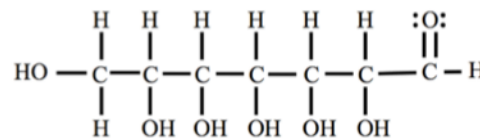
Stereochemistry of Monosaccharides

Except for the *ketotriose*, **monosaccharides** contain ____ _____ *one chiral carbon*.

Recall, that a chiral carbon is a carbon that is surrounded by *four **different** groups*.

Molecules with just **one** chiral carbon have a pair of **geometric isomers** called **enantiomers**.

Enantiomers have the same atomic connections, but a different three-dimensional arrangement of atoms, and are **nonsuperimposable mirror images** of each other.

If a molecule has _____ **than one** *chiral carbon*, then it will have **more than one** pair of enantiomers.

If a monosaccharide has **n** chiral carbons, then it will have 2^n stereoisomers. For example, if a molecule has **three** chiral carbons, then it will have $2^3 = (2 \times 2 \times 2) =$ **8** stereoisomers (**four** pairs of enantiomers).

Nonsuperimposable Mirror Images: *Enantiomers*

3
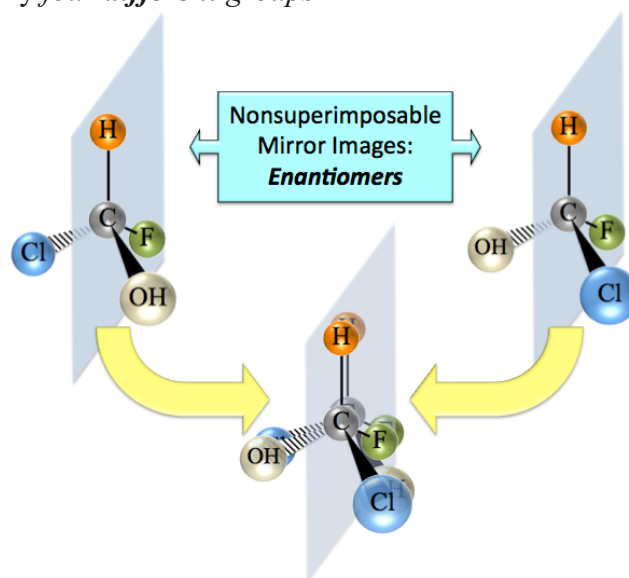
Example: How many stereoisomers are possible for the monosaccharide shown below?
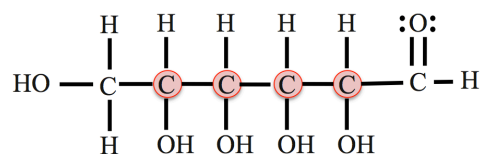
Solution: Identify the number of *chiral carbons*, and then calculate the number of stereoisomers.

- There are *four* chiral carbons in this molecule. The chiral carbons are highlighted in the structure below.

Since this monosaccharide structure has *four* chiral carbons, there are $2^4 = (2 \times 2 \times 2 \times 2) = $ **16 possible stereoisomers (*eight pairs of enantiomers*).**

We found that there are **16** different molecules (stereoisomers) that share this molecular formula **and** structural formula.

Most of the physical properties of these **16** stereoisomers are quite similar; however, the way they each behave in _____ *systems* can be very _____.

Let's consider the three dimensional arrangement of the atoms in the smallest monosaccharide, *glyceraldehyde*. Glyceraldehyde has only _____ *chiral carbon*.
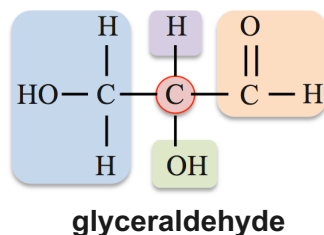
glyceraldehyde

Since there is *one* chiral carbon in glyceraldehyde, then there are $2^n = 2^1 = 2$ stereoisomers (one pair of enantiomers/nonsuperimposable mirror images).

**the pair of glyceraldehyde enantiomers
(nonsuperimposable mirror images)**
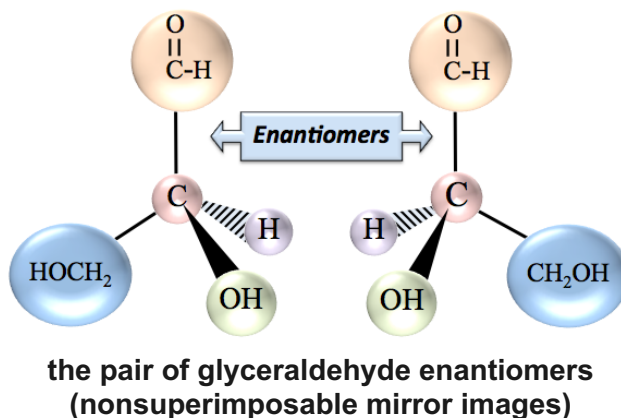
In order for professionals in healthcare, engineering, and science fields to discuss and depict the various monosaccharide stereoisomers, it is necessary to be able to draw two-dimensional (flat) structural formulas on a page or computer display, such that they still contain the ***three-dimensional information*** particular to each stereoisomer.

In previous chapters, we used the **wedge and dash system** to retain the three-dimensional information on a flat surface.

4

For monosaccharides, _____ _____ are used for this purpose.

Fischer Projections

Fisher projections are related to an imaginary "_____" that would be produced if a *chiral carbon* and its four bonded groups were placed in a *particular orientation* between a light source and a surface.

In Fischer projections, *chiral carbons are* _____ to *be at the* _____ *of a vertical and horizontal line*.

Fischer's choice of the particular orientation of the chiral carbon and its four groups was arbitrary, *any* orientation could have been used; *however*, for consistency, one specific orientation needed to be chosen.

The chosen orientation of a chiral carbon and the four groups that are bonded to it *relative to the drawing surface/page in all Fischer Projections* is as follows:

The *bonds* from the *chiral carbon* to the _____ *carbon* atoms *point at a downward angle*, and their shadows form _____ *lines* on the Fischer projection.

- In this model, these are the bonds from the *chiral carbon* to groups **Y** and **W**.

The *bonds* from the *chiral carbon* to *the* _____ *carbon groups point at an upward angle*, and their shadows form _____ *lines* on the Fischer projection.

- In this model, these are the bonds from the *chiral carbon* to groups **X** and **Z**.

For *aldoses*, the *aldehyde group* is positioned at the end of the molecule that is closest to the top of the page (position **W**).

For *ketoses*, the *carbonyl carbon* is positioned as close as possible to the end molecule that is nearest the top of the page.

5
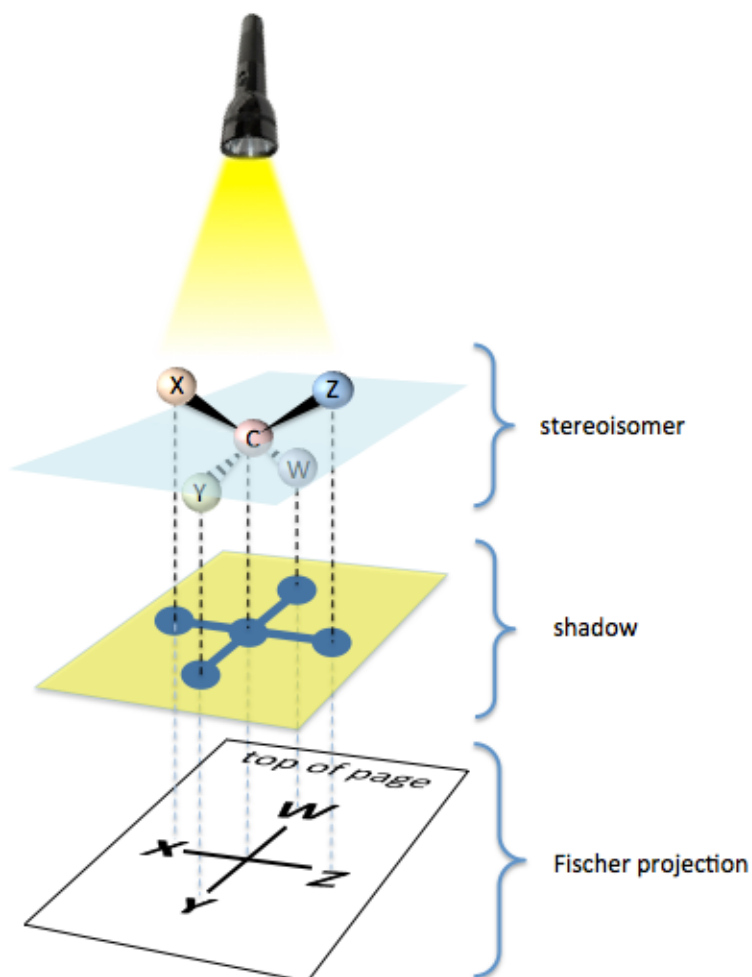
Let's consider the **Fischer projections** for both of the *glyceraldehyde* stereoisomers.

Recall that *glyceraldehyde* has **one chiral carbon**.

Because the **other two carbons** in *glyceraldehyde* are **not chiral**, shorthand notation is used to simplify the structure.

glyceraldehyde

The *aldehyde group* is represented by "**CHO.**"
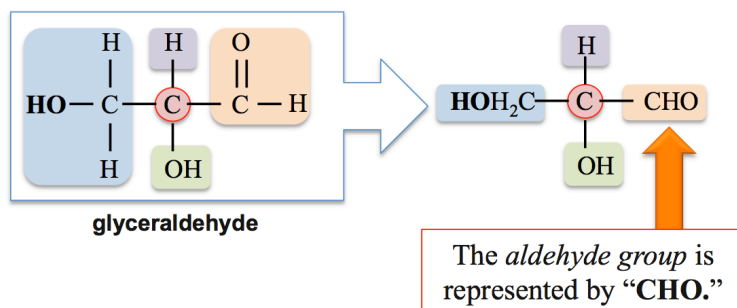
The derivation for the Fischer projections of glyceraldehyde's enantiomers is illustrated below.
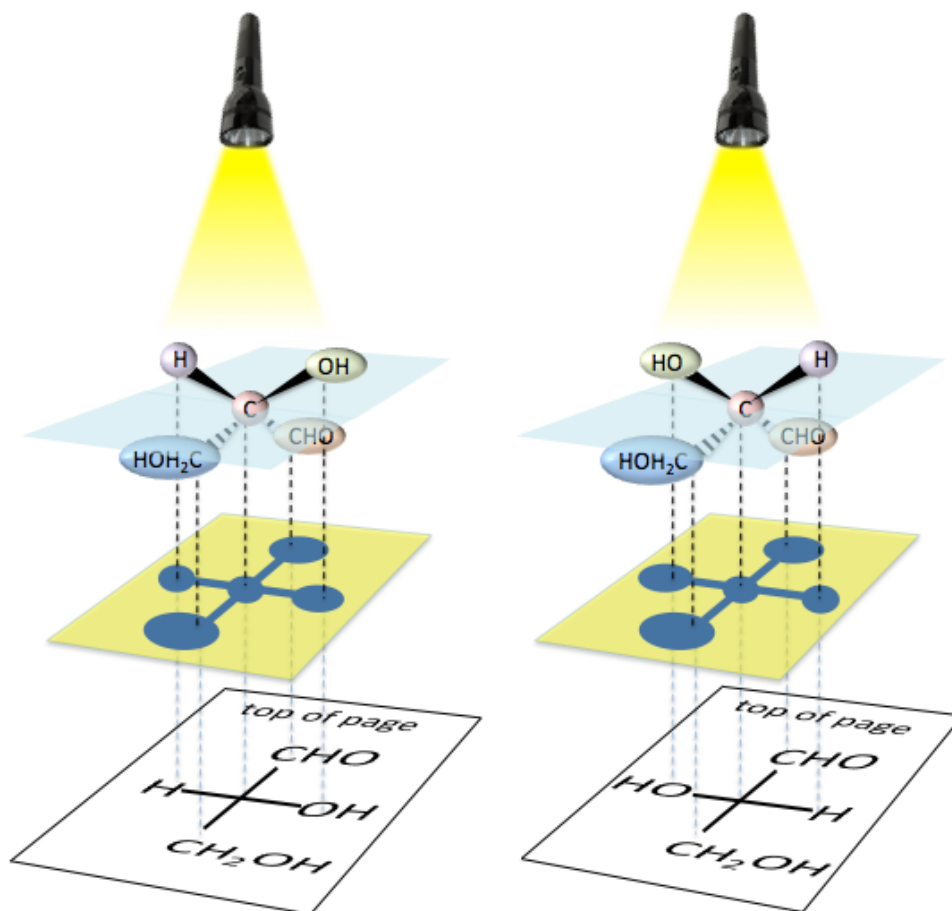
The Fischer projections for the two enantiomers of glyceraldehyde are:
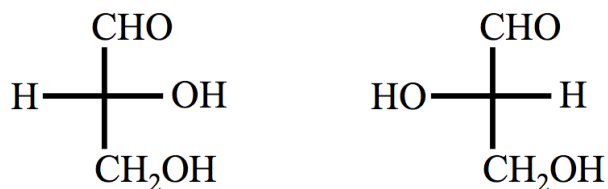
We do not need to draw the bonds around the top or bottom carbon atoms because they are **not chiral**.

Note that we draw the hydroxyl groups that are on the **left-hand side** of Fischer projections as "**HO.**"

6

For monosaccharides with ***more than one*** chiral carbon, Fischer projections must be drawn (or interpreted) by considering the orientation around _____ of the ***chiral carbons***.

This is done one chiral carbon at a time. As an example, let's consider aldotetroses, which contain ***two chiral carbons***:
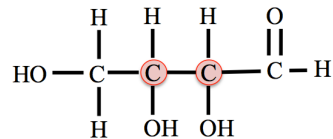
an aldotetrose

Since aldotetroses each have ***two*** chiral carbons, there are $2^2 = (2 \times 2) = $ **4 stereoisomers (*two pairs of enantiomers*).**
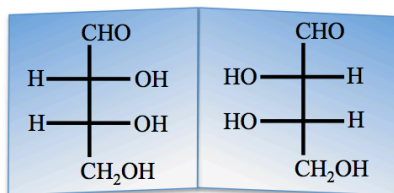
an enantiomer pair
(mirror images)
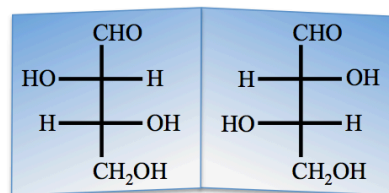
an enantiomer pair
(mirror images)

Note that the hydrogen (**H**) and the hydroxyl group (**OH**) positions are reversed on chiral carbons for each particular enantiomer pair.

Implication of a Fischer Projection:

Wedge and Dash Representation

Fischer Projection
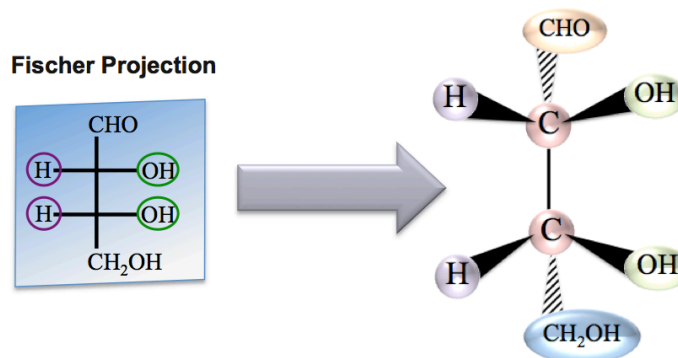
Understanding Check: An aldopentose contains ***three chiral carbons***, and therefore there are $2^3 = 8$ aldopentose stereoisomers. Draw Fischer projections of the ***eight*** stereoisomers.

D- and L- Designations for Monosaccharides

Carbohydrates are most often referred to by their *common names*, all of which use the "_____" suffix.

- A *common name* is assigned to each pair of enantiomers.

In order to differentiate the *two* individual monosaccharides of an enantiomer pair, 'D-' or 'L-' designations are used with the common name.

- The 'L-' designation is used for the enantiomer in which **the *chiral carbon* that is furthest from the top of the Fischer projection** has its _____ *group* on the _____.

- The 'D-' designation is used for the _____ *enantiomer* of the pair.

D-erythrose   L-erythrose
(an enantiomer pair)

D-threose   L-threose
(an enantiomer pair)
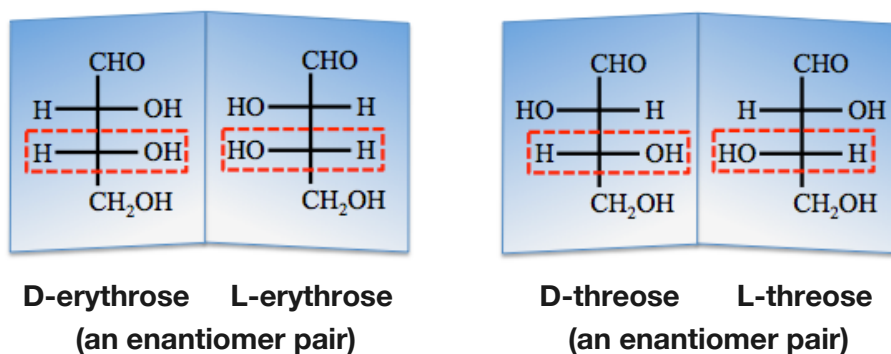
Monosaccharides with the **L-** designation are sometimes referred to as "**L-sugars**," and those with the **D-** designation are sometimes referred to as "**D-sugars**."

Monosaccharides are produced in living organisms by chemical reactions, some of which require enzymes that can only produce _____ particular enantiomer.

For example, the stereoisomer of *glucose* that is made in photosynthesis is **D-glucose**.

Fischer projections for both of the glucose enantiomers are shown below.

Dashed boxes are shown around the chiral carbons and hydroxyl groups responsible for the **D-** and **L-** designations.

D-glucose   L-glucose
(an enantiomer pair)
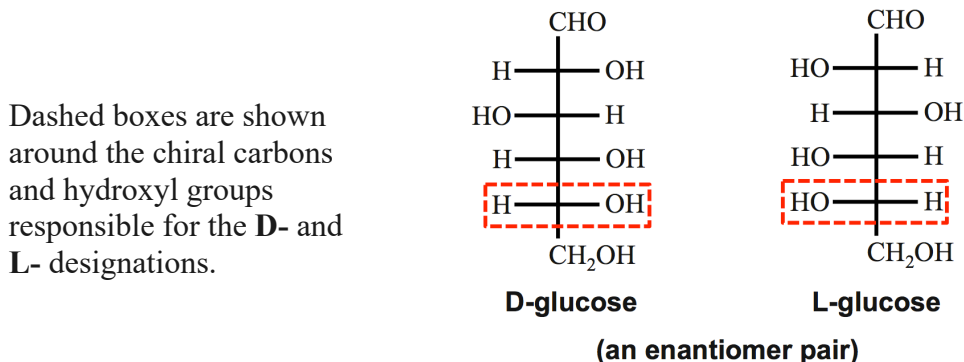
The glucose enantiomer pair (D-glucose and L-glucose) are *two* of the *sixteen* aldohexose stereoisomers.

- There are *seven* more aldohexose enantiomer pairs that can be drawn by varying the positions of the **H** and **OH** on each side of a Fischer projection.

- These seven other *enantiomer pairs* are differentiated from glucose, and each other, by their *common names*.

I *do not* require my students to memorize the common names and structures for particular monosaccharides, however, you should check with your own instructor to see if you are required to do so.

8

An example of a _____ is **fructose**. **D-Fructose** is one of our major dietary carbohydrates.

```
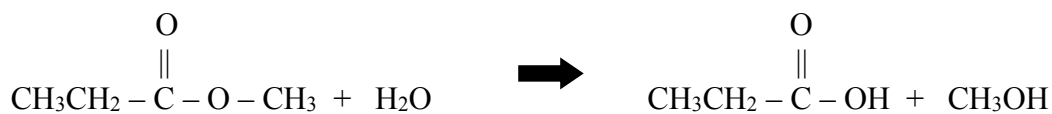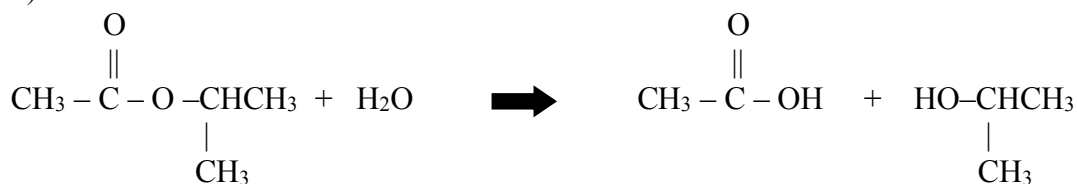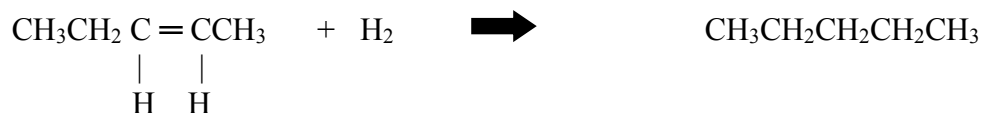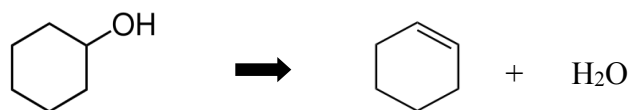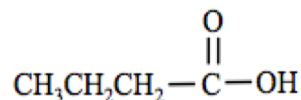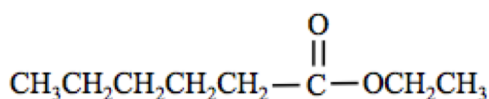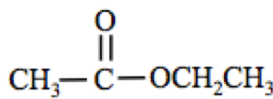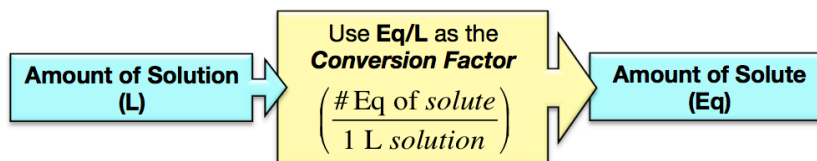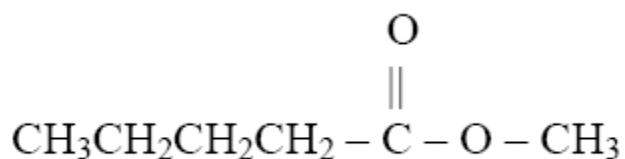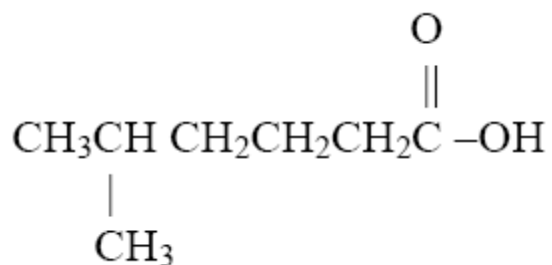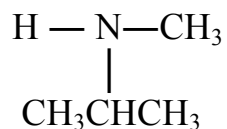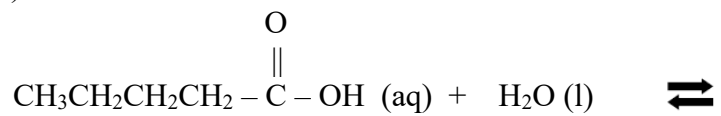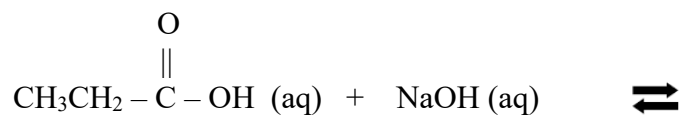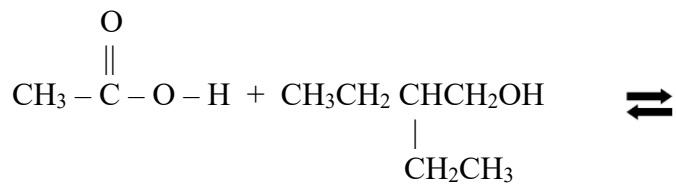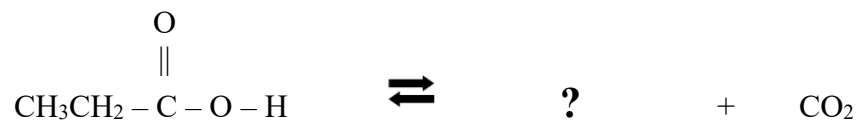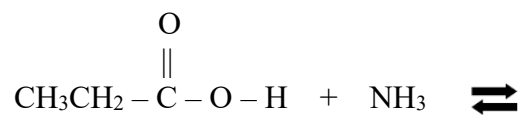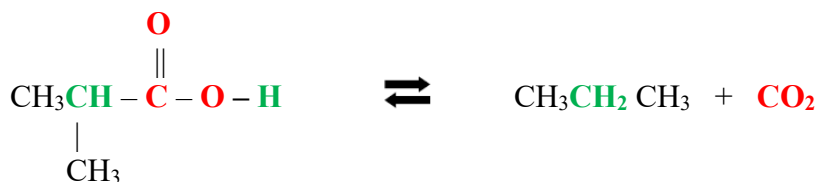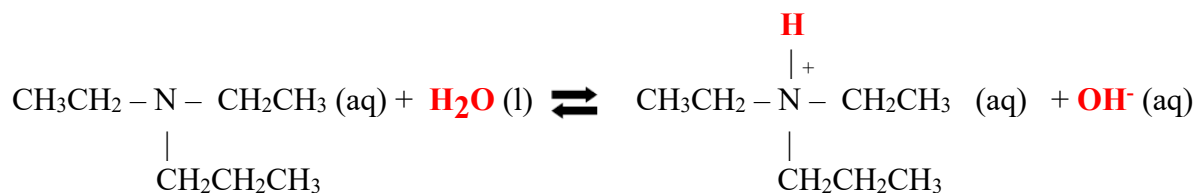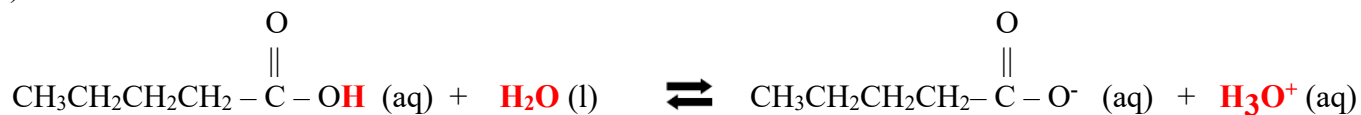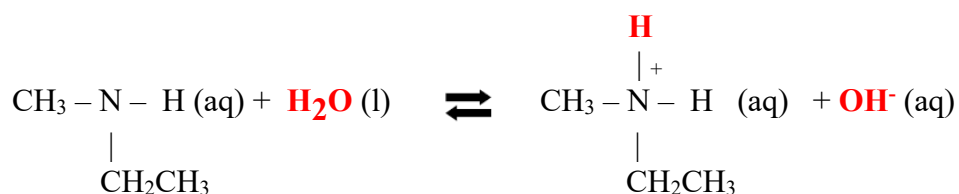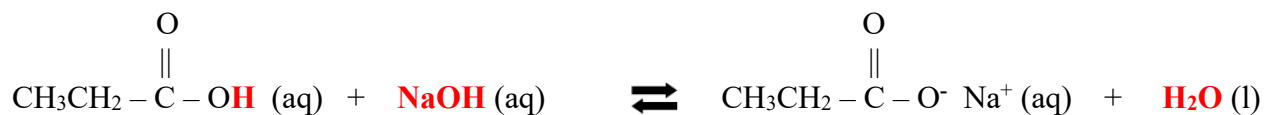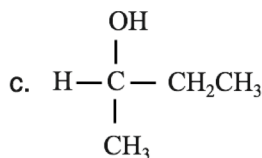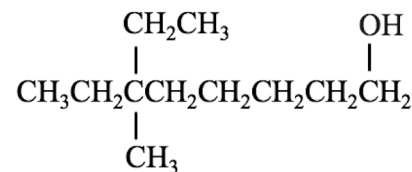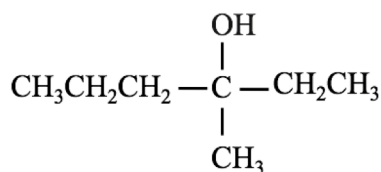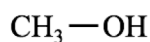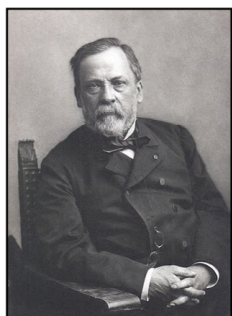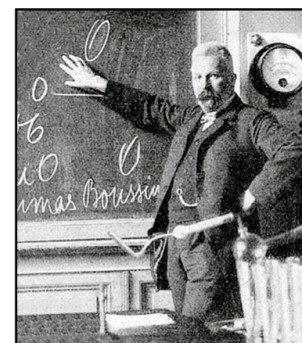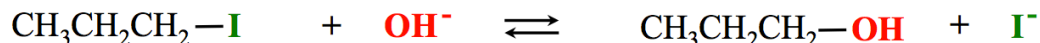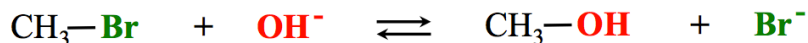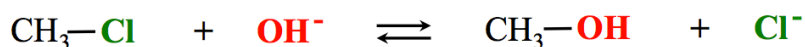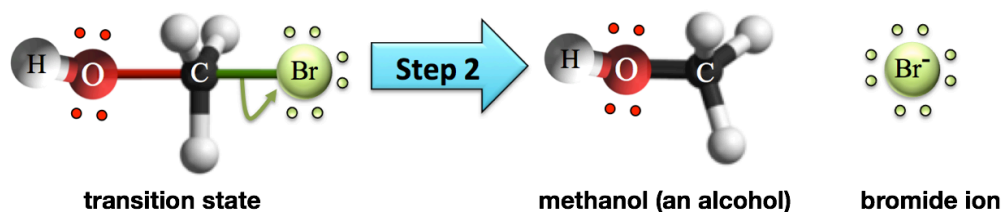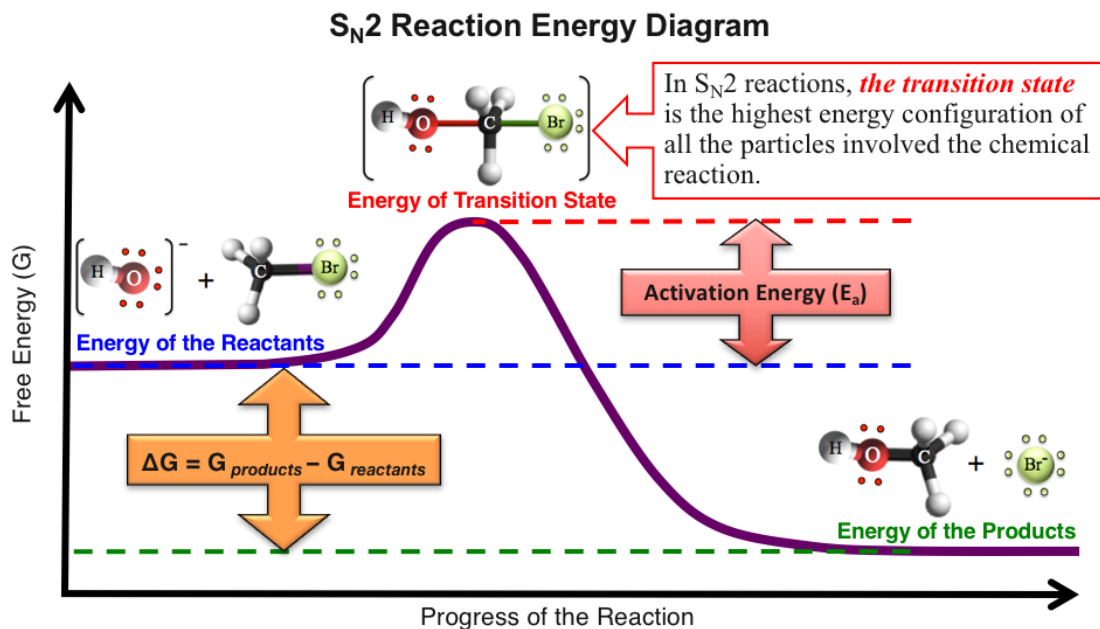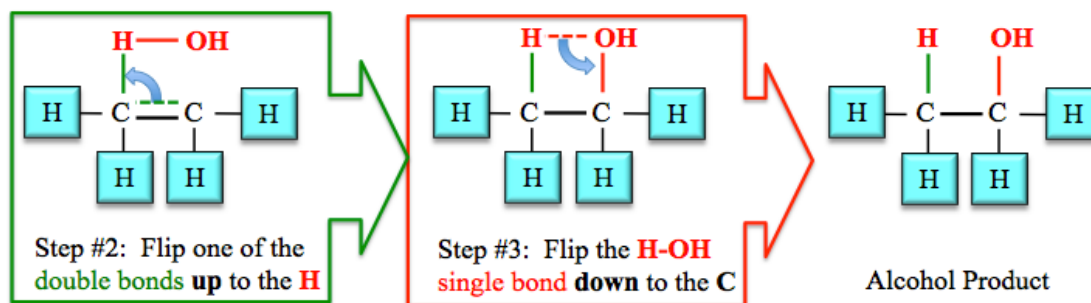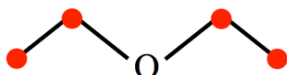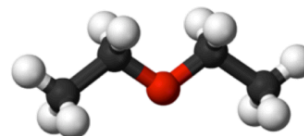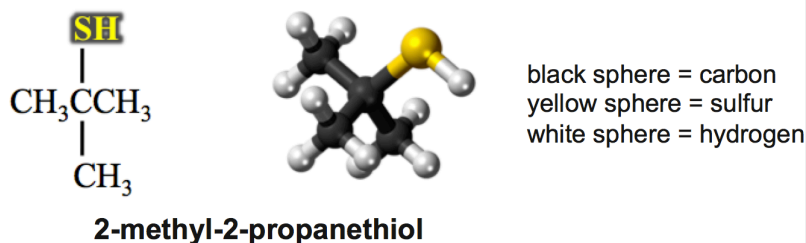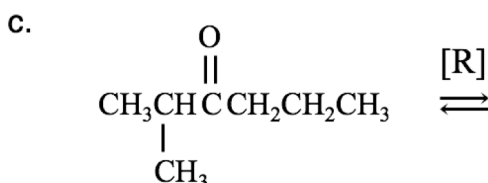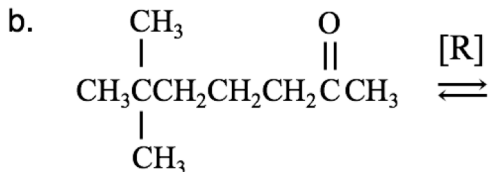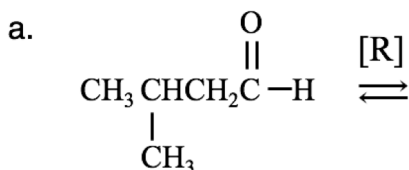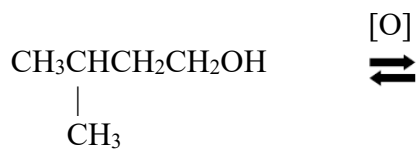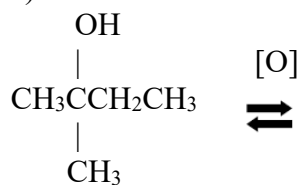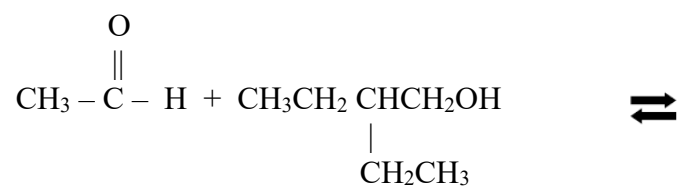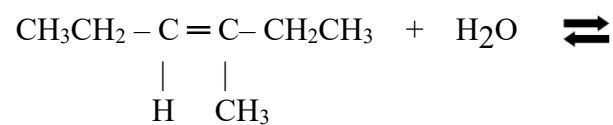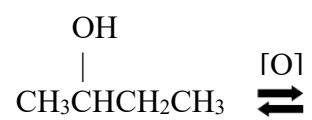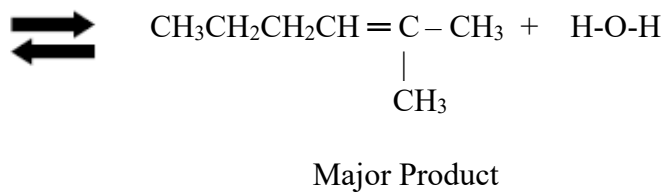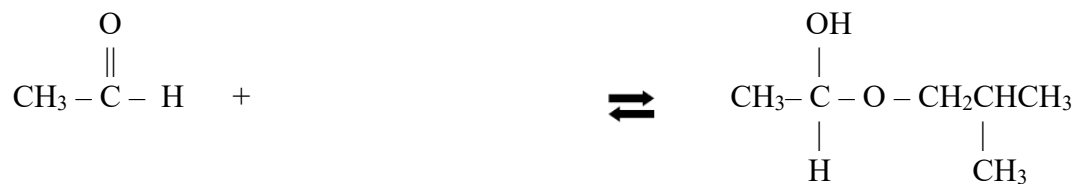        CH2OH              CH2OH
        C=O                C=O
  HO ——— H            H ——— OH
   H ——— OH          HO ——— H
   H ——— OH          HO ——— H
        CH2OH              CH2OH

      D-fructose         L-fructose
```

(an enantiomer pair)
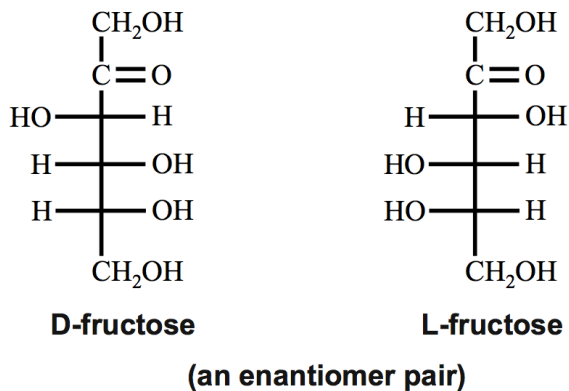
Understanding Check
Classify each of the eight stereoisomers shown below as either **D-** or **L-** stereoisomers.

```
      CHO                CHO                CHO                CHO
 H ——— OH          HO ——— H          HO ——— H           H ——— OH
 H ——— OH          HO ——— H           H ——— OH          HO ——— H
 H ——— OH          HO ——— H           H ——— OH          HO ——— H
      CH2OH              CH2OH              CH2OH              CH2OH
```

```
      CHO                CHO                CHO                CHO
HO ——— H            H ——— OH           H ——— OH          HO ——— H
HO ——— H            H ——— OH          HO ——— H           H ——— OH
 H ——— OH          HO ——— H           H ——— OH          HO ——— H
      CH2OH              CH2OH              CH2OH              CH2OH
```
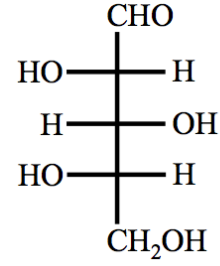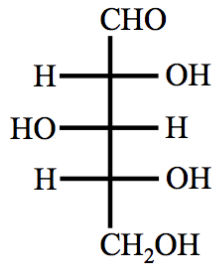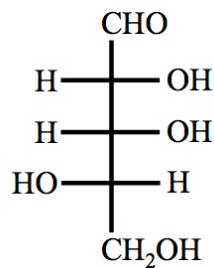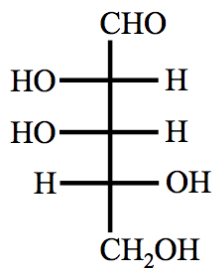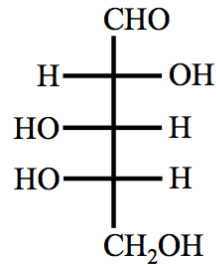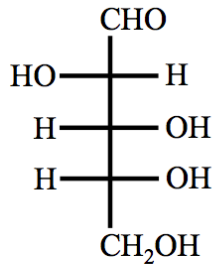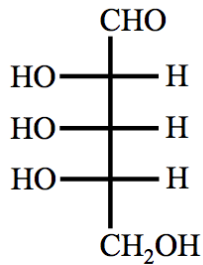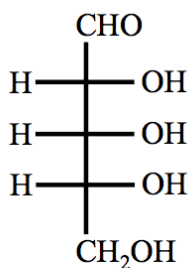
The Cyclic Forms of Monosaccharides

When monosaccharides that contain five to seven carbons are in aqueous solutions, they can undergo a reaction in which they _____ their bonding pattern to form _____ *structures*.

It is a ***reversible*** reaction in which the _____ *form* is interconverted with the _____ *form*.

- **Example:** The *cyclization* rearrangement reaction is shown below for a **D-glucose** molecule.

D-glucose
Fischer projection
(open-chain form)

D-glucose
Haworth projection
(cyclic form)
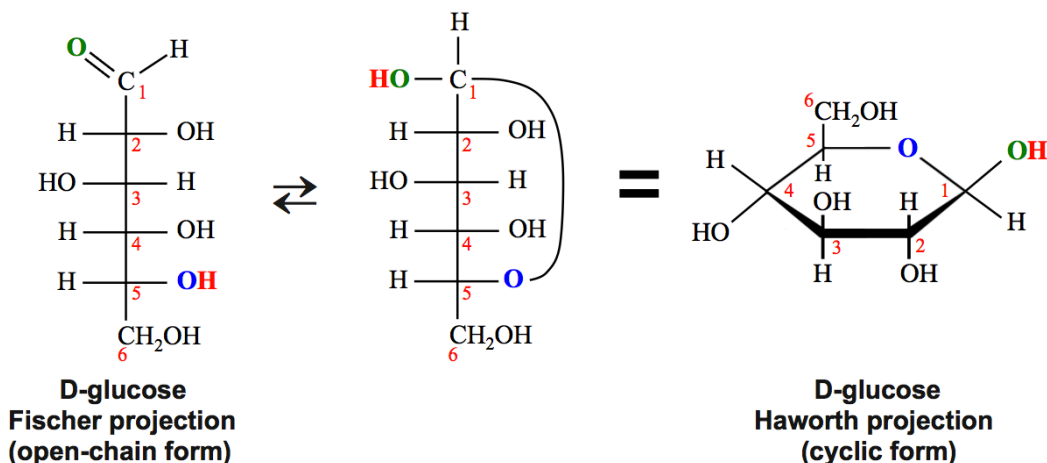
The ***cyclic form*** is *lower in energy* and is therefore the predominant form.

- In most solutions, the equilibrium ratio of ***cyclic form*** to ***open-chain form*** is about *one hundred* to *one*.

The *side view structures* of cyclic monosaccharides (above, right), are called _____ **projections** *or* **Haworth structures**.

- The carbon atoms that form the ring are not drawn explicitly, but are implied to occur where lines/bonds meet.

To help you understand the *three-dimensional* implications of Haworth projections, I have drawn a ball-and-stick model that shows the actual geometry/bond angles of the cyclic form of D-glucose, next to its Haworth Projection representation:

ball-and-stick model
(actual molecular geometry)

Haworth projection
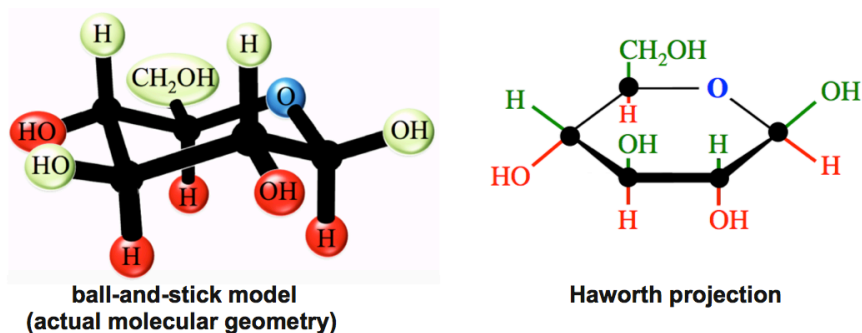
- I used large black dots at the ring-carbon positions in both structures.
- Each ring-carbon is bonded to **two** *other ring-atoms* ***and*** **two** *other groups*.
- Groups that are oriented ***upward*** relative to the ring-carbons are shaded ***green***.
- Groups that are oriented ***downward*** from ring-carbons are shaded ***red***.

The rearrangement/cyclization reaction of a monosaccharide is actually a form of the **hemiacetal formation** reaction that you learned about at the end of the previous chapter.

Let's take a moment to review that reaction.

A *hemiacetal* is a molecule that contains **both** an **OR** group *and* **OH** group that are bonded to the *same* carbon.
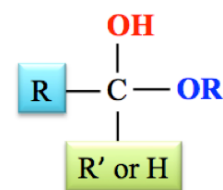
general form of a hemiacetal

An *aldehyde or a ketone* will react with an *alcohol* to form a **hemiacetal**.

The **OR"** from the *alcohol* forms a bond to the *carbonyl-carbon* of the aldehyde or ketone, the **H** from the *alcohol* bonds to the *carbonyl-oxygen*, and the carbonyl group's double bond is changed to a single bond.

aldehyde or ketone   alcohol   hemiacetal
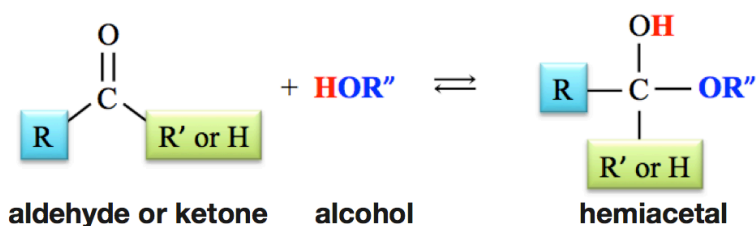
Now let's think about how this reaction can occur **for a monosaccharide.**

A *hemiacetal* is formed when a monosaccharide's *hydroxyl group* reacts with its *carbonyl group*.

D-glucose
(open-chain form, drawn curved)

D-glucose
(cyclic form)
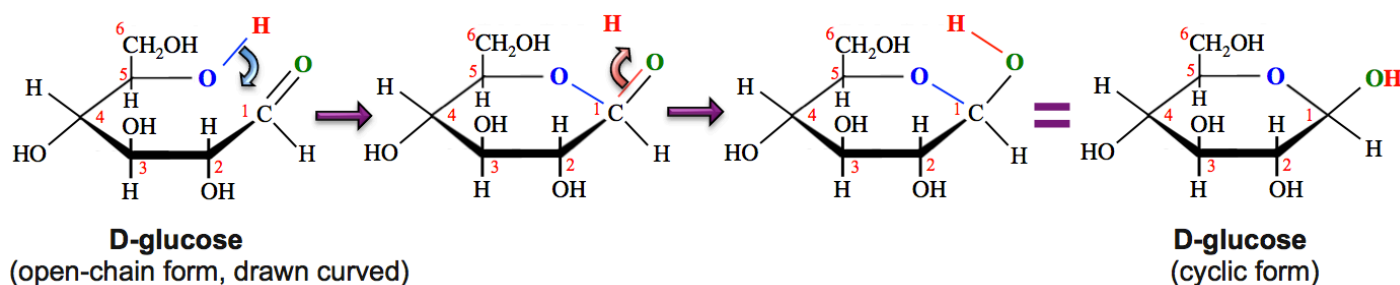
- The *hydroxyl group* is added "across" the carbonyl double bond.

D-glucose
(cyclic form)
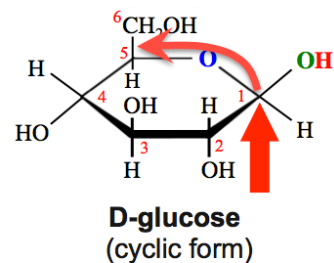
Note that, beginning at carbon number **1** and moving *counter-clockwise*, as indicated by the **red arrow**, the **OR** bonding pattern is seen.

When the **OR** bonding pattern occurs in this way, *forming a ring*, the

molecule is referred to as a _____ *hemiacetal.*
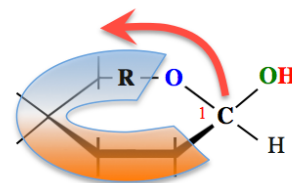
An example of the cyclization of a **ketose** (*fructose*) is shown below.

D-fructose
Fischer projection
(open-chain form)

D-fructose
Haworth projection
(cyclic form)
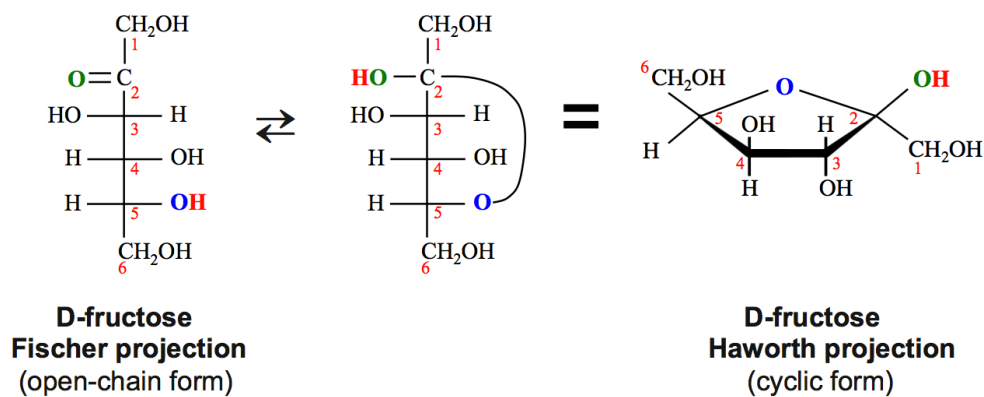
The most common cyclic monosaccharide structures are _____ and _____ member rings.

Cyclic monosaccharides with five-member rings are called _____, and those with six-member rings are called _____.

- These terms are often used as *suffixes* when naming cyclic monosaccharide structures.

    - **Examples:**

A six-member ring

A five-member ring

D-glucopyranose
(a pyranose)

D-fructofuranose
(a furanose)

12
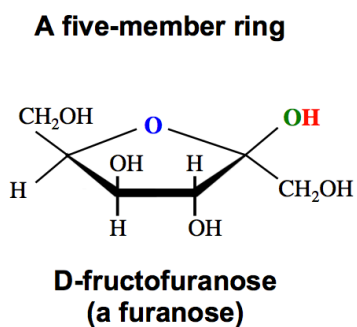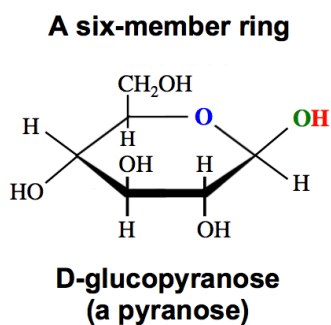
The cyclization reaction is reversible; the *cyclic form* interconverts with the *open-chain form* when monosaccharides are in _____.

Each time that the *open-chain form* is converted to the *cyclic form*, one of two cyclic **enantiomers** will be formed.

- **Example:** The *cyclization* of D-glucose.

Rotation of the Aldehyde Group

Caused by rotation around the bond between carbon **1** and carbon **2**.

D-glucose
(open-chain form)

D-glucose
(open-chain form)

β-D-glucopyranose
(cyclic form)

**Enantiomers
(a cyclic enantiomer pair)**

α-D-glucopyranose
(cyclic form)
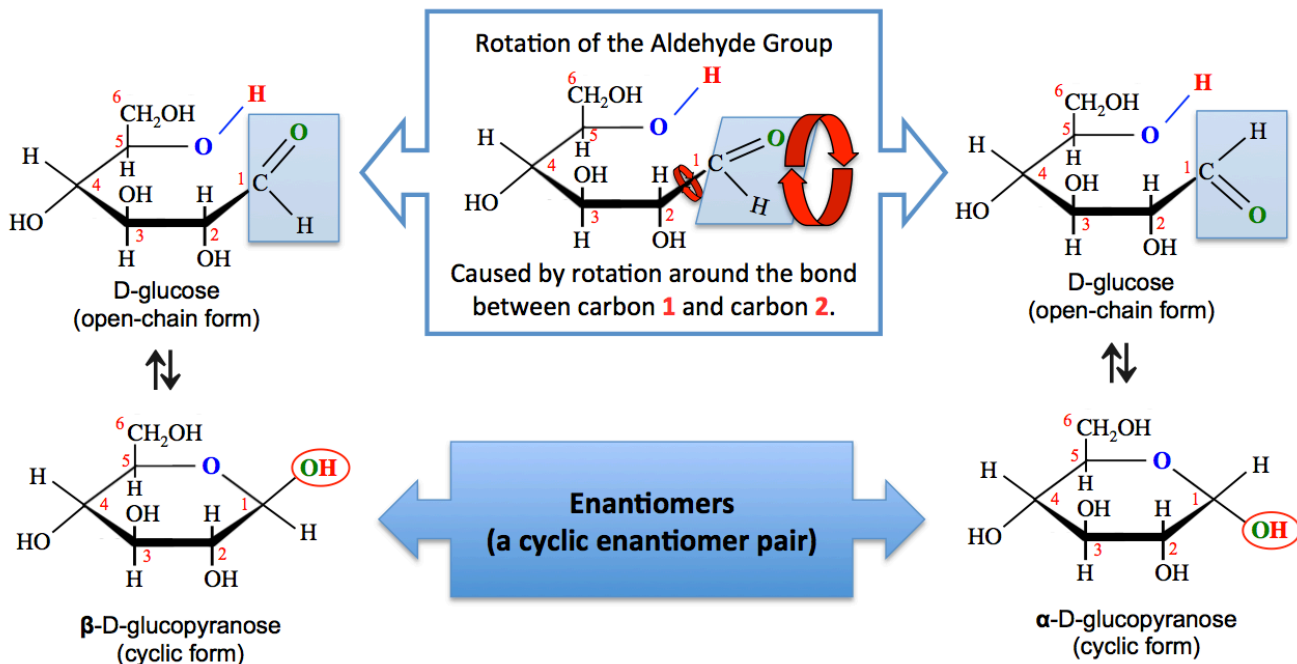
In the open-chain form of D-glucose that is shown in **top-left** of the illustration above, the carbonyl group (**C=O**) is oriented **upward** from the ring; therefore, when the *cyclic hemiacetal* is formed (**bottom, left**), the *new* hydroxyl group (**OH**) will be oriented **upward** from carbon number **1**. *Free rotation* occurs around single bonds in the open-chain form (as depicted in the box in the **top-middle** of the illustration). Rotation around the bond between carbon number **1** and carbon number **2** of the open-chain form causes the carbonyl group to, at times, be oriented **downward** from the ring (as seen in the open-chain form in the **top-right** of the illustration). In this arrangement, when the cyclization reaction occurs, the cyclic hemiacetal is formed with the *new* hydroxyl group (**OH**) oriented **downward** from carbon number **1** (as seen in the **bottom-right** structure of the illustration).

The formation of either of two different cyclic structures, **a *cyclic enantiomer pair*,** is possible because of the **four different groups** bonded to a ***chiral hemiacetal carbon*** (the carbon which contains an **OH** and an **OR**).

This carbon is called the _____ *carbon*.

The cyclic enantiomers are *almost identical*; the **only** difference is that the bonding pattern around the *anomeric carbons* are mirror images.

anomeric carbons

β-D-glucopyranose
(cyclic form)

**Enantiomers
(a cyclic enantiomer pair)**

α-D-glucopyranose
(cyclic form)

13
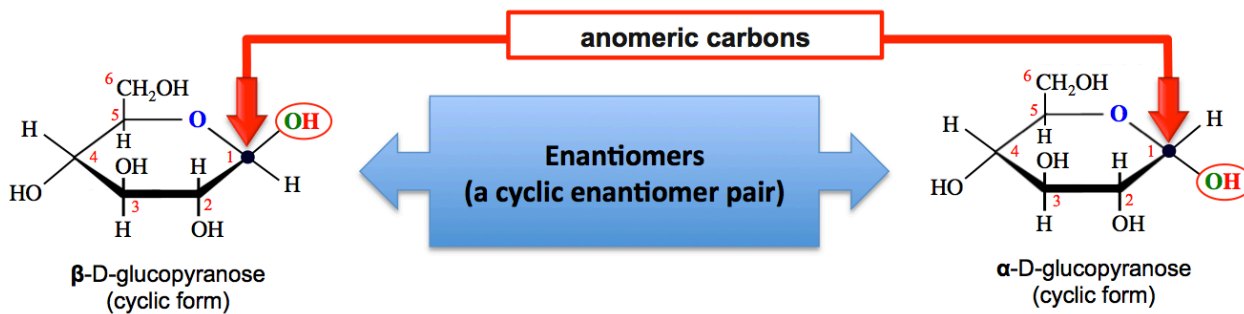
The sugar produced in photosynthesis, and almost all of the other monosaccharides found in plants and animals, are **D-sugars**. At some point in the history of Earth, nature showed a preference for **D-sugars**.

For the *remainder of this course*, you will only see **D-sugars**.

It is easy to identify the *anomeric carbon* in a Haworth projection of a D-sugar; it is the ring-carbon to the _____-*hand side* of the *ring-*_____.

The two enantiomers that can be formed during the cyclization process are called _____.

They are classified, based on the orientation of the _____ *group* (**OH**) on the *anomeric carbon*, as the **α-anomer** or the **β-anomer**.

- The **α-anomer** has the **OH** on the anomeric carbon oriented _____ from the ring.
- The **β-anomer** has the **OH** on the anomeric carbon oriented _____ from the ring.

β-anomer
β-D-glucopyranose
(cyclic form)

anomeric carbons

Anomers

α-anomer
α-D-glucopyranose
(cyclic form)
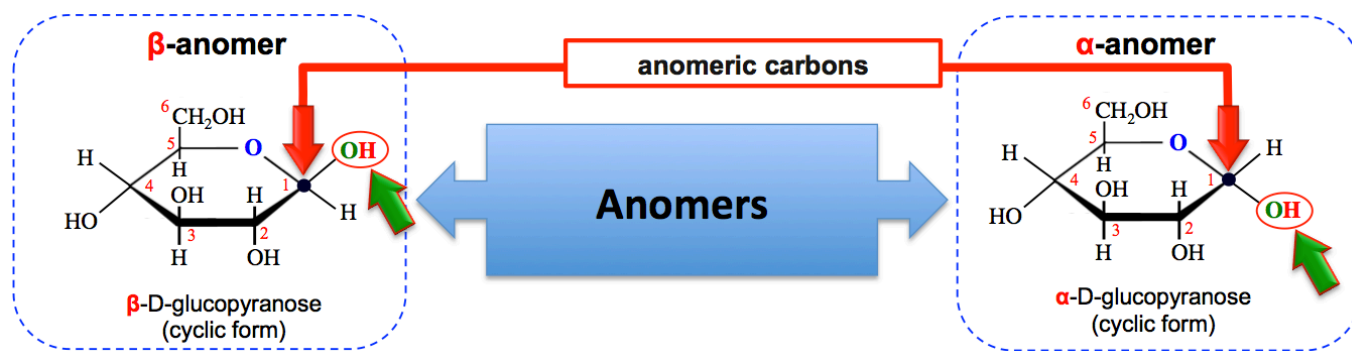
The conversion from **α-anomer**, to the ***open-chain form***, then to the **β-anomer** (and vice versa) is called _____.

The formation of **β-anomers** or **α-anomers** also occurs, for the same reason, for **ketoses**.

- For example, the cyclization of *D-fructose* results in the formation of two possible **anomers**, as shown below.

anomeric carbons

β-anomer
(**β-D-fructofuranose**)

α-anomer
(**α-D-fructofuranose**)
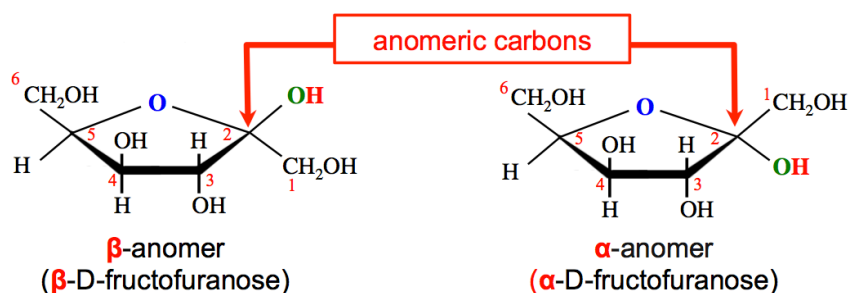
Understanding Check: For the molecules shown below,
   a) Classify each of the molecules as either a **pyranose** *or* a **furanose**.
   b) Label the **anomeric carbon**.
   c) Classify each as either a **β-anomer** *or* an **α-anomer**.

14
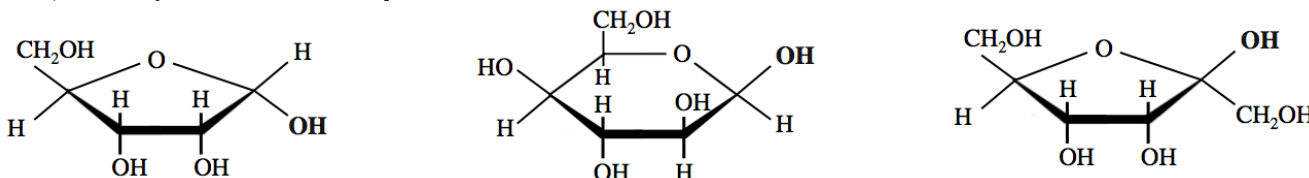
I would like you to be able to do the following on an examination:

Given a **Haworth projection** of a **D-**monosaccharide:

1. Identify the molecule as a **pyranose** or a **furanose**.
2. Identify the **anomeric** carbon.
3. Identify the molecule as the **β-anomer** or the **α-anomer**.
4. Understand the definition of **mutarotation**.
5. Understand how the three-dimensional arrangement of atoms in a monosaccharide (as seen in a ball-and-stick model) is implied by a **Haworth projection**.

Summary of Monosaccharides Stereochemistry

Monosaccharide Stereochemistry	
open-chain form	**cyclic form**
In the Fischer projection, the OH on the chiral carbon that is furthest from the carbonyl group is *on the right*: **D-Sugar**	In the Haworth projection, the OH on the anomeric carbon is oriented *downward from the ring*: **α-anomer**
In the Fischer projection, the OH on the chiral carbon that is furthest from the carbonyl group is *on the left*: **L-Sugar**	In the Haworth projection, the OH on the anomeric carbon is oriented *upward from the ring*: **β-anomer**

Monosaccharide Derivatives and Reactions

Monosaccharide derivatives are compounds that are _____ from monosaccharides.

I will introduce you to *four* classes of monosaccharide derivatives:

1) **Amino Sugars**
2) **Carboxylic Acid Sugars**
3) **Alcohol Sugars**
4) **Deoxy Sugars**

Amino Sugars

In an **amino sugar**, a hydroxyl group (**OH**) of a monosaccharide has been replaced by an _____ *group* (**NH₂**).

An example of an amino sugar is **D-glucosamine**. *D-Glucosamine* is derived when the hydroxyl group on carbon number **2** of *D-glucose* is replaced by an *amino group*.
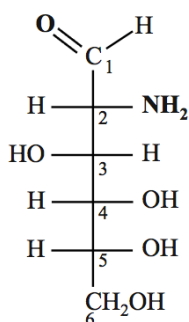
open-chain D-glucosamine

Like monosaccharides, *amino sugars* undergo *mutarotation*.
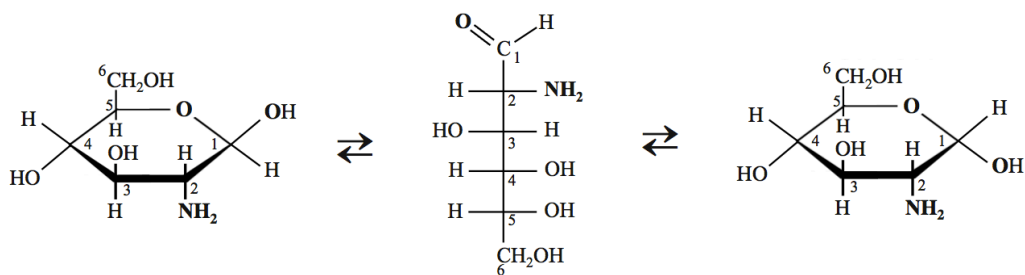
β-D-glucosamine   **open-chain D-glucosamine**   **α-D-glucosamine**

D-Glucosamine of the larger monosaccharide-containing polymers that make up the exoskeletons of crustaceans (e.g. shrimp, lobster, crab) and other arthropods. D-glucosamine is purified for commercial use by processing exoskeletons or other organic material that contains it. Although it has been deemed safe for human consumption and sold as a "dietary supplement," its *actual effectiveness* in the treatment of any health/medical condition, according to the US National Institutes of Health, *has not been established*.

Carboxylic Acid Sugars

In a **carboxylic acid sugar**, an aldehyde group (**CHO**) of a monosaccharide has been replaced by a _____ *group* (**COOH**).

This is done by a reaction that you have previously seen, *oxidation* of *aldehydes* to *carboxylic acids*.

- **Example:** *D-glucose* can be **oxidized** to produce *D-gluconic acid*:

This *oxidation of aldoses* reaction was used for about 50 years in the measurement of blood sugar levels.

Stanley Benedict first discovered and published a method in which a solution containing Cu^{2+} ions acts as an oxidizing agent in the conversion of _____ to *carboxylic acid sugars*.

This solution is now referred to as _____ *reagent*.

It is used as a test for aldoses since it will oxidize the aldehyde groups *but* _____ the hydroxyl groups **or** the *ketone bonding patterns*.

Cu^{2+} ions appear clear-blue when in solution. If a sample that contains an *aldose* is placed in a test tube that contains hot Benedict's reagent, the Cu^{2+} will be reduced to Cu^{1+}. The Cu^{1+} then reacts with hydroxide to form a colored solid. As the aldose concentration in a sample increases, more of the colored solid is made and the color of the Benedict's test goes from blue to green to orange to red to brown. When a color change is observed, we say that it is a "positive" test.
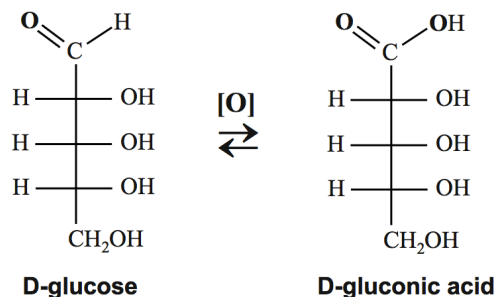
Exception: Although *fructose* is a **ketose** (*not an aldose*), it gives a positive Benedict's test result.

Sugars that produce a color change in Benedict's reagent are called "_____ _____," since they reduce Cu^{2+} to Cu^{1+}.

Because Benedict's reagent is *not specific* for D-glucose, which is the important blood sugar species in diabetes monitoring, its use in most medical diagnostic work has been replaced by glucometers. Glucometers are much more specific in sensing *only* D-glucose since they are based on a naturally-occurring enzyme which only catalyzes a reaction of D-glucose.

> **Understanding Check:** Draw the Fischer projection of the *carboxylic acid sugar* that is formed when the aldehyde group of D-ribose (shown below) is oxidized.
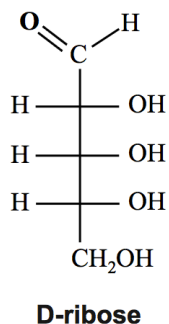
Alcohol Sugars

Alcohol sugars, sometimes called "***sugar alcohols***," are derived when the carbonyl group (**C=O**) of a monosaccharide is ***reduced*** to a _____ (OH) ***group***.

This is done by a reaction that you have previously seen, ***reduction*** of *aldehydes* and *ketones* to *alcohols*.

- Example of the reduction of a monosaccharide (*D-glucose*) to form an *alcohol sugar* (*sorbitol*):

D-glucose   **sorbitol**
                                  (an alcohol sugar)
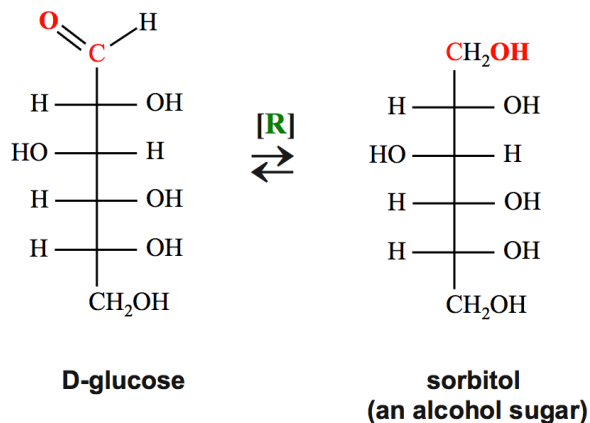
Alcohol sugars are used in the food and beverage industry as thickeners and sweeteners. Unlike sugars, alcohol sugars cannot be metabolized by oral bacteria, and therefore do not cause tooth decay. Unfortunately for chefs, alcohol sugars do not caramelize, as do natural sugars.

Sorbitol can be manufactured by the reduction of *D-glucose* and it also occurs naturally in pears, peaches, prunes, and apples. *Sorbitol* is used as a sugar substitute, mostly to replace natural sugars in order to prevent tooth decay. It is not so effective as a dietary aid because it can be metabolized by humans for energy. On a per gram basis, it provides 65% of the energy of natural sugars, yet is only 60% as sweet as table sugar (*sucrose*). *Sorbitol* is used in toothpaste, mouthwash, and chewing gum. It is also used, in greater quantities, as an orally or rectally administered laxative.

- Other examples of alcohol sugars are *mannitol* and *xylitol*:
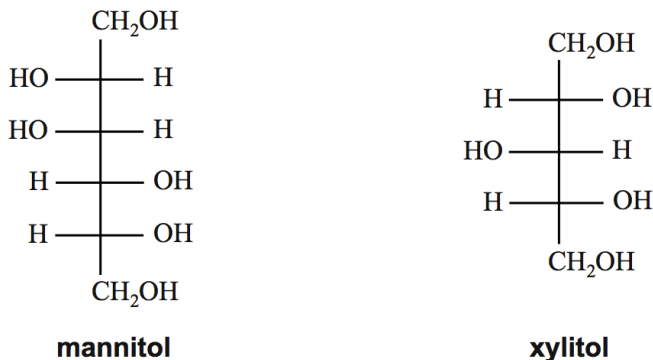
mannitol   **xylitol**

Mannitol is used as a sweetener and has many applications in medicine. It is frequently used as a filler in the production of tablets of medicine.

Xylitol is used as a sweetener in chewing gum. Like other alcohol sugars, it is unusable by oral bacteria. However, unlike the other alcohol sugars, *xylitol* aids in the recalcification of teeth.

Understanding Check: Draw the Fischer projection of the **alcohol sugar** that is formed when D-ribose (shown below) is **reduced**.
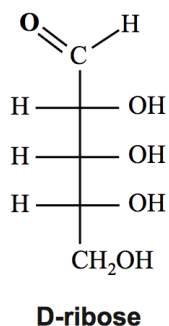
D-ribose

Deoxy Sugars

Deoxy sugars are derived when a hydroxyl group (OH) in a monosaccharide is replaced by a _____ *atom*.

- **Example:** D-*2-deoxyribose* (a deoxy sugar) is derived when the hydroxyl group on carbon number **2** of D-ribose (a monosaccharide) is replaced by a **hydrogen atom**:

D-ribose
(a monosaccharide)

D-2-deoxyribose
(a deoxy sugar)
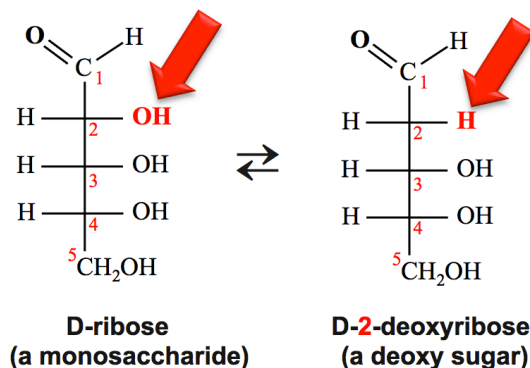
The "**2**" in D-**2**-deoxyribose indicates the carbon position where a hydrogen (**H**) replaces a hydroxyl group (**OH**) of the D-ribose monosaccharide.

Like monosaccharides, *deoxy sugars* undergo *mutarotation*.

α-D-2-deoxyribofuranose

D-2-deoxyribose
(a deoxy sugar)

β-D-2-deoxyribofuranose
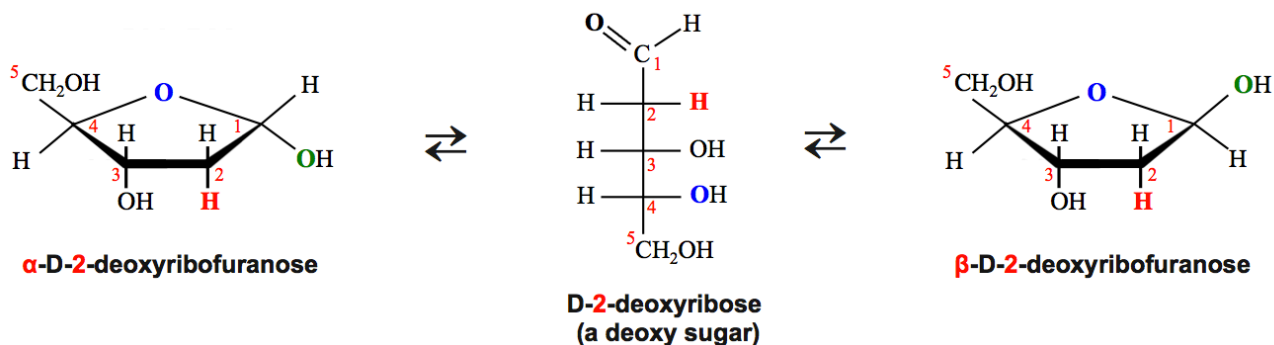
D-**2**-deoxyribofuranose is one of the residues that make deoxyribonucleic acids (DNA).

Understanding Check

D-2-deoxyglucose is currently being used in the development of anticancer strategies.

Using the Fischer projection of **D-glucose** (shown below) as the *starting point*, draw the **Fischer projection** of D-2-deoxyglucose.

$$\begin{array}{c}
O = C_1 - H \\
H - C_2 - OH \\
HO - C_3 - H \\
H - C_4 - OH \\
H - C_5 - OH \\
CH_2OH \; (6)
\end{array}$$

D-glucose
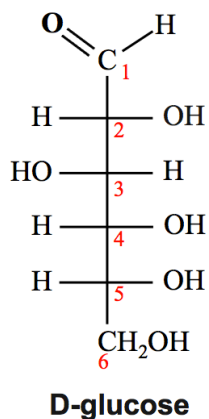
Table for the Review of Monosaccharide Derivatives

Monosaccharide Derivative	Defining Structural Trait
Amino Sugar	A hydroxyl group (OH) of a monosaccharide is replaced by an amino group (NH_2)
Carboxylic Acid Sugar	The aldehyde group (CHO) of an aldose is oxidized to a carboxyl group $(COOH)$.
Alcohol Sugar	The carbonyl group $(C=O)$ of a monosaccharide is reduced to a hydroxyl (OH) group
Deoxy Sugar	A hydroxyl group (OH) of a monosaccharide is replaced by a hydrogen.

Understanding Check:

Identify each of the molecules shown below as either a monosaccharide, amino sugar, carboxylic acid sugar, alcohol sugar, or a deoxy sugar.
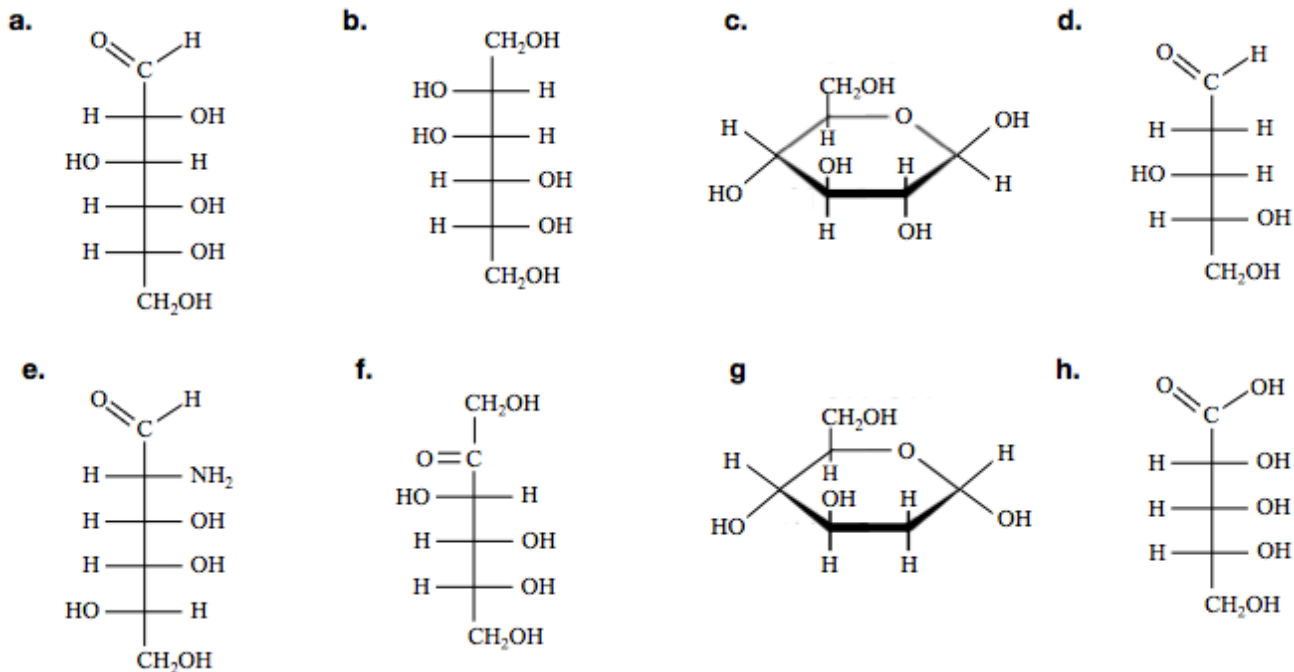
a.

$O=C-H$
$H-OH$
$HO-H$
$H-OH$
$H-OH$
CH_2OH

b.

CH_2OH
$HO-H$
$HO-H$
$H-OH$
$H-OH$
CH_2OH

c.

(cyclic structure: CH_2OH, OH, H, H, OH, HO, H, OH)

d.

$O=C-H$
$H-H$
$HO-H$
$H-OH$
CH_2OH

e.

$O=C-H$
$H-NH_2$
$H-OH$
$H-OH$
$HO-H$
CH_2OH

f.

CH_2OH
$O=C$
$HO-H$
$H-OH$
$H-OH$
CH_2OH

g

(cyclic structure: CH_2OH, H, H, OH, H, OH, HO, H, OH)

h.

$O=C-OH$
$H-OH$
$H-OH$
$H-OH$
CH_2OH

Carbohydrates can be classified into three major groups based on their size:

1) **monosaccharides**

2) **oligosaccharides**

3) **polysaccharides**

Oligosaccharides

Oligosaccharides are molecules that are made when _____ to _____ *monosaccharides* chemically bond to each other.

Molecules from particular organic families (such as monosaccharides) are referred to as "_____" when they bond together to form a large molecule.

Oligosaccharides are often subcategorized by the number of monosaccharide *residues* that they contain.

- For example, an oligosaccharide that is composed of *two* monosaccharide *residues* is called a

  _____.

- Likewise, an oligosaccharide made from *three* monosaccharide *residues* is called a

  _____.

Let's consider the bond formed between two **α-D-glucose** monosaccharides.

I will sometimes use **large black dots** at the position of the *anomeric carbons* in order to draw your attention to them.

α-D-glucose   **α-D-glucose**

Step 1: An **H** atom is removed from the hydroxyl group (**OH**) *that is bonded to the anomeric carbon* of the left-most residue, and an **OH** is removed from *any carbon* in the right-most residue.

- The **H** and **OH** that were removed form a water molecule.

Step 1

Step 2: Draw a *new bond* from the oxygen (**O**) that remains on the *anomeric carbon* in the left-most residue **to the** carbon from which the **OH** was removed in the right-most residue.

- This *new bond* is oriented in the same direction as *was* the bond to **OH** that was removed.

Step 2

maltose (a disaccharide)
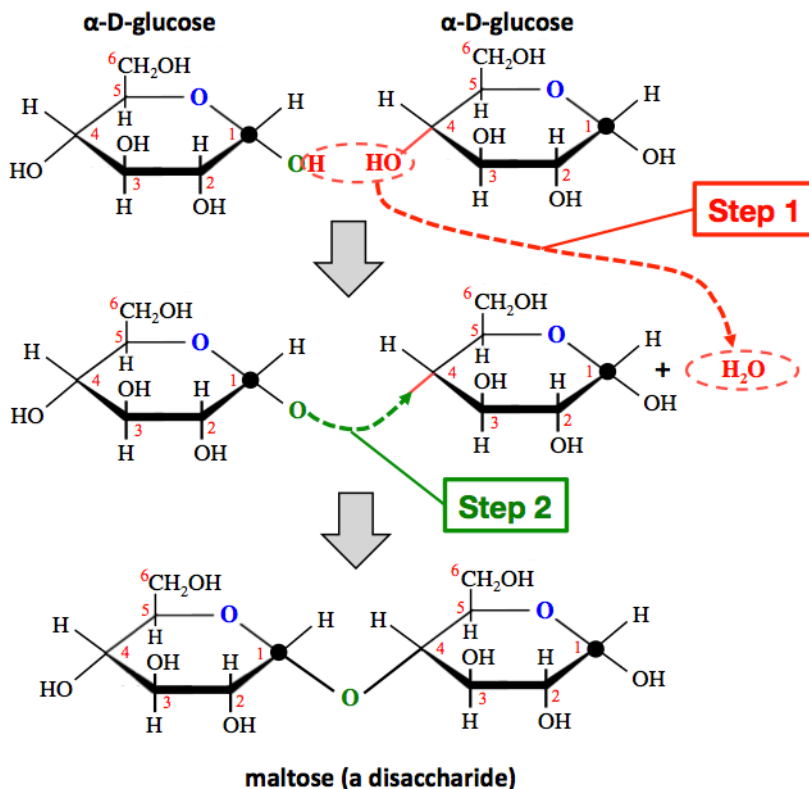
This method can be used to form a bond *between any two sugar residues*.

The *disaccharide* that is formed in *this* example is called **maltose**.

Maltose is found in malt, which is purified from germinated grains. Brewers interrupt the barley grain germination to obtain what is referred to as *malted barley*. Malted barley has a high concentration of *maltose*, which is fermentable, and therefore used in making beer and some other adult beverages. It is also used as a sweetener and thickener in frozen beverages called "malts."

The covalent bonding pattern linking the *anomeric carbon* of one residue to an *oxygen*, then to a carbon in the *other* sugar residue is referred to as a _____ _____.
(even though it actually contains *two* single bonds)

a *glycosidic bond*

maltose (a disaccharide)
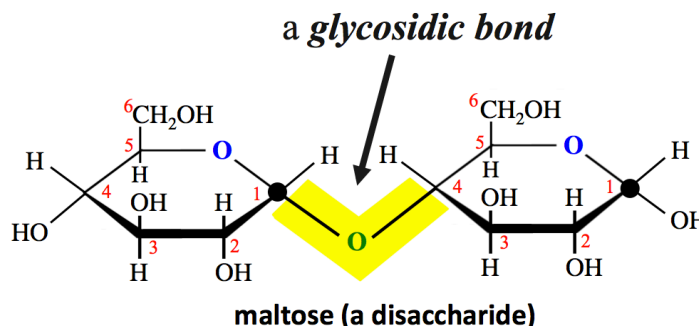
The Glycosidic Bond

Glycosidic bonds are described using **alpha (α)** or **beta (β)**.

- The **alpha (α)** designation indicates that the bond *from the anomeric carbon to the oxygen* (**O**) *in the glycosidic bond* is oriented _____ from the ring.

- The **beta (β)** designation indicates that the bond *from the anomeric carbon to the oxygen* (**O**) *in the glycosidic bond* is oriented _____ from the ring.
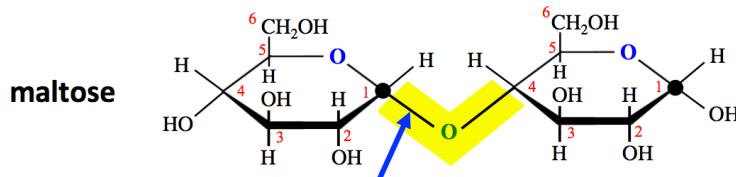
maltose

Maltose has the "**α**" designation because the bond *from the anomeric carbon to the oxygen* (**O**) *of the glycosidic bond* is oriented *downward* from the ring.

A glycosidic bond is characterized by its **α/β** orientation, *and* a description of _____ *two carbons are linked* by the glycosidic bond.

For example, the glycosidic bond in *maltose* is classified as **α-(1→4)**.

The numbers and arrow that are seen in the parenthesis (the "**1→4**" in the case of *maltose*) begins with the position number of the ***anomeric carbon*** where the glycosidic bond **originates**, then the arrow followed by the carbon position number where the glycosidic bond **terminates** in the *other* residue.

an **α-(1→ 4)** glycosidic bond
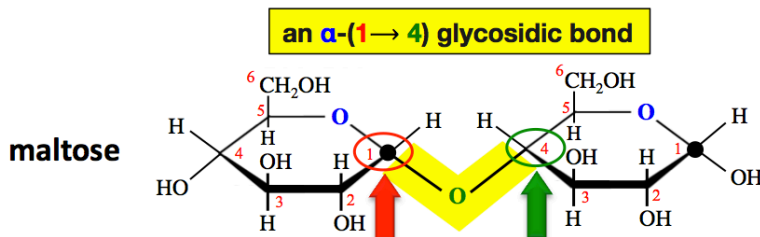
maltose

Maltose has the **(1→4)** designation because the ***glycosidic bond*** links the *anomeric* carbon (carbon number **1**) to carbon number **4** of the *other* residue.

Note that the glycosidic bond in *maltose* has the **α** designation because it was constructed from **α**-monosaccharides.

Later in this video, you will see that a glycosidic bond constructed from **β**-monosaccharides will have the **β** orientation.

α-D-glucose   **α-D-glucose**

maltose

an **α-(1→ 4)** glycosidic bond

23

maltose

This residue can no longer interconvert between open-chain and cyclic forms.
- It is "locked" in the cyclic form.

acetal carbon bonded to two OR groups.

hemiacetal carbon bonded to to an OR and an OH group

This residue can undergo **mutarotation**
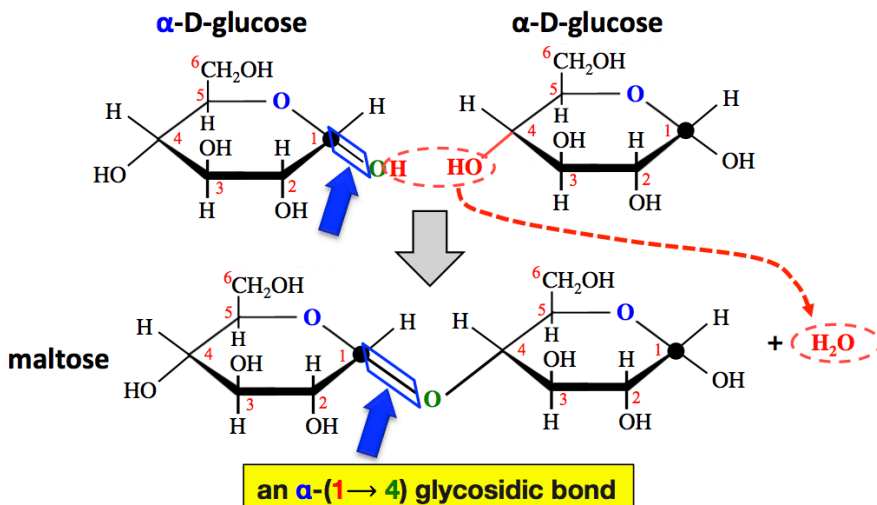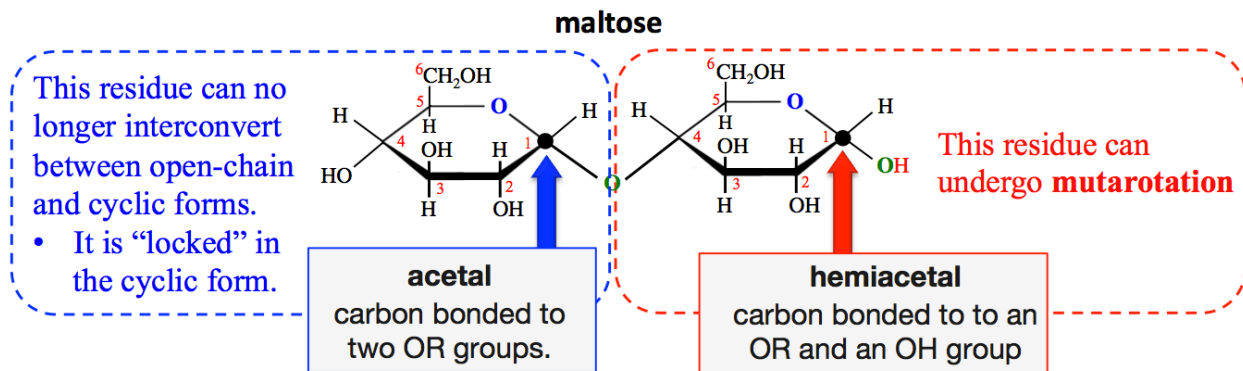
Oligosaccharides, such as maltose, *with a residue that contains a hemiacetal anomeric carbon* will interconvert (*mutarotate*) between closed anomers and an open-form.

mutarotation of maltose

OH in the α orientation

the **open-form** of maltose contains an *aldehyde group*

OH in the β orientation
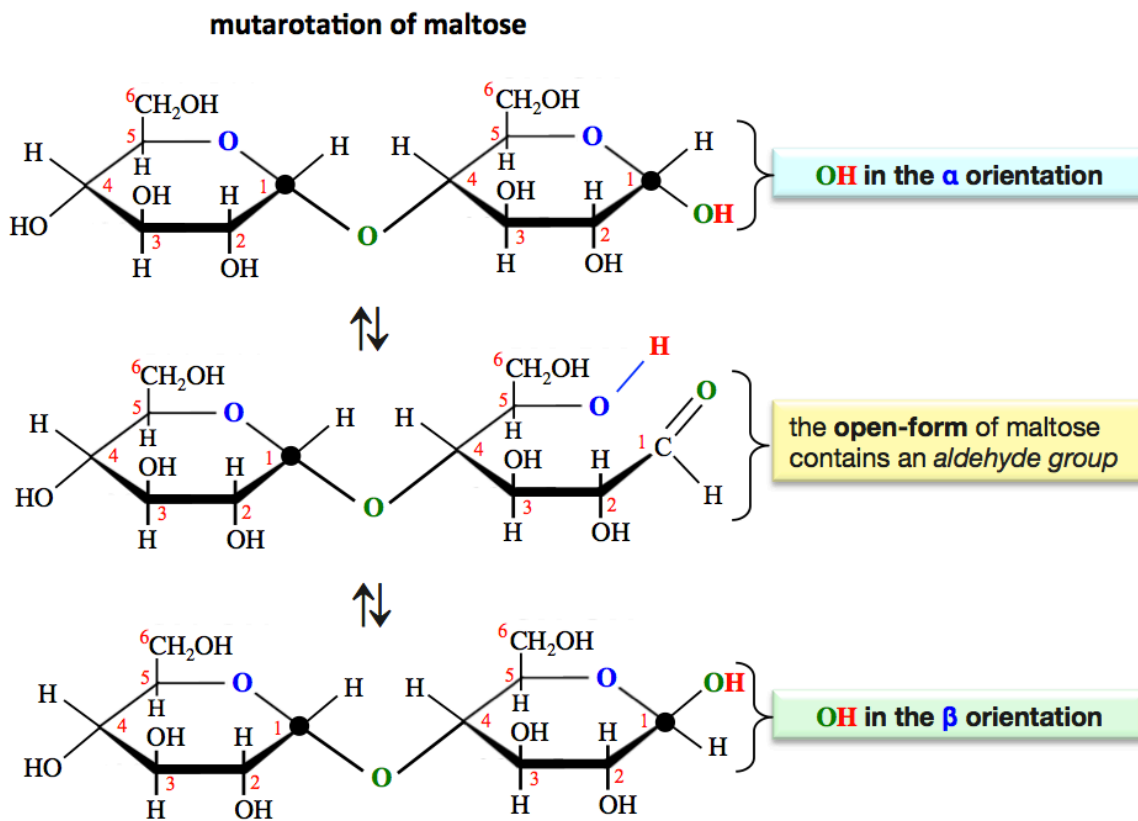
Note that the mutarotation **does not** change the **α/β** designation of a glycosidic bond.

If the **open-chain form** of an oligosaccharide contains an *aldehyde group*, it will give a positive _____ test.

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Let's now visualize the way that a glycosidic bond connects two **β-D-glucose** monosaccharides.

- We will use the same two steps as we did for the formation of a disaccharide in our previous example.

Step 1: An **H** atom is removed from the hydroxyl group (**OH**) *that is bonded to the anomeric carbon* of the left-most residue, and an **OH** is removed from *any carbon* in the right-most residue.

The **H** and **OH** that were removed form a water molecule.

Step 2: Draw a *new bond* from the oxygen (**O**) that remains on the *anomeric carbon* in the left-most residue **to** the carbon from which the **OH** was removed in the right-most residue.

- This *new bond* is oriented in the same direction as *was* the bond to **OH** that was removed.

The *disaccharide* that is formed in **this** example is called **cellobiose**.
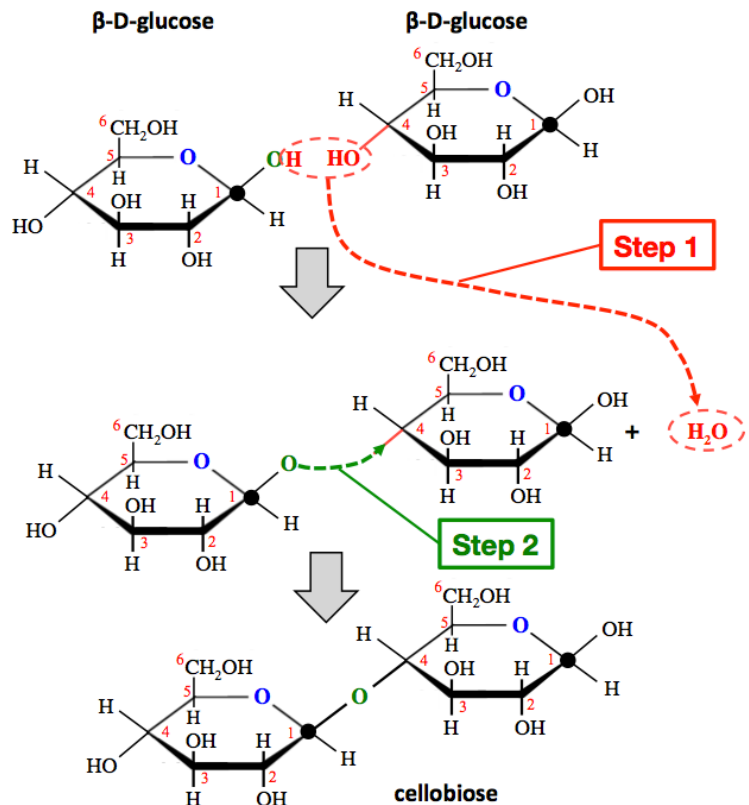
Cellobiose has the "**β**" designation because the bond *from the anomeric carbon to the oxygen (**O**) of the glycosidic bond* is oriented **upward** from the ring.

Cellobiose has the (1→4) designation because the glycosidic bond links the anomeric carbon (carbon number 1) to carbon number 4 of the other residue.
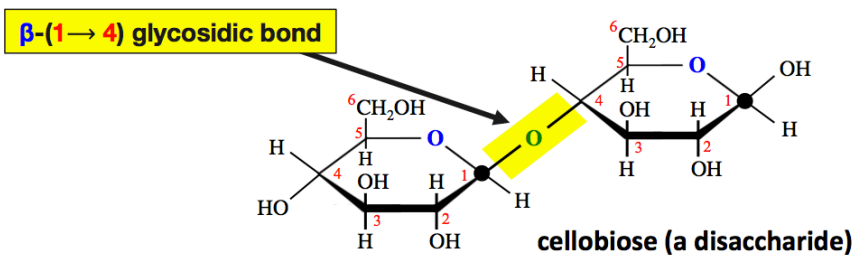
Note that since we began with **β**-monosaccharides, the glycosidic bond, necessarily, has the **β** orientation.

25
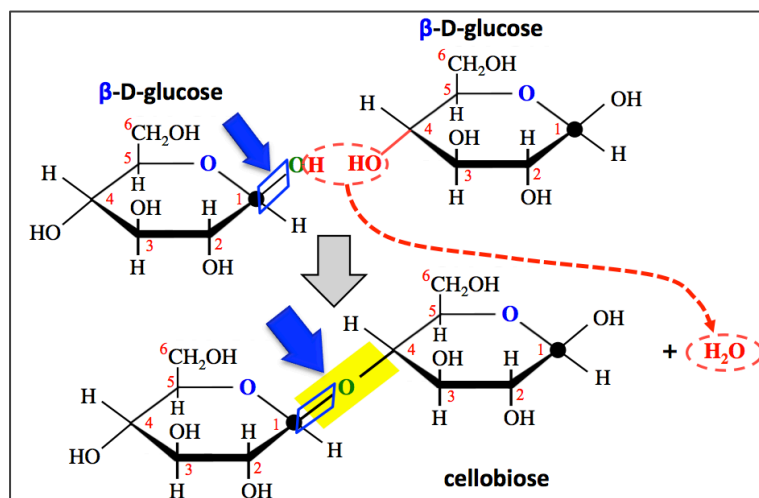
Examples of Other Oligosaccharides

Lactose is a disaccharide that contains a β-D-galactose residue bonded to a D-glucose residue by a **β-(1→4)** glycosidic bond.
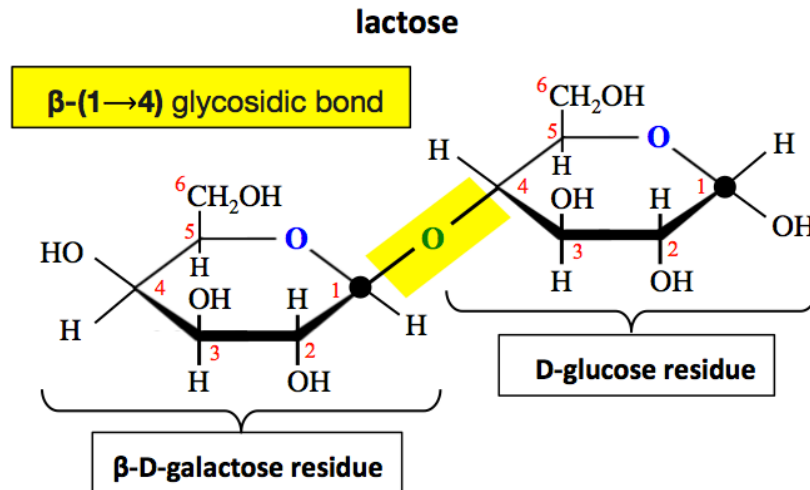
lactose

Most of us have an enzyme, called lactase, that will break *galactose*-glucose **β-(1→4)** glycosidic bonds so that we can digest and metabolize *lactose*. Lactose is a nutrient that is found in milk and dairy food made from milk. A small percentage of individuals are born with a mutation in the gene that is responsible for the production of the lactase enzyme, and are therefore unable to metabolize lactose. This condition is called **congenital lactose intolerance**. In many mammals, including humans, production of the lactase enzyme ceases at a very young age, this condition is known as **primary lactose intolerance**.

Over the last five to ten thousand years, human populations have evolved a genetic variant in a "lactose persistence DNA sequence" that allows them to continue to produce the lactase enzyme, and therefore continue *lactose* metabolism into adolescence and adulthood. The presence of this DNA variation was evolutionarily beneficial and has spread to about half of the world's population. Individuals who lack the lactose persistent DNA variation suffer from *primary lactose intolerance*. Both congenital and primary lactose intolerance results in the build-up of undigested lactose in the large intestine. Intestinal bacteria ferment the lactose and produce gases such as carbon dioxide, hydrogen, and methane. The presence of these gases is quite uncomfortable since it results in flatulence and bloating. In order for individuals with lactose intolerance to enjoy dairy foods, they can add the lactase enzyme (produced by fungi or yeast) directly to their food or ingest it in tablet form. Milk that has been supplemented with the yeast lactase enzyme is sold in many countries for lactose intolerant consumers.

Sucrose, also referred to as *"table-sugar"* or just *"sugar,"* is a *disaccharide* formed from an α-D-glucose residue and a **β**-D-fructose residue.
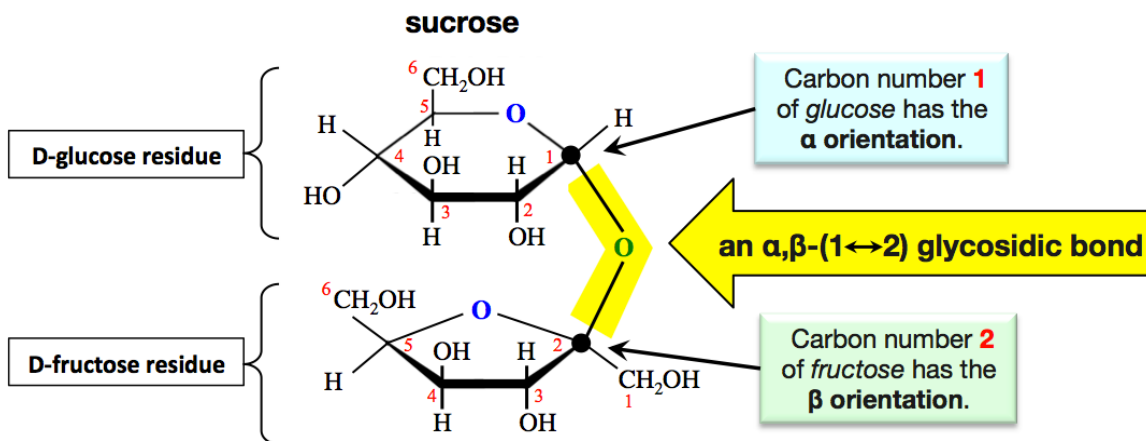
sucrose

Its glycosidic bonding pattern is a bit different from the ones that you have seen so far because it involves *two anomeric carbons*.

The glycosidic bond in sucrose links the *anomeric carbon* in the glucose residue to the *anomeric carbon* in the fructose residue.

- Note that the *anomeric carbon* in the D-fructose residue is carbon number **2**.

The glycosidic bond in *sucrose* is classified as **α,β-(1⟷2)**.

- This is because the stereochemistry at the anomeric carbon of the *glucose* residue (position number **1**) has the **α** orientation, and the anomeric carbon of the *fructose* residue (position number **2**) has the **β** orientation.

- The double arrow (⟷) used in this notation indicates that the glycosidic bond is between *two anomeric carbons*.
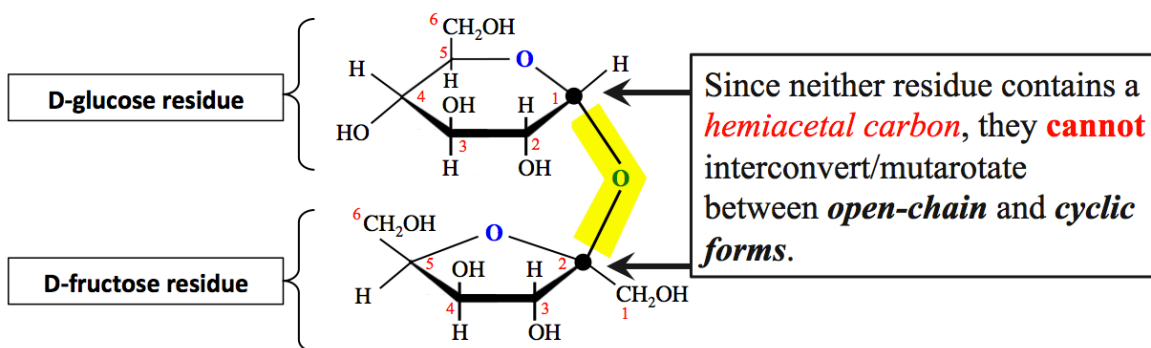
Both residues are "locked" in their **cyclic forms**.

For this reason, *sucrose*, *unlike* the other disaccharides that you have seen, will give a _____ Benedict's test and is therefore **not** classified as a **reducing sugar**.

Sucrose is consumed in relatively large quantities because of its desired "sweet" taste. It is manufactured by purification from sugar cane or sugar beets. Overconsumption of sucrose has been linked to tooth decay and obesity.

Examples of oligosaccharides that contain **more than two** monosaccharide residues are **raffinose** (a trisaccharide) and **stachyose** (a tetrasaccharide).

- **Raffinose** is made from a *galactose*, a *glucose*, and a *fructose* residue.

raffinose

D-galactose residue

α-(1→6) glycosidic bond

Note that *raffinose* contains an **α-(1→6)** glycosidic bond.

D-glucose residue

α,β-(1↔2) glycosidic bond
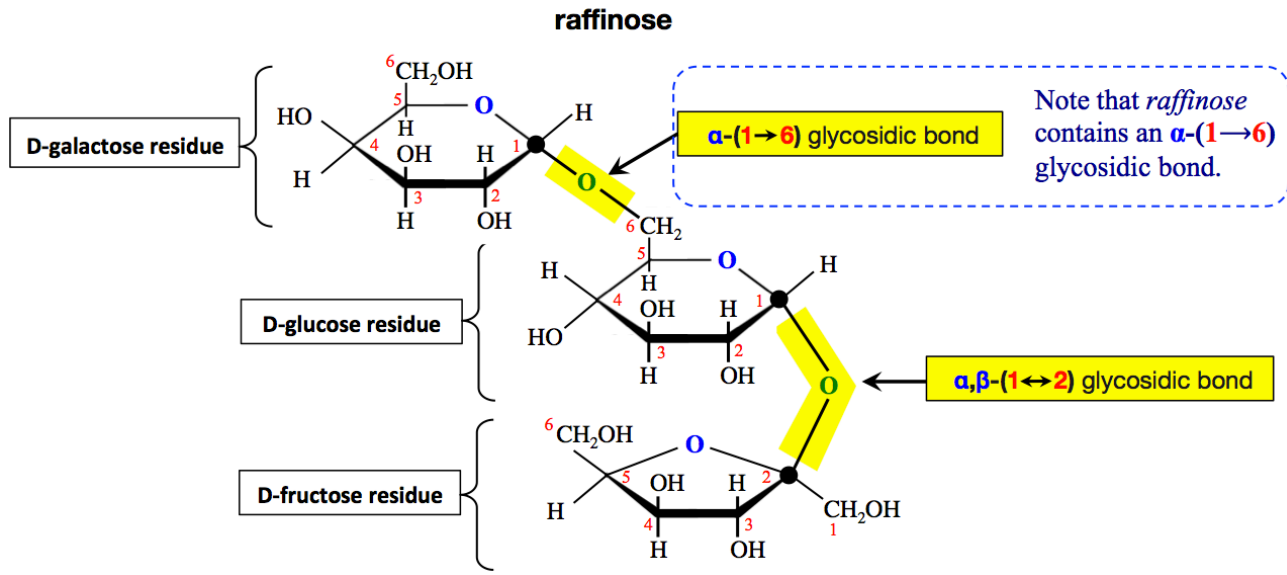
D-fructose residue

- It is categorized as a _____ because it contains **three** monosaccharide residues.

- **Stachyose** is made from **two** *galactose* residues, a *glucose* residue, and a *fructose* residue.

stachyose

D-galactose residue

D-galactose residue

α-(1→6) glycosidic bonds

D-glucose residue

α,β-(1↔2) glycosidic bond

D-fructose residue
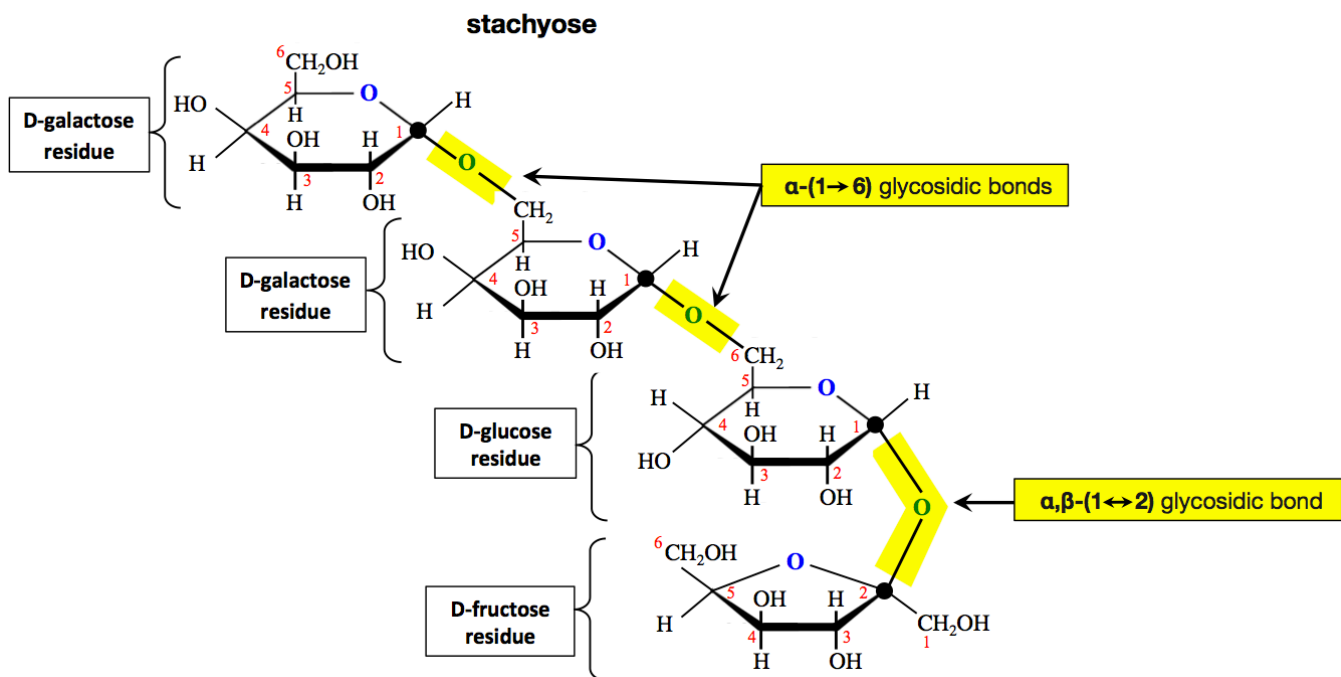
- It is categorized as a _____ because it contains **four** monosaccharide residues.

Raffinose and **Stachyose** are found together in many foods, most notably legumes (e.g. beans and peanuts) and cruciferous vegetables (e.g. broccoli, cauliflower, brussels sprouts, and cabbage). Monogastric (single stomach) animals, including humans, pigs, and poultry, cannot completely digest *raffinose* or *stachyose* because we do not have the enzyme, α-galactosidase, that is needed to break their α-galactose glycosidic bonds. Because *raffinose* and *stachyose* pass through the digestive track without being completely digested, they can be fermented by digestive microbes to produce gases. To avoid the discomfort of bloating and flatulence associated with such gases, the α-galactosidase enzyme can be taken as a nutritional supplement (marketed by Prestige Holdings Inc.) using the brand name of Beano.

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Understanding Check

Classify each of the highlighted glycosidic bonds using the **alpha "α-(X→Y)"** *or* **beta "β-(X→Y)"** designation.
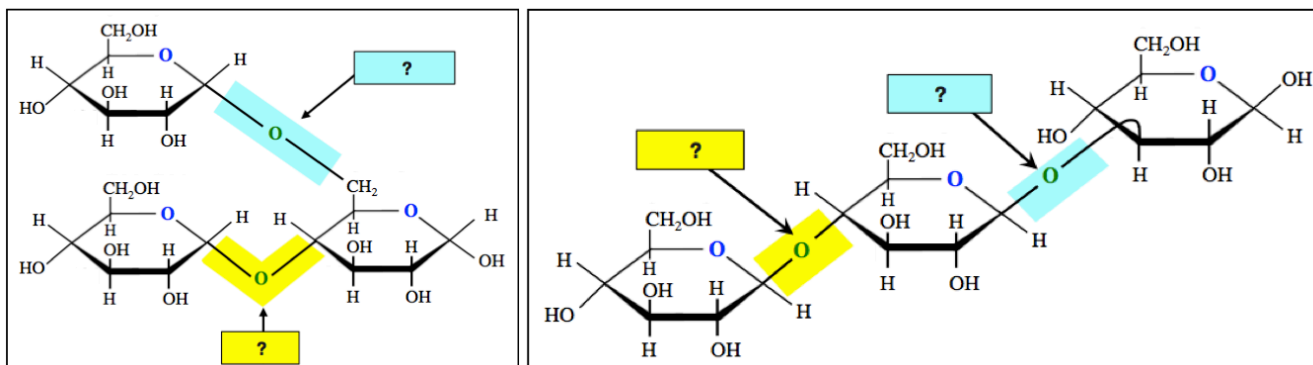
Understanding Check

Draw the disaccharide that is formed when the two monosaccharide molecules below are connected by a **β-(1→4)** glycosidic bond.
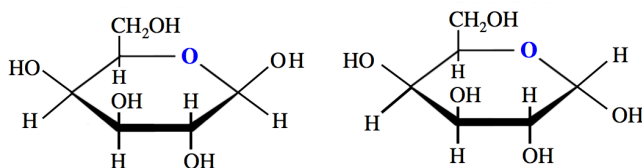
Sweeteners

A sweetener is a compound that is added to food in order to impart the sweet taste of sucrose, but with significantly fewer calories.

Sweeteners can be classified as "_____ *sweeteners*" or "_____ *sweeteners*."

- *Natural sweeteners* are carbohydrates, *naturally* occurring carbohydrate derivatives, or other *naturally* occurring non carbohydrate compounds.

    - **Example** of a *natural sweetener*: fructose

$$CH_2OH$$
$$C=O$$
$$HO-H$$
$$H-OH$$
$$H-OH$$
$$CH_2OH$$
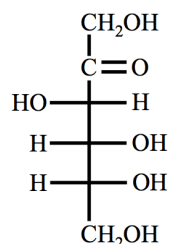
D-fructose

- *Artificial sweeteners* do not occur in nature; they are *synthesized* in commercial laboratories.

    - The structural formulas of some *artificial sweeteners* are shown below.
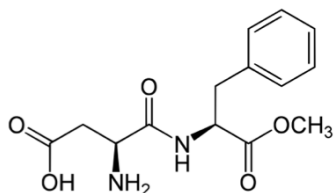
aspartame
(Equal, NutraSweet)
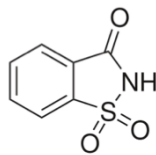
saccharin
(Sweet'N Low)
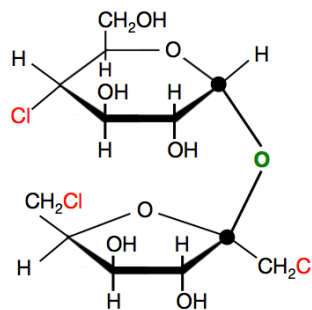
sucralose
(Splenda)
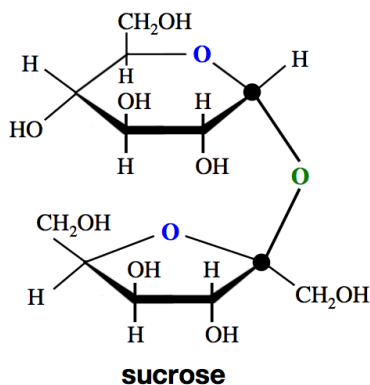
sucrose

Sucrose is the reference standard for "sweetness."

A "*sweetness value*" of **100** is assigned to sucrose, and then *other* sweeteners are assigned *sweetness values* relative to the taste of the same mass of sucrose.

| Sweetness Relative to the Same Mass of Sucrose ||
Sweetener	Sweetness Value
Natural Sweeteners	
Fructose	170
Xylitol (an alcohol sugar)	100
Glucose	75
Sorbitol (an alcohol sugar)	55
Maltose	32
Galactose	30
Lactose	15
Stevia (a plant extract)	25,000
Artificial Sweeteners	
Sucralose (Splenda, Kaltame)	60000
Saccharin (Sweet'N Low)	30000
Aspartame (Equal, NutraSweet)	18,000

The sweeteners that are currently approved for sale in the US are: stevia, aspartame, sucralose, neotame, acesulfame potassium (Ace-K), saccharin, and advantame.

Although there are **rumors** to the contrary, *none of these sweeteners*, artificial or natural, *have ever been shown to cause cancer in humans.*

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Carbohydrates can be classified into three major groups based on their size:

1) **monosaccharides**
2) **oligosaccharides**
3) **polysaccharides**

Polysaccharides

Polysaccharides are composed of *more than* _____ residues.

- The residues can be monosaccharides **or** monosaccharide derivatives.

Polysaccharides are often subcategorized as either **homopolysaccharides** or **heteropolysaccharides**.

- *Homopolysaccharides* are composed of *only* _____ *type of* residue.

- *Heteropolysaccharides* are composed of _____ *than one type* of residue

Homopolysaccharides

Example of a Homopolysaccharide: Cellulose

Cellulose is composed of multiple D-glucose residues (only), bonded to each other by **β-(1→4)** glycosidic bonds.
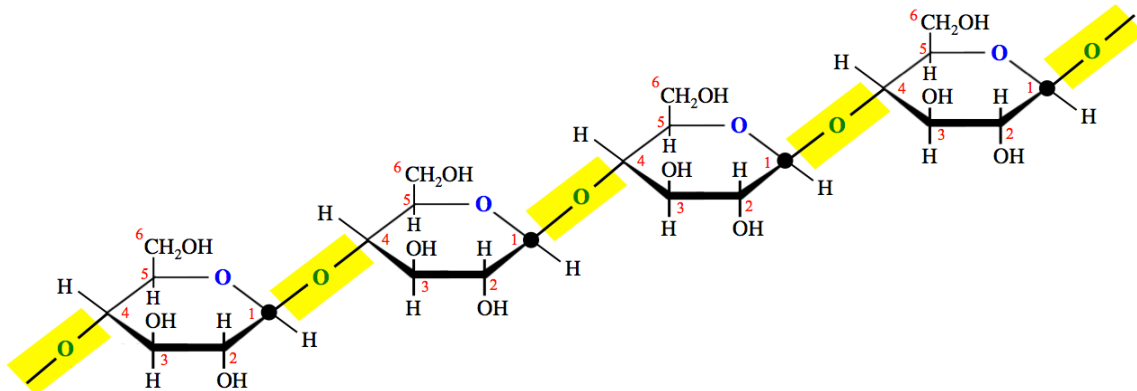
The structure shown above represents a ***small section*** of a *cellulose* molecule.

- A *cellulose* molecule contains *hundreds* (sometimes *thousands*) of glucose residues.

Cellulose is found in the cell walls of green plants, some algae, and oomycetes.

Cellulose accounts for approximately 45% of the mass of dry wood and about 90% of the mass of cotton fibers.

The major industrial use for *cellulose* is the production of paper.

Humans lack the enzyme necessary to break the *glucose-glucose* β-(1→4) glycosidic bond, therefore we cannot metabolize cellulose to get energy. It is for this reason that we do not eat paper, cotton, wood, and many other plants. Some animals (ruminants and termites) are able to metabolize cellulose, not because they produce an enzyme that can break the *glucose-glucose* β-(1→4) glycosidic bond, but because they contain bacteria in their digestive track that can do so. In humans, dietary *cellulose* acts as a bulking agent for feces, and eases defecation. When consumed, it is classified as a ***dietary fiber.***

Much of the rigidity of plant cell walls comes from the strong intermolecular forces, especially hydrogen bonding, that are present between the very long and straight cellulose molecules that lie next to each other in a side-by-side fashion.

Example of a Homopolysaccharide: Starch

Starch is a common component of plants.

- The excess *glucose* produced in photosynthesis is stored as *starch* in plants.

Starch is composed of _____ different polysaccharides, both of which are ***homopolysaccharides***.

The two components of *starch* are _____ and _____.

Amylose

Amylose is composed of multiple D-glucose residues (only), bonded to each other by **α-(1→4)** glycosidic bonds.
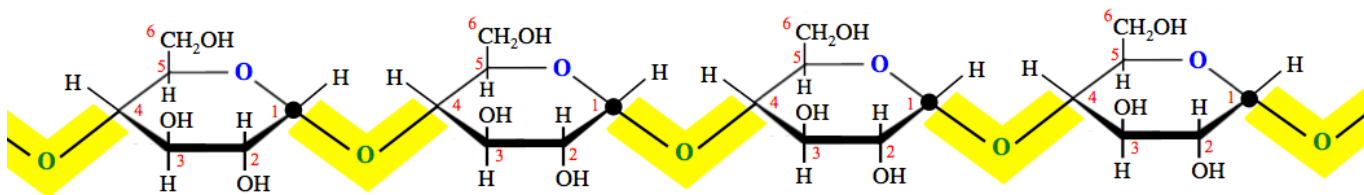
The structure shown above represents a ***small section*** of an amylose molecule. An *amylose* molecule contains *hundreds* to many *thousands* of D-glucose residues.

Note that *amylose* and *cellulose* have the same bonding pattern except for the **α** vs. **β** orientation of their glycosidic bonds.

- The difference in stereochemistry (**α** vs. **β**) in *amylose* vs. *cellulose* makes a big difference in our ability to digest these two compounds. Humans (and many other animals) have digestive enzymes (called amylases) that are capable of breaking *glucose-glucose* **α-(1→4)** glycosidic bonds.

- The difference in stereochemistry (**α** vs. **β**) *does* result in a significant difference in the three-dimensional arrangement of the residues. While *cellulose* molecules are relatively straight, the residues in amylose form a helical coil (helix) as illustrated below.
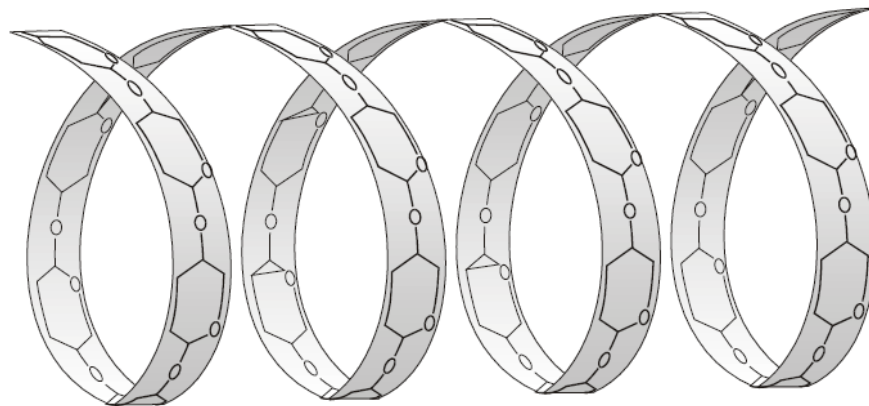
Amylopectin

The second component of starch, **amylopectin**, is also a *homopolysaccharide* composed of multiple D-glucose residues (only), bonded to each other by **α-(1→4)** glycosidic bonds (as in *amylose*) **with other chains of D-glucose that _____ from carbon number 6**.

The branching occurs as an **α-(1→6)** glycosidic bond, as shown below.
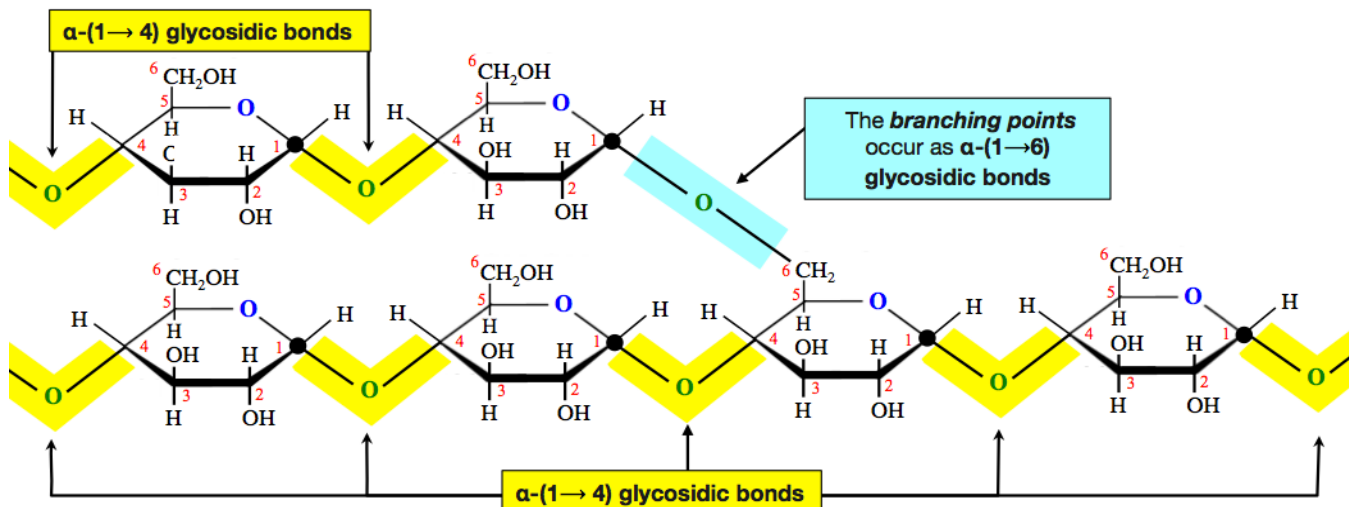
The structure shown here represents a **small section** of an *amylopectin* molecule. An *amylopectin* molecule typically contains 2,000 to 200,000 D-glucose residues.

Branching usually occurs every **24 to 30 glucose residues** in *amylopectin*, as illustrated below.
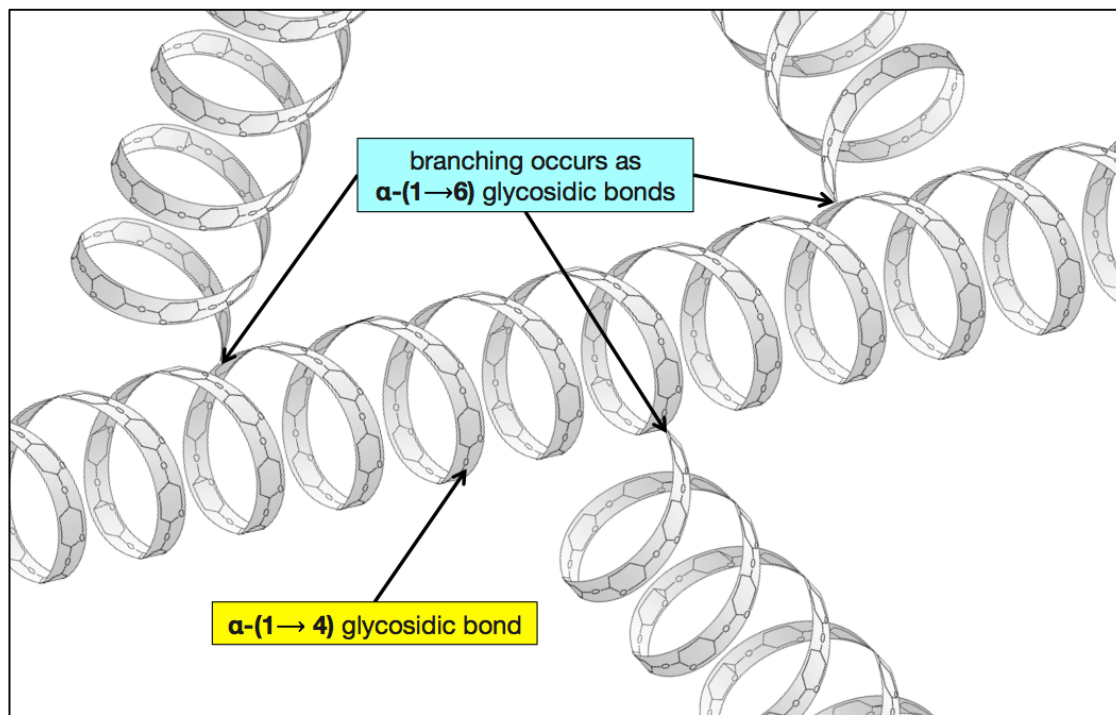
Because of branching, *amylopectin* molecules have a large number of *endpoints*. Since the *amylase digestive enzymes* attach to starch molecules at the endpoints, *amylopectin* can be digested more quickly than *amylose*. Starch contains about 70-80% *amylopectin* and 20-30% *amylose*. One of the three *amylase digestive enzymes* is capable of breaking the branching **α-(1→6)** glycosidic bonds.

Example of a Homopolysaccharide: Glycogen

Plants store excess glucose as *starch*; animals and fungi store excess glucose as **glycogen**.

Glycogen is a ***homopolysaccharide*** composed of multiple D-glucose residues (only).

It is almost identical to *amylopectin*, the only difference is that it ***branches more*** _____.

- Branching in *glycogen* usually occurs every ***8 to 10 glucose residues***.

In humans, *glycogen* is made and stored primarily in liver and muscle cells.

Understanding Check: Amylose vs. Amylopectin

Identify the following as properties of either **amylose**, **amylopectin**, **or** *both* **amylose** and **amylopectin**.

- a. contains **α-(1→4)** glycosidic bonds
- b. homopolysaccharide
- c. contains glucose residues only
- d. contains **α-(1→6)** glycosidic bonds
- e. contains branching points
- f. more quickly digested (amylose or amylopectin?)

Understanding Check: Amylose vs. Cellulose

Identify the following as properties of either amylose, cellulose, or **both** amylose *and* cellulose.

- a. contains **α-(1→4)** glycosidic bonds
- b. contains glucose residues only
- c. found in plants
- d. has a helical structure
- e. is a homopolysaccharide
- f. contains **β-(1→4)** glycosidic bonds
- g. can be digested by humans
- h. is a major component of cell walls

Understanding Check: Glycogen vs. Amylopectin

Identify the following as properties of either glycogen, amylopectin, or **both** glycogen *and* amylopectin.

- a. contains **α-(1→4)** glycosidic bonds
- b. contains glucose residues only
- c. contains **α-(1→6)** glycosidic bonds
- d. contains branching points
- e. is a homopolysaccharide
- f. produced by plants
- g. produced by animals
- h. branching occurs more frequently (glycogen *or* amylopectin)

Heteropolysaccharides

Heteropolysaccharides are composed of *more than one type* of residue.

The residues can be *monosaccharides* and/or *monosaccharide derivatives*.

Example of a Heteropolysaccharide: Hyaluronic acid

Hyaluronic acid contains *D-glucuronic acid* and *N-acetyl-D-glucosamine* residues, connected to each other in the bonding pattern shown below.
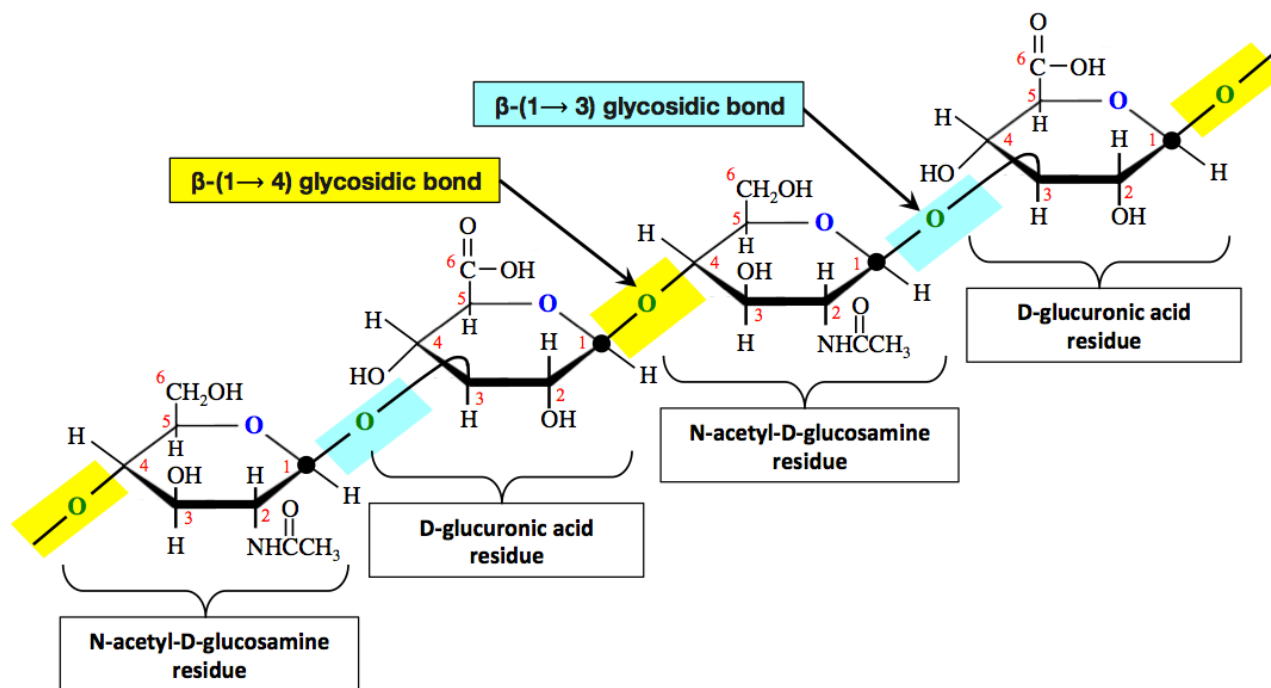
The D-glucuronic acid and N-acetyl-D-glucosamine residues are connected by alternating **β-(1→4)** and **β-(1→3)** glycosidic bonds.

The structure shown above represents only a ***small section*** of a *hyaluronic acid* molecule, *which* can contain *up to* about 50,000 residues.

Hyaluronic acid is found in the lubricating fluid that surrounds joints, and also in the vitreous humor inside the eye.

Review: Homopolysaccharides vs. **Heteropolysaccharides**

Homopolysaccharides contain ***only one type*** *of* residue.

Heteropolysaccharides contain ***more than one type*** of residue.

Summary of Carbohydrate Classification

Carbohydrates

Contains 3-7 carbon atoms

Contains *2 to 10* monosaccharide residues

Contains *more than 10* monosaccharide residues

Monosaccharides

Oligosaccharides

Polysaccharides

Contains *an aldehyde group*

Contains *a ketone bonding pattern*

Aldoses

Ketoses

Contains *only one type* of residue

Contains *more than one* type of residue

Homopolysaccharides

Heteropolysaccharides

Carbohydrates Worksheet and Key

1) Define: aldoses, ketose, hexose, aldopentose, ketotetrose, alcohol sugar, deoxy sugar, amino sugar, carboxylic acid sugar, anomeric carbon, glycosidic bond, hemiacetal, acetal, and cyclic hemiacetal

Compare and contrast: Haworth Projection vs. Fischer Projection

Compare and contrast: monosaccharide, oligosaccharide, and polysaccharide

Compare and contrast: D-sugar vs. L-sugar

Compare and contrast: starch vs. glycogen

Compare and contrast: amylose vs. amylopectin

Compare and contrast: cellulose vs. amylose

2) Identify the following as D- or L- monosaccharides:
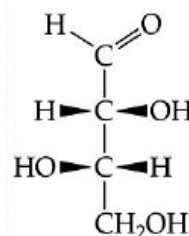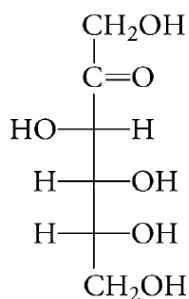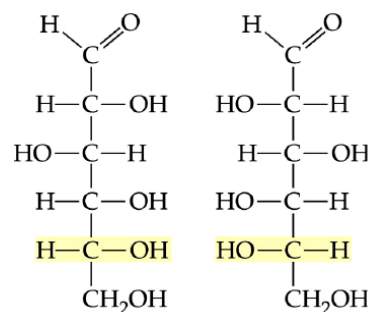
3) Identify the following as the α or β anomer:
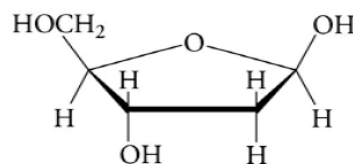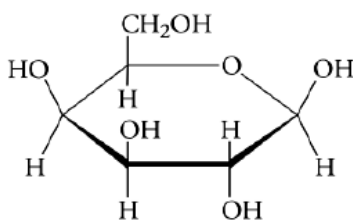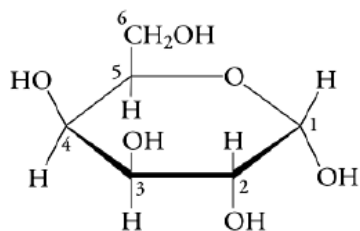
4) Identify the type of glycosidic bond for each of the following sugars. Choose from α-(1→2), α-(1→3), α-(1→4), α-(1→5), α-(1→6), β-(1→2), β-(1→3), β-(1→4), β-(1→5), β-(1→6), or α,β-(1↔2)

a)
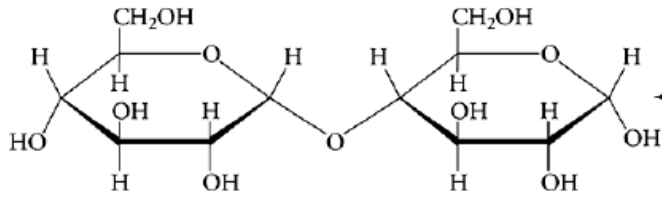
b)
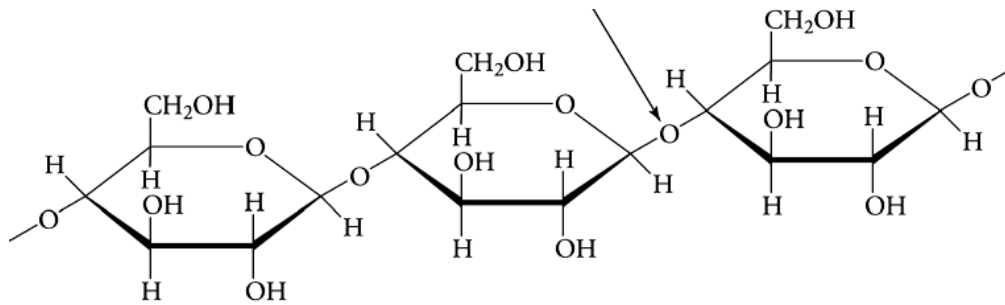
c)
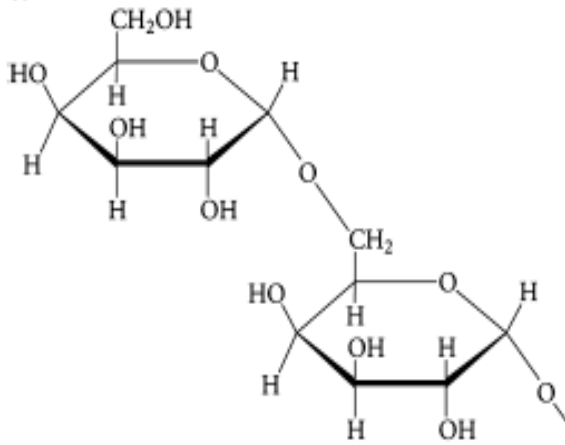
d)
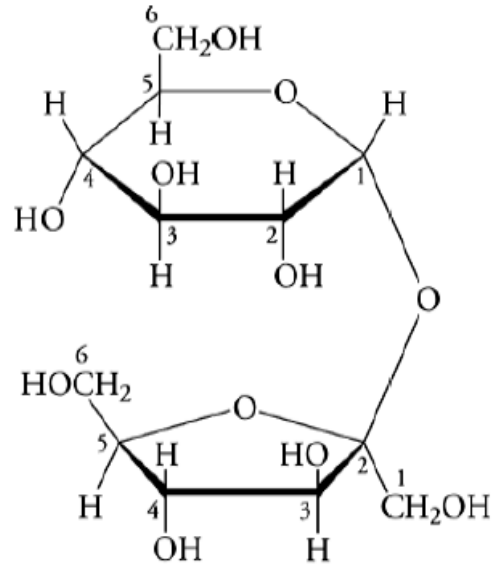
e)
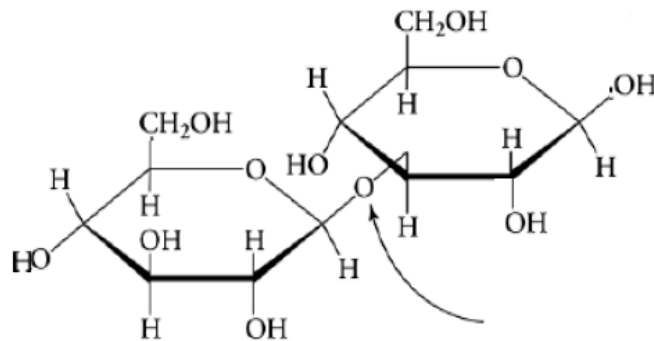
KEY

1) SEE YOUR LECTURE NOTES or the TEXBOOK

2) Identify the following as D- or L- monosaccharides:

D   L   D   L

3) Identify the following as the α or β anomer:

α   β   β

4) Identify the type of glycosidic bond for each of the following sugars. Choose from α-(1→2), α-(1→3), α-(1→4), α-(1→5), α-(1→6), β-(1→2), β-(1→3), β-(1→4), β-(1→5), β-(1→6), or α,β-(1↔2)

a) α-(1→4)

b) β-(1→4)

c) α-(1→6),

d) α,β-(1↔2)

e)) β-(1→3)

Chapter 12 Lecture Notes: Lipids and Membranes

Educational Goals

1. Know the *factors* that characterize a compound as being a **lipid**.

2. Describe the structure of **fatty acids** and explain how *saturated, monounsaturated, and polyunsaturated fatty acid* structures differ from one another.

3. Predict how the *number of carbons* and *the degree of unsaturation* affect the melting points of fatty acids.

4. Describe the *structure* of waxes, how they are made, and understand the *biological function* of waxes.

5. Describe the general **structure of triglycerides** and list their biological functions.

6. Describe the reaction involved in the *formation of triglycerides* from fatty acid residues and glycerol.

7. Describe three reactions in which *triglycerides are reactants*.

8. Explain how the structures of *saturated* and *unsaturated triglycerides* differ from one another.

9. Explain the difference in melting points of **vegetable oils** vs. **animal fats**.

10. Distinguish **phospholipids** from **glycolipids**.

11. Distinguish **glycerophospholipids** from **sphingophospholipid.**

12. Distinguish **glyceroglycolipids** from **sphingoglycolipids.**

13. Identify the structural component that is common to all **steroids** and identify *three important members* of this class of lipids.

14. Describe the *structure and function* of **bile salts**.

15. Describe the *structure and function* of **lipoproteins**. List *five types* of lipoproteins.

16. Understand what is meant by the terms "total cholesterol," "good cholesterol," and "bad cholesterol" as they relate to lipid panel blood tests.

17. Understand the structural basis of the lipid class called **eicosanoids**.

18. Explain how *aspirin, ibuprofen, and acetaminophen* work to reduce fever, swelling, and pain.

19. Describe the *components and structure* of a **cell membrane**.

20. Compare and contrast **passive transport** and **active transport**.

21. Compare and contrast **simple diffusion** and **facilitated diffusion**.

Lipids are used as: cell membrane components, energy storage compounds, insulation, signaling compounds, and hormones.

Introduction to Lipids

Lipids *are not* defined by the presence of specific functional groups.

Lipids are defined as _____ *compounds* that are _____ in _____ but soluble in nonpolar solvents.

- *Biological compounds* are organic compounds that occur in *living* organisms.

- *There* are three *solubility classes* for biological compounds: **hydrophilic, hydrophobic,** and **amphipathic**.

    - Of these three classes, **hydrophobic *and* amphipathic** are *water-<u>in</u>soluble*.

        - Amphipathic molecules are *water-<u>in</u>soluble* because they do not dissolve when placed in water; they form *monolayers* and *micelles*.

You will be introduced to *seven* **classes of lipids** in this chapter:

1) **Fatty Acids**
2) **Waxes**
3) **Triglycerides**
4) **Steroids**
5) **Phospholipids**
6) **Glycolipids**
7) **Eicosanoids**

Fatty Acids

Fatty acids are _____ *acids* with _____-*chain* hydrocarbon parts.

$$\underset{\text{long-chain hydrocarbon}}{\boxed{}} \overset{\displaystyle O}{\underset{}{\overset{\|}{-C}}} - OH$$

general form of a fatty acid

Fatty acids typically *contain between twelve and twenty carbon atoms*.

A specific example of a fatty acid is *lauric acid*.

lauric acid

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{O}{\overset{\|}{C}}-OH$$

In order to save time when drawing structural formulas for large molecules such as fatty acids, an *abbreviated condensed structure* is used. Repeating units are shown in parenthesis with a subscripted number where the subscript is equal to the number of times that the structural unit *within the parenthesis* is repeated.

$$CH_3(CH_2)_{10}\overset{O}{\overset{\|}{C}}-OH$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{O}{\overset{\|}{C}}-OH$$

- For example, carbons that are single bonded to each other in a linear sequence, along with the hydrogens that are bonded to them, are abbreviated as $(CH_2)_n$, where **n** is equal to the number of times that the CH_2 is repeated.

Fatty acids usually contain an _____ *number of carbon atoms* because they are made in nature by combining *two-carbon* molecules.

Fatty acids can differ from one another in the _____ *of carbon atoms* they contain, and in the **number of** _____ _____ **bonds** they contain.

Some Fatty Acids that are Frequently Encountered in Biological Systems				
Number of Carbons	**Number of Carbon-Carbon Double Bonds**	**Common Name**	**Condensed Structure**	**Major Source**
12	0	lauric acid	$CH_3(CH_2)_{10}COOH$	coconut
14	0	myristic acid	$CH_3(CH_2)_{12}COOH$	nutmeg
16	0	palmitic acid	$CH_3(CH_2)_{14}COOH$	palm
16	1	palmitoleic acid	$CH_3(CH_2)_5CH{=}CH(CH_2)_7COOH$	macadamia, animals
18	0	stearic acid	$CH_3(CH_2)_{16}COOH$	animal fat
18	1	oleic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$	olives
18	2	linoleic acid	$CH_3(CH_2)_4(CH{=}CHCH_2)_2(CH_2)_6COOH$	safflower, soy
18	3	linolenic acid	$CH_3CH_2(CH{=}CHCH_2)_3(CH_2)_6COOH$	flax, corn

Classification of Fatty Acids

Fatty acids are classified as **saturated**, **monounsaturated**, or **polyunsaturated** based on the number of *carbon-carbon* double bonds they contain.

- **Saturated fatty acids** contain *no* carbon-carbon double bonds.
- **Monounsaturated fatty acids** contain *one* carbon-carbon double bond.
- **Polyunsaturated fatty acids** contain *more than one* carbon-carbon double bond.

Classification of Fatty Acids Based on the Degree of Saturation

Contain *no* carbon-carbon double bonds.

Contain *one* carbon-carbon double bond.

Contain *more than one* carbon-carbon double bond.

Saturated Fatty Acids

lauric acid	$CH_3(CH_2)_{10}COOH$
myristic acid	$CH_3(CH_2)_{12}COOH$
palmitic acid	$CH_3(CH_2)_{14}COOH$
stearic acid	$CH_3(CH_2)_{16}COOH$

Monounsaturated fatty acids

palmitoleic acid
$CH_3(CH_2)_5CH{=}CH(CH_2)_7COOH$

oleic acid
$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$

Polyunsaturated fatty acids

linoleic acid
$CH_3(CH_2)_4(CH{=}CHCH_2)_2(CH_2)_6COOH$
(*two* C=C double bonds)

linolenic acid
$CH_3CH_2(CH{=}CHCH_2)_3(CH_2)_6COOH$
(*three* C=C double bonds)

Classification of Fatty Acids

Another way in which fatty acids can be classified is by their _____.

They are categorized as either *cis* or *trans*, based on the stereochemistry of the carbon-carbon double bonds in their hydrocarbon parts.

- Fatty acids that contain *one or more* double-bonded carbons with the **trans geometry** are referred to as *trans* **fatty acids**.

- Fatty acids that contain *only* the **cis geometry** are called *cis* **fatty acids**.

Most of the fatty acids that are produced in nature are _____; the only known exceptions are the fatty acids produced by some bacteria.

- Examples of **cis fatty acids**:

palmitoleic acid
(a *cis* fatty acid)

linolenic acid
(a *cis* fatty acid)
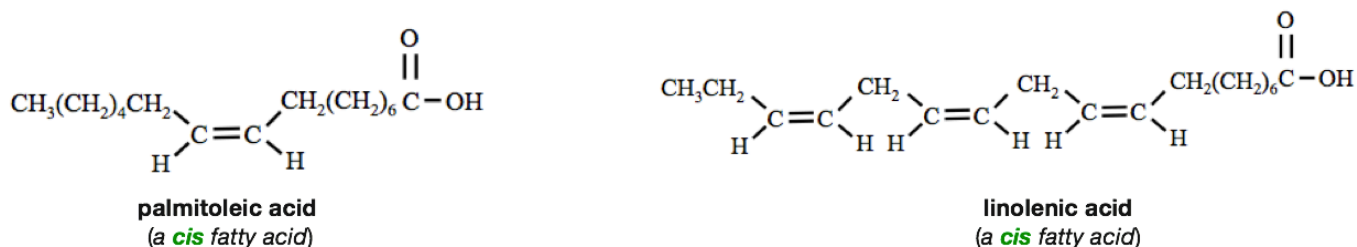
Omega Notation and Classification of Unsaturated Fatty Acids

Although not used in IUPAC naming, *omega notation* is frequently seen in popular nutrition literature.

In omega notation, the carbon at the _____ of a fatty acid's hydrocarbon chain is designated as the "*omega* carbon" or "ω-carbon."

- Omega (ω) is the last letter of the Greek alphabet, making the omega designation appropriate for the "last" carbon in a fatty acid's hydrocarbon chain.

Unsaturated fatty acids are put into omega notation classes by the position of the *first* **double bond** that occurs, **counting from the omega carbon**.

Example: If a carbon-carbon double bond in a fatty acid occurs at the *seventh* carbon, counting from the *omega* carbon, then it is classified as an *omega-7* fatty acid (or ω-7 fatty acid).

palmitoleic acid (an *omega-7* fatty acid)
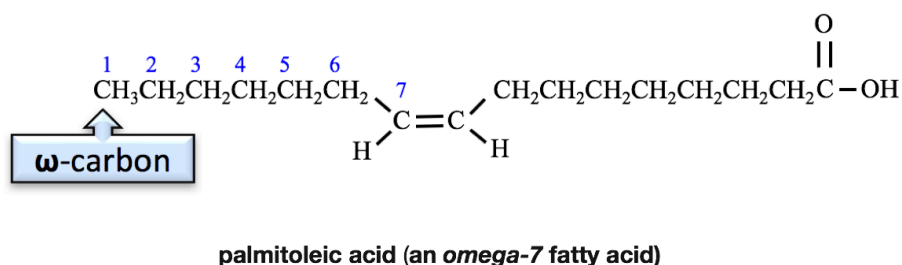
An example of an *omega-3* fatty acid is linolenic acid.
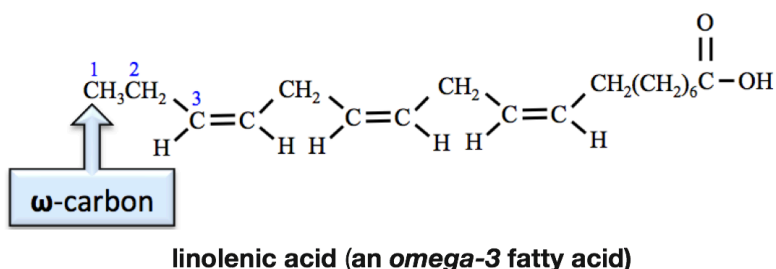
linolenic acid (an *omega-3* fatty acid)

4

Properties of Fatty Acids: Melting Points of Fatty Acids

All fatty acids are attracted to each other through hydrogen bonding, dipole-dipole interactions of their carboxyl groups, and through London forces.

The melting points of fatty acids are related to the _____ of their hydrocarbon part - as are, in general, the melting points of all organic compounds.

The larger the nonpolar hydrocarbon part, the stronger the _____ *forces* and the higher the melting point.

Melting Points of some Saturated Fatty Acids			
Number of Carbons	Common Name	Condensed Structure	Melting Point (°C)
12	lauric acid	$CH_3(CH_2)_{10}COOH$	43
14	myristic acid	$CH_3(CH_2)_{12}COOH$	54
16	palmitic acid	$CH_3(CH_2)_{14}COOH$	62
18	stearic acid	$CH_3(CH_2)_{16}COOH$	69

Another factor that influences the melting points of fatty acids is their ***degree of saturation***.

The more carbon-carbon _____ *bonds* that are present in a fatty acid, the _____ the melting point.

The inability of rotation around double bonds prevents less saturated molecules from getting as close to each other as is possible for more highly saturated molecules. The strength of London forces - and all other noncovalent interactions - are distant dependent; the closer the particles are to each other, the stronger the attractive force.

If two fatty acids have the same number of carbon atoms but differ in degree of saturation, molecules of the fatty acid with more carbon-carbon double bonds cannot pack as close to to each other as the molecules of the more saturated fatty acid, and will therefore have a lower melting point than the more saturated fatty acid.

Example:
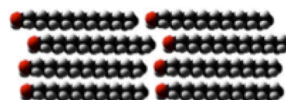
Stearic Acid

18 carbons
no C=C double bonds
melting point = 69 °C

Linolenic Acid

18 carbons
three C=C double bonds
melting point = -17 °C

> **Understanding Check:** Which fatty acid would you expect to have the higher melting point, oleic acid or palmitoleic acid?

> **Understanding Check:** Which fatty acid would you expect to have the higher melting point, oleic acid or linoleic acid?

Properties of Fatty Acids: Water Solubility of Fatty Acids

Fatty acids are _____ and therefore ***do not dissolve in water***.

- This is because they contain eleven or more carbon atoms in their *hydrocarbon part*.
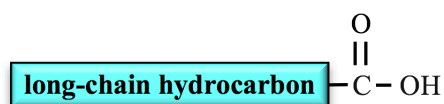
general form of a fatty acid

Properties of Fatty Acids: Formation of Carboxylate Ions from Fatty Acids

Fatty acids, *like all carboxylic acids*, will react with water to produce their corresponding _____ *ion* forms (**base forms**).

- **Example:** Lauric acid and its corresponding carboxylate ion (laurate ion).

lauric acid (a fatty acid)
(acid form)

laurate ion (a carboxyate ion)
(base form)
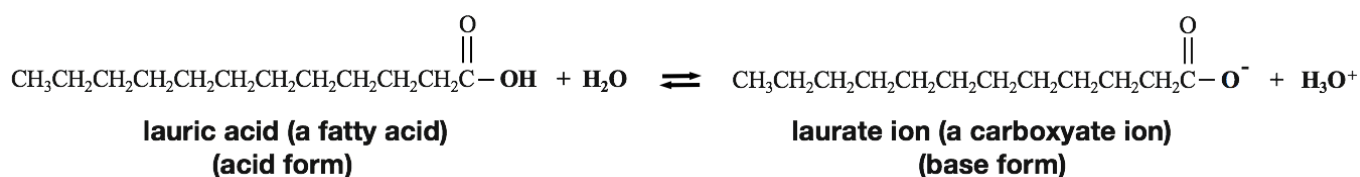
In previous chapters, you learned that the relative amounts of a conjugate pair's ***acid form*** and ***base form*** that are present in an aqueous solution depends on the pH of the solution ***and*** the pK_a of the particular acid (as described by the Henderson-Hasselbalch Equation). The pK_a of carboxylic acids (including fatty acids) is about **5**. Since the physiological pH in cells, blood, and intercellular solutions is *greater than* **5**, the *carboxylate form* of fatty acids are predominant in these solutions ($pH > pK_a$).

Carboxylate ions are named by replacing the "-ic acid" suffix of the ***fatty acid*** name with "-ate ion."

- **Examples:**

lauric acid ⟶ laurate ion

oleic acid ⟶ oleate ion

palmitic acid ⟶ palmitate ion

6
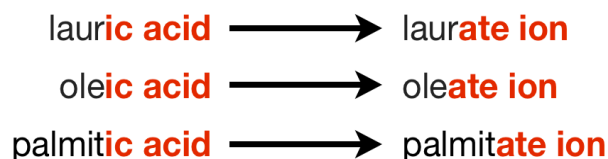
Waxes

Waxes are members of the _____ family of organic compounds.
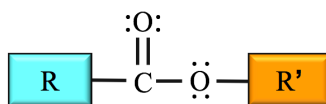
general form of an *ester*

Waxes are **e*sters*** with ***relatively*** _____ ***hydrocarbon parts***.
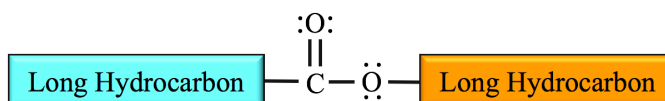
general form of a *wax*

Waxes are produced by plants and animals.

- Insects use wax to contain their larvae and store food or pollen. Examples of waxes are the esters in beeswax.

- Beeswax is a mixture of compounds, of which about 80% are waxes. The condensed and skeletal structural formulas for the *most abundant wax* molecule found in beeswax are shown below.

$$CH_3(CH_2)_{14}-\overset{\overset{\displaystyle O}{\|}}{C}-O-CH_2(CH_2)_{28}CH_3$$
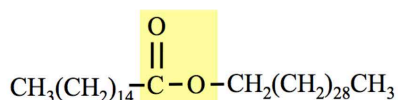
Waxes are ***hydrophobic*** because of their large and nonpolar hydrocarbon parts.

- Sheep secrete a wax called *lanolin* which protects their wool and skin from the environment and helps shed water from their coats.

- Plants secrete waxes which help them control hydration and evaporation.

Examples of Esters Found in Waxes			
Common Name	**Most Abundant Ester**	**Source**	**Uses**
beeswax	$CH_3(CH_2)_{13}COOCH_2(CH_2)_{27}CH_3$	honeycomb	candles, shoe polish, wax paper
carnauba wax	$CH_3(CH_2)_{24}COOCH_2(CH_2)_{27}CH_3$	Brazilian palm	furniture, car, and floor wax
insect wax	$CH_3(CH_2)_{24}COOCH_2(CH_2)_{27}CH_3$	insects	shoe polish
spermaceti	$CH_3(CH_2)_{30}COOCH_2(CH_2)_{14}CH_3$	whale's head	lubricant
jojoba wax	$CH_3(CH_2)_{18}COOCH_2(CH_2)_{18}CH_3$	jojoba bush	candles, cosmetics, soap additive

Formation of Waxes

In chapter 9, you learned that in *esterification*, carboxylic acids react with alcohols to form esters.

Waxes are formed by the *esterification* reaction of *fatty acids* with *large alcohols*.

- In this reaction, the **OH** from the fatty acid and an **H** from the alcohol are removed, and then combined to form **H₂O**. The oxygen (**O**) and hydrocarbon that was originally part of the alcohol, forms a new bond to the fatty acid's carbonyl carbon.

$$\underset{\text{fatty acid}}{\boxed{\text{Long Hydrocarbon}}-\overset{\overset{\text{O}}{\|}}{\text{C}}-\text{OH}} + \underset{\text{large alcohol}}{\text{H}-\text{O}-\boxed{\text{Long Hydrocarbon}}} \rightleftharpoons \underset{\text{wax}}{\boxed{\text{Long Hydrocarbon}}-\overset{\overset{\text{O}}{\|}}{\text{C}}-\text{O}-\boxed{\text{Long Hydrocarbon}}} + \underset{\text{water}}{\text{H}_2\text{O}}$$
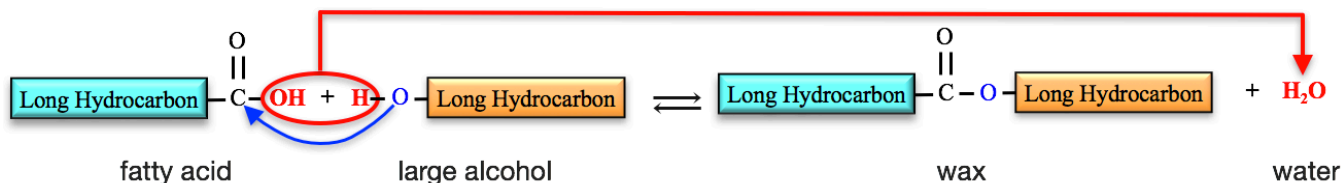
A specific example of the formation of a wax molecule in an esterification reaction is shown below.

$$CH_3(CH_2)_{14}\,\overset{\overset{\text{O}}{\|}}{C}-\text{OH} + \text{H}-\text{O}-CH_2(CH_2)_{28}CH_3 \rightleftharpoons CH_3(CH_2)_{14}\,\overset{\overset{\text{O}}{\|}}{C}-\text{O}-CH_2(CH_2)_{28}CH_3 + H_2O$$
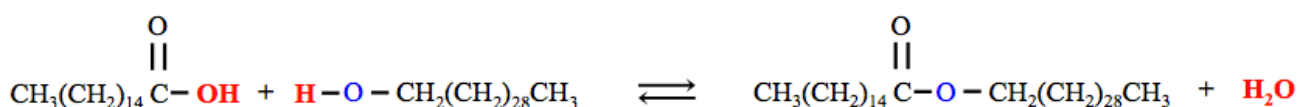
Understanding Check

Draw the condensed structure of the wax that is produced in the reaction shown here.

$$CH_3(CH_2)_{22}\,\overset{\overset{\text{O}}{\|}}{C}-\text{OH} + \text{H}-\text{O}-CH_2(CH_2)_{26}CH_3 \rightleftharpoons$$
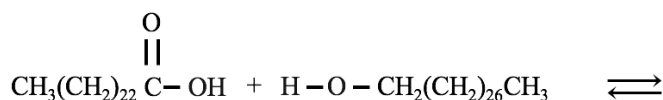
Triglycerides

The Structure of Triglycerides

Triglycerides - also referred to as *triacylglycerides* - are **triesters**.

- The reason for this classification is that they contain **three** _____-*type bonds*.

The triglyceride bonding pattern can be seen in the line bond, condensed, and space-filling structures shown here. The ester bonding patterns are highlighted in yellow.
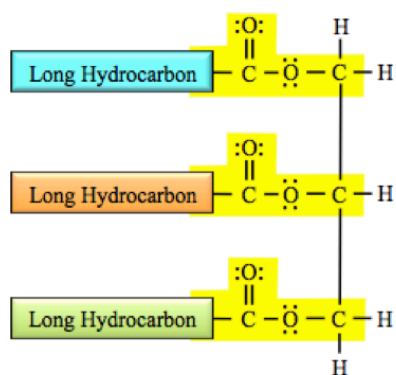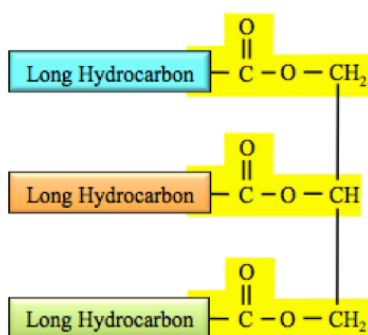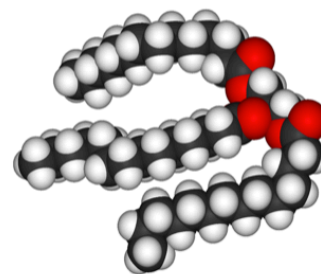
line bond structure   condensed structure   space-filling model

The Formation of Triglycerides

Triglycerides are formed in the esterification reaction of *three fatty acid molecules* with _____ (an alcohol with three hydroxyl groups – a *tri*ol).

three fatty acid molecules   a glycerol molecule   a triglyceride   +   **three** H_2O molecules
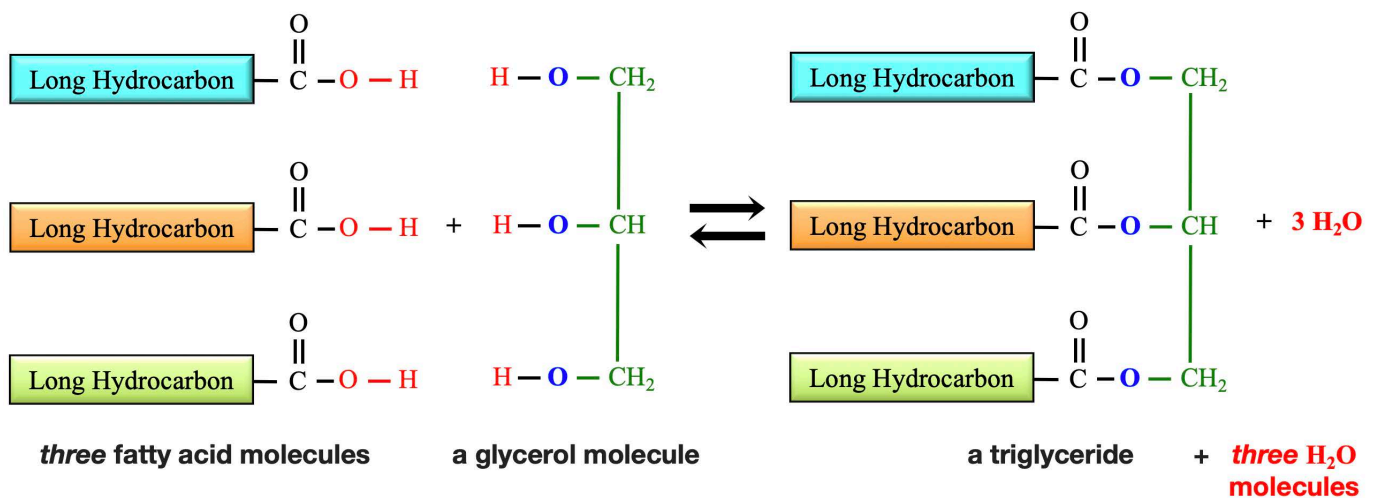
When molecules from particular organic families - such as the three fatty acids and glycerol in the formation of a triglyceride - react to form a large molecule, or when a large molecule is broken down to form them, they are often referred to as "_____."

- For example, a *triglyceride* contains *three* **fatty acid residues** and a **glycerol residue**.
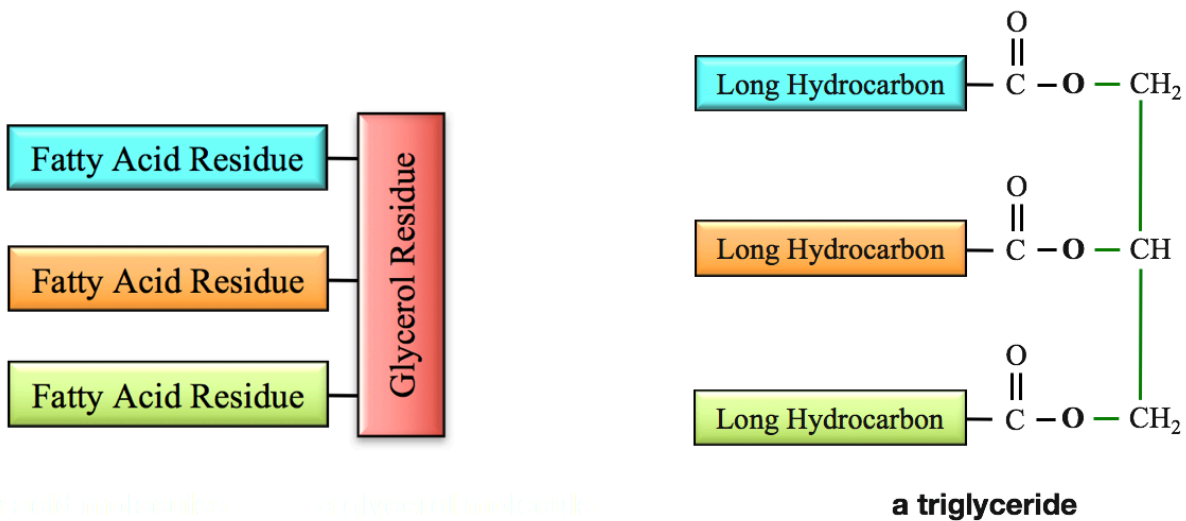
a triglyceride

The part that was originally from glycerol – the glycerol residue - is sometimes called the "**glycerol backbone**."

9

$$CH_3(CH_2)_{10}\overset{\displaystyle O}{\overset{\displaystyle \|}{C}}-OH$$
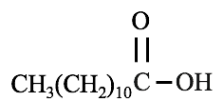
lauric acid

Classification of Triglycerides: Fat vs. Oil

The terms "fat" and "oil" can each have multiple meanings and, worse, are often used ambiguously.   In the most general sense, the term "*oil*" is defined as any nonpolar, viscous liquid.

In the context of *triglycerides*:

- The term "_____" is generally used for a triglyceride that is _____ *at room temperature.*

- The term "_____" is generally used for a triglyceride that is _____ *at room temperature.*

Our use of the term "fat" in this context should not be confused with the common practice using the term "fat" for adipose tissue in humans and animals.   Adipose tissue is composed of cells that store triglycerides.

Solid triglycerides made by *animals* are referred to as **animal fat**.

- Animal fat can be separated from other animal parts in a process called **rendering**. Fat from *pigs* is used in food products and is called **lard**. Fat from *chickens* that is used in food products is called **schmaltz**. Fat from *beef and sheep* is called **tallow**, and is used primarily for producing soap and in animal feed.   Fat from *milk* is called **butterfat**, **clarified butter**, or **ghee**. The food product that is commercially marketed as "butter" contains about 80% fat, 15% water, and 5% protein and other substances. Butterfat is usually, but not always, made from *cow's milk*.

    Important Roles of Triglycerides in Animals:

    - Energy storage

    - Production of **ATP**

    - Provision of fatty acids for the production of other lipids

    - Insulation

10

Liquid triglycerides that are made by plants are referred to as **vegetable oils**. Vegetable oils are used for cooking and in food products, biofuels, cosmetics, and soaps. Evidence of human purification of vegetable oils goes as far back as 4000 years (*"4,000-year-old 'kitchen' unearthed in Indiana". Archaeo News. January 26, 2006*).

Some Vegetable Oils and Their World Consumption, Primary Uses, and Sources

Vegetable Oil	Worldwide Consumption (metric tons)	Primary Uses and Sources
palm oil	41.3	cooking oil, biofuel (from palm fruit mesocarp pulp)
soybean oil	41.3	cooking oil
canola oil	18.2	cooking oil (comes from a variety of rapeseeds)
sunflower oil	9.9	cooking oil, biodiesel (from sunflower seed)
cottonseed oil	5.0	food products
palm kernel oil	4.8	cooking oil, food products (from palm seed)
peanut oil	4.8	cooking oil
coconut oil	3.5	cooking oil and soap making
olive oil	2.8	cooking oil, cosmetics, soaps, fuel for traditional oil lamps (from whole olives)

Worldwide Consumption data is from the US Department of Agriculture for 2007/2008

Fish oil is purified from tissue and belly cavities of oily fish, such as sardines, herring, anchovies, salmon, trout, tuna, and mackerel. Some fish, such as shark and cod, have significant amounts of oil stored in their liver.

In nutritional labeling, **all triglycerides,** *whether from plants or animals, solid or liquid*, are often grouped together and called "**fat**" or included in the "**total fat**" category.

Sample label for
Macaroni & Cheese

Nutrition Facts
Serving Size 1 cup (228g)
Servings Per Container 2

Amount Per Serving

Calories 250   Calories from Fat 110

% Daily Value*

Total Fat 12g	**18%**
Saturated Fat 3g	**15%**
Trans Fat 3g	
Cholesterol 30mg	**10%**
Sodium 470mg	**20%**
Total Carbohydrate 31g	**10%**
Dietary Fiber 0g	**0%**
Sugars 5g	
Protein 5g	

Vitamin A	4%
Vitamin C	2%
Calcium	20%
Iron	4%

* Percent Daily Values are based on a 2,000 calorie diet. Your Daily Values may be higher or lower depending on your calorie needs.

	Calories	2,000	2,500
Total Fat	Less than	65g	80g
Sat Fat	Less than	20g	25g
Cholesterol	Less than	300mg	300mg
Sodium	Less than	2,400mg	2,400mg
Total Carbohydrate		300g	375g
Dietary Fiber		25g	30g

Classification of Triglycerides: Saturated vs. Unsaturated Triglycerides

We classify triglyceride molecules as either **saturated** or **unsaturated** using the same criteria as we used for **fatty acids**.

- **Saturated triglyceride** molecules ___ _____ contain *carbon-carbon* _____ *bonds*.

- **Unsaturated triglyceride** molecules contain ____ __ _____ *carbon-carbon double bonds*.

    o **Unsaturated triglycerides** are often further subcategorized as either _____*unsaturated* or _____*unsaturated*.

    - *Monounsaturated* triglycerides contain only _____ carbon-carbon double bond.

    - *Polyunsaturated* triglycerides contain ____ __ _____ carbon-carbon double bonds.

Just like *fatty acids*, triglycerides with higher degrees of saturation (fewer carbon-carbon double bonds) are more flexible and can pack closer to each other than less saturated triglycerides.

- It is for this reason that the noncovalent interactions, and therefore the melting points of triglycerides increase with the degree of saturation.

Since animal fats have a relatively **high** *degree of saturation*, they are solid at room temperature.

- Consider beef-fat or butter.

Vegetable oils and fish oils have a **lower** *degree of saturation* than animal fats, and are therefore **liquid** at room temperature.

- Consider olive or corn oil.

- Palm and coconut oil are *semi-solid* at room temperature because they contain a higher degree of saturation than the other vegetable oils.

Understanding Check

Categorize each one of these triglycerides as being either **saturated** or **unsaturated**.
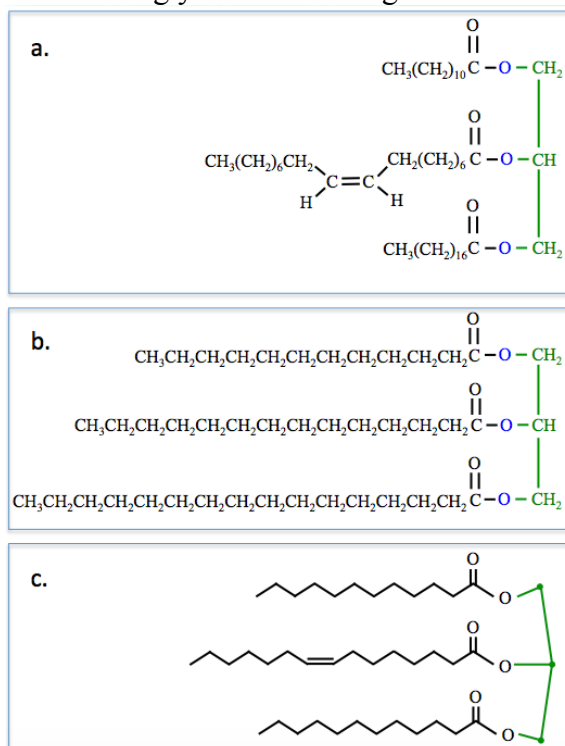
Understanding Check

Using table of fatty acids shown below, draw the *skeletal structure* of a *saturated triglyceride*.

	Some Fatty Acids that are Frequently Encountered in Biological Systems			
Number of Carbons	Number of Carbon-Carbon Double Bonds	Common Name	Condensed Structure	Major Source
12	0	lauric acid	$CH_3(CH_2)_{10}COOH$	coconut
14	0	myristic acid	$CH_3(CH_2)_{12}COOH$	nutmeg
16	0	palmitic acid	$CH_3(CH_2)_{14}COOH$	palm
16	1	palmitoleic acid	$CH_3(CH_2)_5CH=CH(CH_2)_7COOH$	macadamia, animals
18	0	stearic acid	$CH_3(CH_2)_{16}COOH$	animal fat
18	1	oleic acid	$CH_3(CH_2)_7CH=CH(CH_2)_7COOH$	olives
18	2	linoleic acid	$CH_3(CH_2)_4(CH=CHCH_2)_2(CH_2)_6COOH$	safflower, soy
18	3	linolenic acid	$CH_3CH_2(CH=CHCH_2)_3(CH_2)_6COOH$	flax, corn

Reactions of Triglycerides

1) **Catalytic Hydrogenation**

   - unsaturated triglyceride $+$ $H_2 \rightarrow$ more saturated triglyceride

2) **Oxidation**

   - triglyceride $+ O_2 \rightarrow$ small organic molecules

3) **Hydrolysis/Saponification**

   - hydrolysis of the ester group in the presence of hydroxide (OH^-)

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1) Catalytic Hydrogenation

The *carbon-carbon* double bonds of triglycerides will react with hydrogen gas (H_2) in the presence of a catalyst (at high temperatures). In chapter 6, you learned about the ***hydrogenation*** of an alkene's carbon-carbon double bonds. We were able to predict the product by "adding H_2 across the carbon-carbon double bond." *We can do the same for triglycerides*.

If enough H_2 is supplied, the carbon-carbon double bonds in *unsaturated triglycerides* become_____ _____; a *saturated triglyceride* is formed.

A hydrogen atom is added to each of the double-bonded carbons, thereby converting them into single bonds. The reaction must be done at a high temperature and on the surface of a *metal catalyst*. The catalysts used are typically platinum, palladium, rhodium, or ruthenium. An example of a chemical equation for *complete saturation* during a ***catalytic hydrogenation reaction*** is shown below.

an unsaturated triglyceride   **a saturated triglyceride**
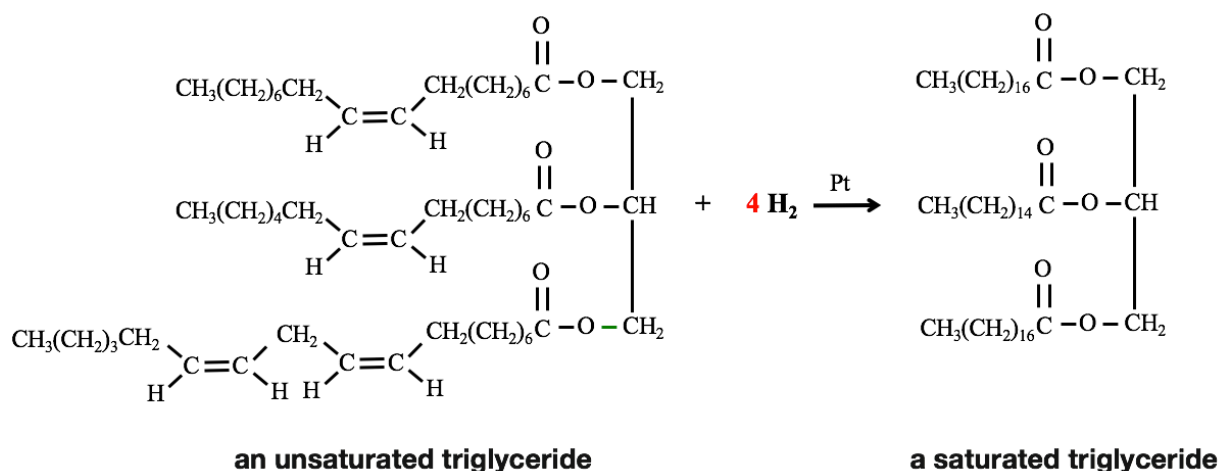
If the amount of H_2 is limited, or the chemical reaction time is reduced, then the triglyceride product will contain *some unreacted* carbon-carbon double bonds.

- We call this process _____ *hydrogenation*.

- **Example** of a *partial hydrogenation reaction*:

an unsaturated triglyceride   a *partially hydrogenated* **triglyceride**
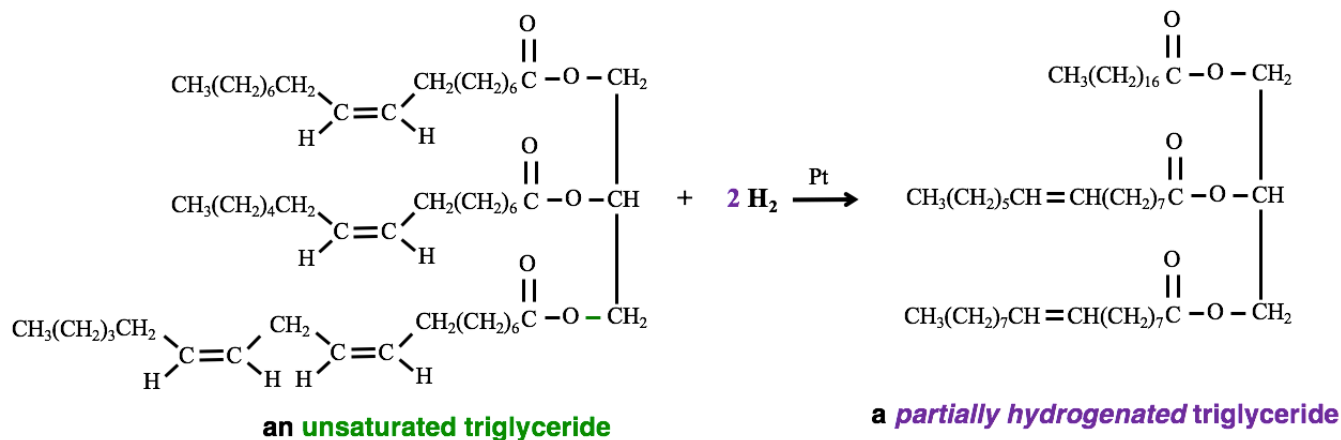
Note that the triglyceride reactant in this example contains **four** double bonds, however, only **two** moles of H_2 were supplied, therefore only **two** of the carbon-carbon double bonds became saturated.

Triglycerides that are found in nature, with few exceptions, contain only *cis* fatty acid residues. Note that the ***reactant*** for the reaction shown above is drawn using *cis* configurations around *all of the carbon-carbon double bonds*.

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The catalytic hydrogenation of vegetable oils is a very important reaction for the food industry.

Solid triglycerides are advantageous in baking because of the texture that is achieved when they are mixed with flour. Animal fat - butter - can be used, however it is more expensive than vegetable oils.

The partial hydrogenation of vegetable oils produces what is referred to as **partially hydrogenated vegetable oil** or **shortening**.

Margarine and *Crisco* are examples of partially hydrogenated vegetable oil products.

An undesirable consequence of *partial hydrogenation* is the formation of *trans* **fats** - fats containing one or more carbon-carbon double bonds that have the *trans* configuration.

- Many of the **unreacted cis** carbon-carbon double bonds are converted to the **trans** configuration.

- **Example:** The partial hydrogenation of a naturally-occurring unsaturated *cis*-triglyceride (vegetable oil) to a partially hydrogenated *trans*-triglyceride.
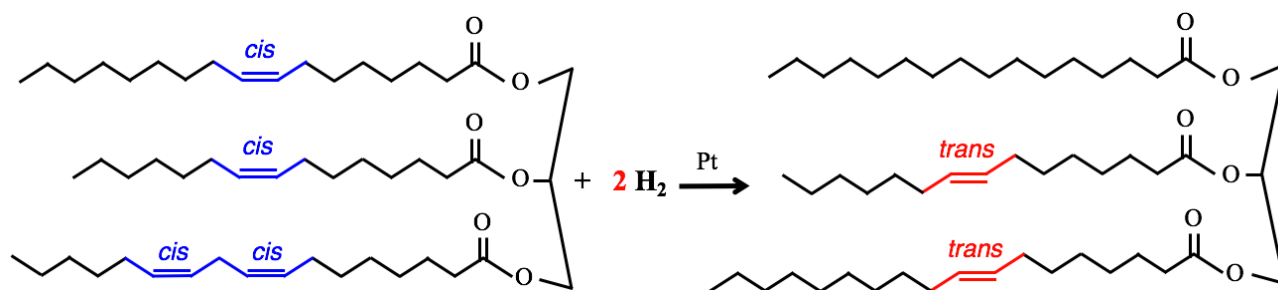
The product is a partially hydrogenated vegetable oil molecule, which typically contains one or more *trans* fatty acid residues.

Understanding Check: Draw the *condensed structure* of the saturated triglyceride that is produced from the **complete hydrogenation** of the triglyceride shown here.
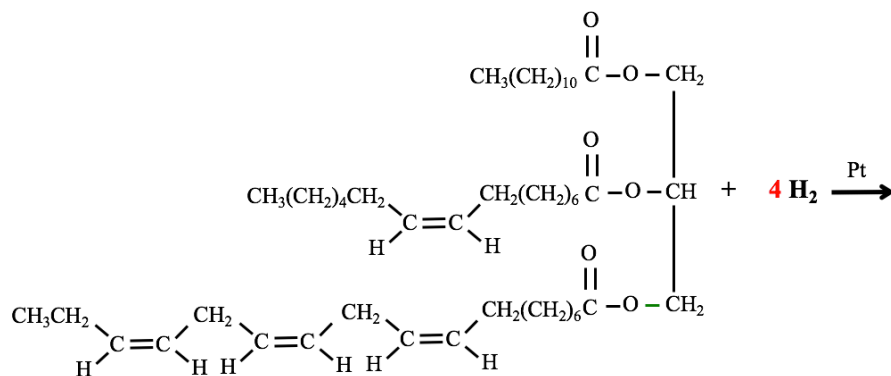
2) Oxidation of Triglycerides

Triglycerides are oxidized by oxygen gas (O_2) to form _____ _____ and _____.

Prediction of the *specific* aldehydes and carboxylic acids that are produced is beyond the scope of this book, however a couple of typical aldehydes and a carboxylic acid that can be produced in this reaction are shown here (below, right).

Many of the aldehydes and carboxylic acids that are produced in this reaction have foul odors.

When triglyceride food products undergo this reaction, it is called "_____"; the food substances are said to become "**rancid**."

In order to prevent or slow the rancidification of foods, the oxygen supply can be limited by air-tight containers and packaging, and the food can be stored at low temperatures.
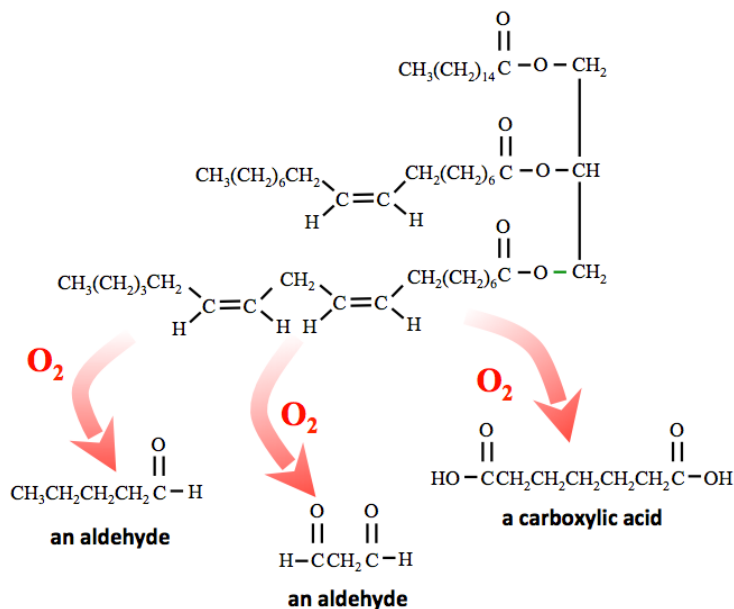
3) Saponification

In the **saponification** reaction**,** a **triglyceride** reacts with **hydroxide ions** to produce _____ **long-chain carboxylate ions** and **glycerol** (an alcohol).

- The general form of this reaction is shown below.
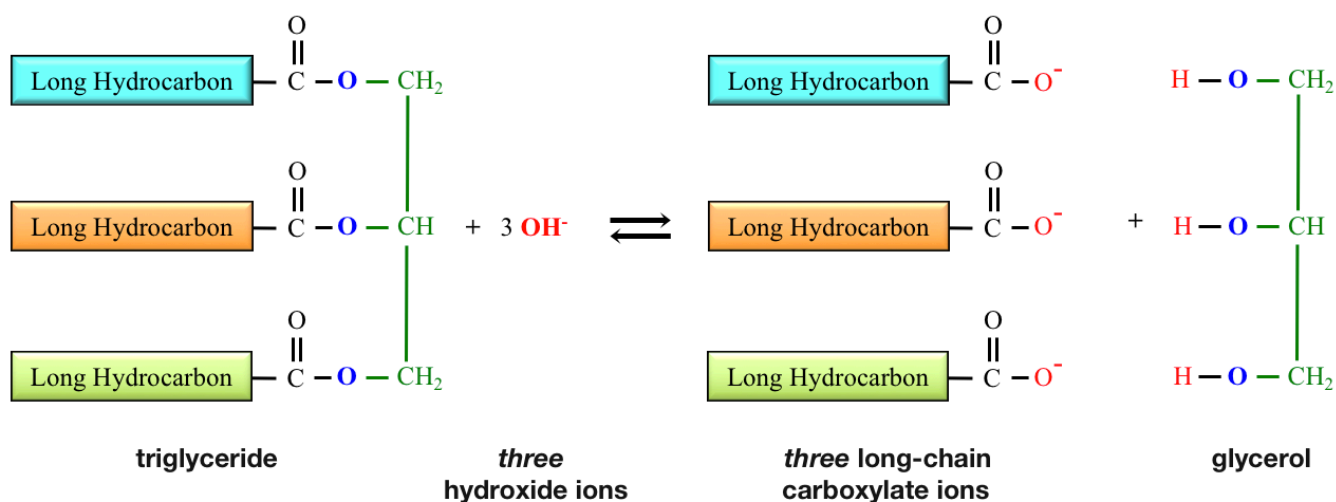
Example *of the hydrolysis of a **specific** triglyceride:*

| triglyceride | three hydroxide ions | three long-chain carboxylate ions | glycerol |
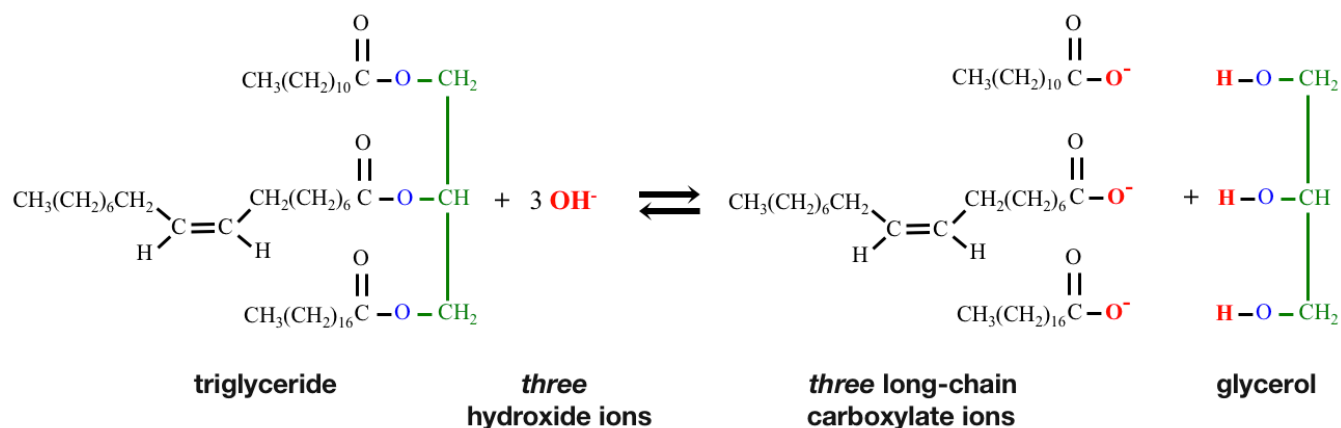
The hydroxide ions in the saponification reaction come from hydroxide-containing ionic compounds, usually sodium hydroxide (**Na**OH) or potassium hydroxide (**K**OH).

- When the cation of the hydroxide-containing compound is specified, it is often written after the long-chain carboxylate ion products as shown below:

| triglyceride | sodium hydroxide | three long-chain carboxylate ions (fatty acid salts) | glycerol |
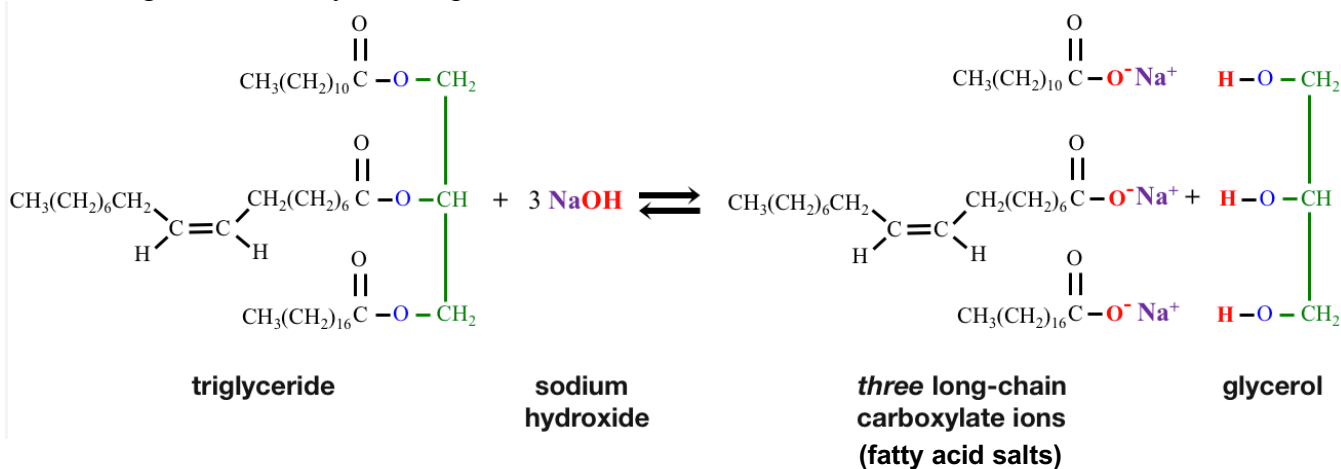
When the **Na⁺** or **K⁺** *cations* are included in chemical equations, as shown above, be careful to avoid the ***common misconception*** of interpreting the negative sign of the carboxylate ion's *formal charge* for a covalent bond to the sodium or potassium ion.

The compounds formed from the long-chain carboxylate anions and the **Na⁺** (or **K⁺**) cations are ***ionic*** and are called _____ _____ _____.

The long-chain carboxylate ions that are produced are_____.
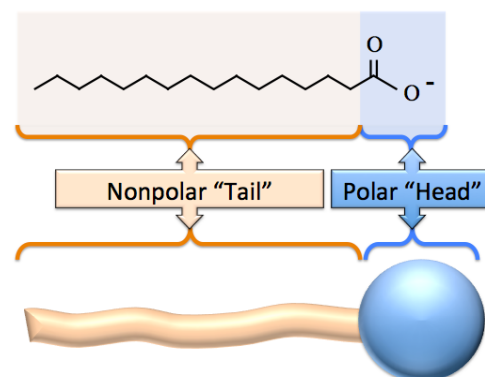
When *fatty acid salts* are formed or placed in water, **only** the cations, **Na⁺** in our example, are solvated (dissolve).

The long-chain carboxylate ions form

_____ and _____ .

Monolayer
Na⁺ ... Water
Micelle
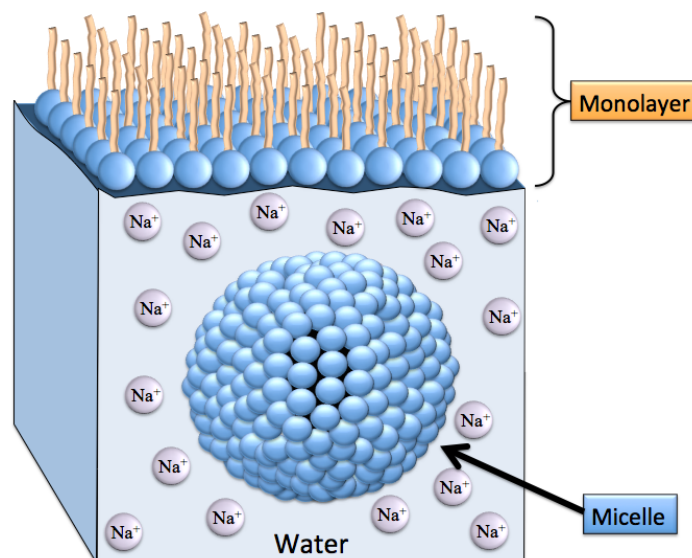
This is an important reaction because it is used to make **soap**.

Because the long-chain carboxylate ions that are produced are **amphipathic**, they act as emulsifying agents to remove nonpolar molecules (i.e. grease or oil) from surfaces, including - very importantly - skin and clothing.
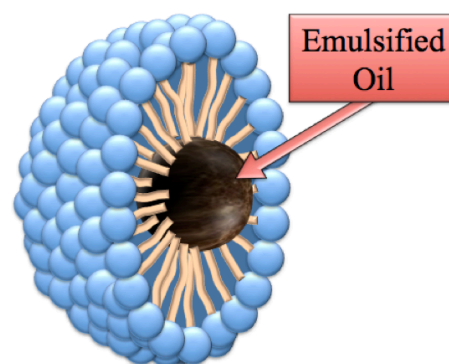
Emulsified Oil

An illustration of an oil droplet emulsified by a long-chain carboxylate ion micelle.

Understanding Check

Draw the *condensed structure* of the products for the saponification of the triglyceride shown below. Include the cations when drawing the fatty acid salts.

$$CH_3(CH_2)_{10} \overset{O}{\overset{||}{C}} - O - CH_2$$
$$CH_3(CH_2)_{12} \overset{O}{\overset{||}{C}} - O - CH \quad + \quad 3\ \textbf{NaOH} \rightleftharpoons$$
$$CH_3(CH_2)_{14} \overset{O}{\overset{||}{C}} - O - CH_2$$
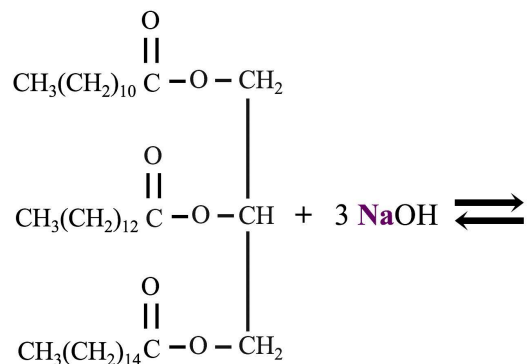
Phospholipids and Glycolipids

Phospholipids and glycolipids are best known for their presence in biological membranes.

They are amphipathic compounds that contain a polar "head" group that is very hydrophilic, and hydrophobic nonpolar "tail" groups.

Phospholipids and glycolipids are found in nature as either monolayers, micelles, or in a layer that is two molecules-thick called a "*lipid* _____ _____ " or a "*lipid* _____."
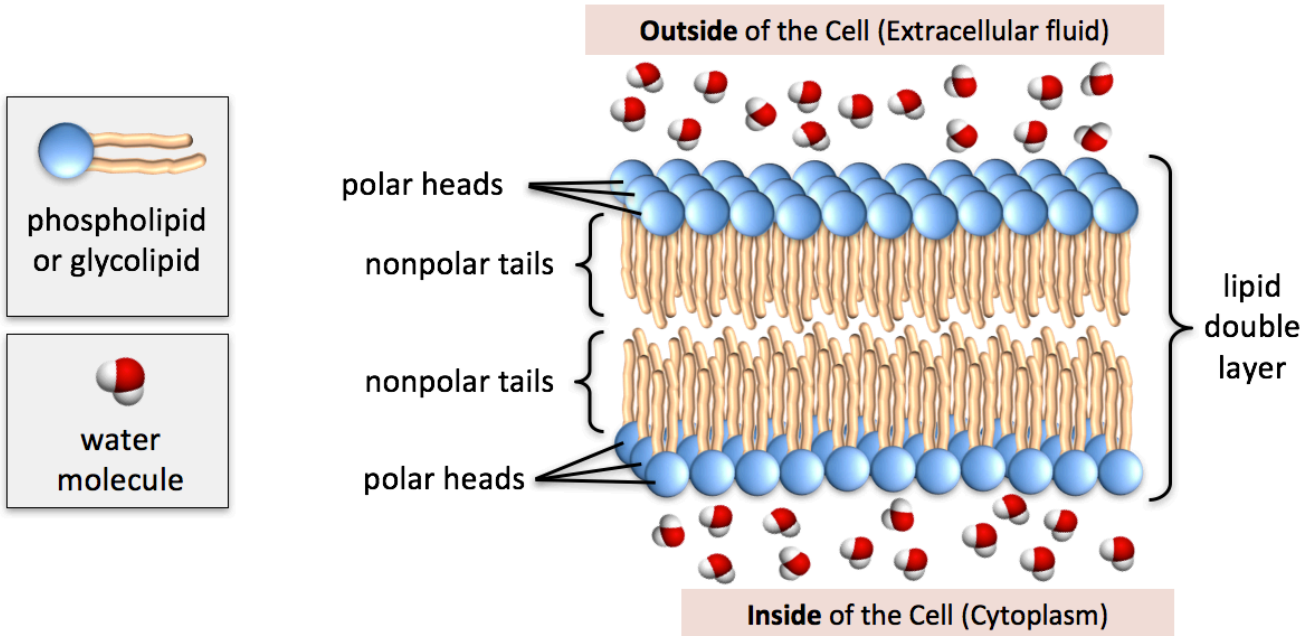
Note that the polar heads are oriented either toward the water that is inside the cell, or toward the water that is outside of the cell. The nonpolar tails in the top of the double layer are much more attracted to the nonpolar tails in the bottom of the double layer than to water or polar head groups. It is for this reason that the two monolayers have the tail-to-tail orientation. Later in this chapter, you will see that there are other components distributed throughout the lipid double layer of biological membranes, however, for simplicity, those other components are not included in the illustration (above).

Lipid double layer membranes not only occur as cell membranes, they also form specialized compartments within cells. For example, intracellular double layer membranes occur in liposomes and form the outer boundary of a cell's nucleus.

Phospholipids

There are two main classes of **phospholipids**: _____*phospholipids* and _____*phospholipids*.

- Both of these classes contain a _____ residue in their structure, it is for this reason that they are called *phospho*lipids.

1) Glycerophospholipids

Glycerophospholipids are made from the components shown here.

one *or* two fatty acids — Long Hydrocarbon $-\overset{\overset{O}{\|}}{C}-OH$; Long Hydrocarbon $-\overset{\overset{O}{\|}}{C}-OH$

glycerol —
$H-O-CH_2$
$H-O-CH$
CH_2-O-H

a phosphate (dihydrogen phosphate ion) —
$HO-\overset{\overset{O}{\|}}{\underset{O^-}{P}}-OH$

an alcohol (X = an organic group) — $HO-X$
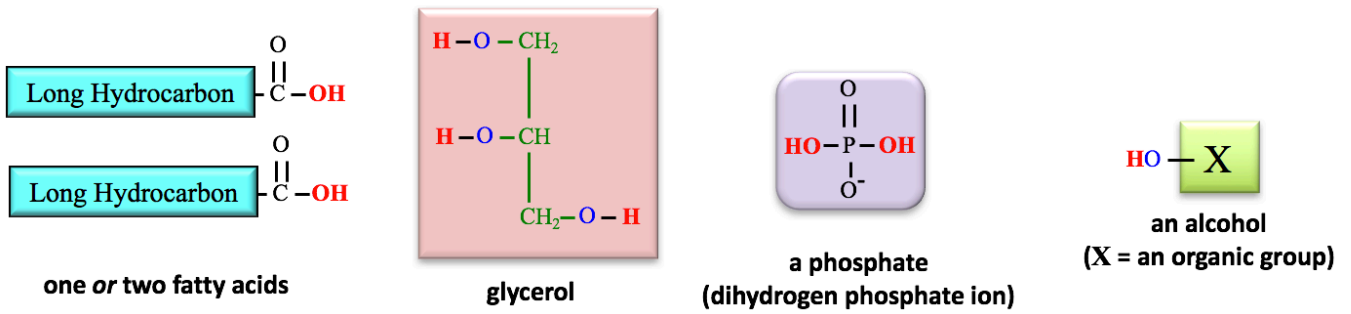
These components are bonded to each other by _____ *reactions* to form glycerophospholipids.

formation of **ester** bonds (esterification)

formation of a **phosphoester** bond

formation of a **phosphoester** bond

H_2O

general form of a glycerophospholipid:

Long Hydrocarbon $-\overset{\overset{O}{\|}}{C}-O-CH_2$
Long Hydrocarbon $-\overset{\overset{O}{\|}}{C}-O-CH$
$CH_2-O-\overset{\overset{O}{\|}}{\underset{O^-}{P}}-O-X$
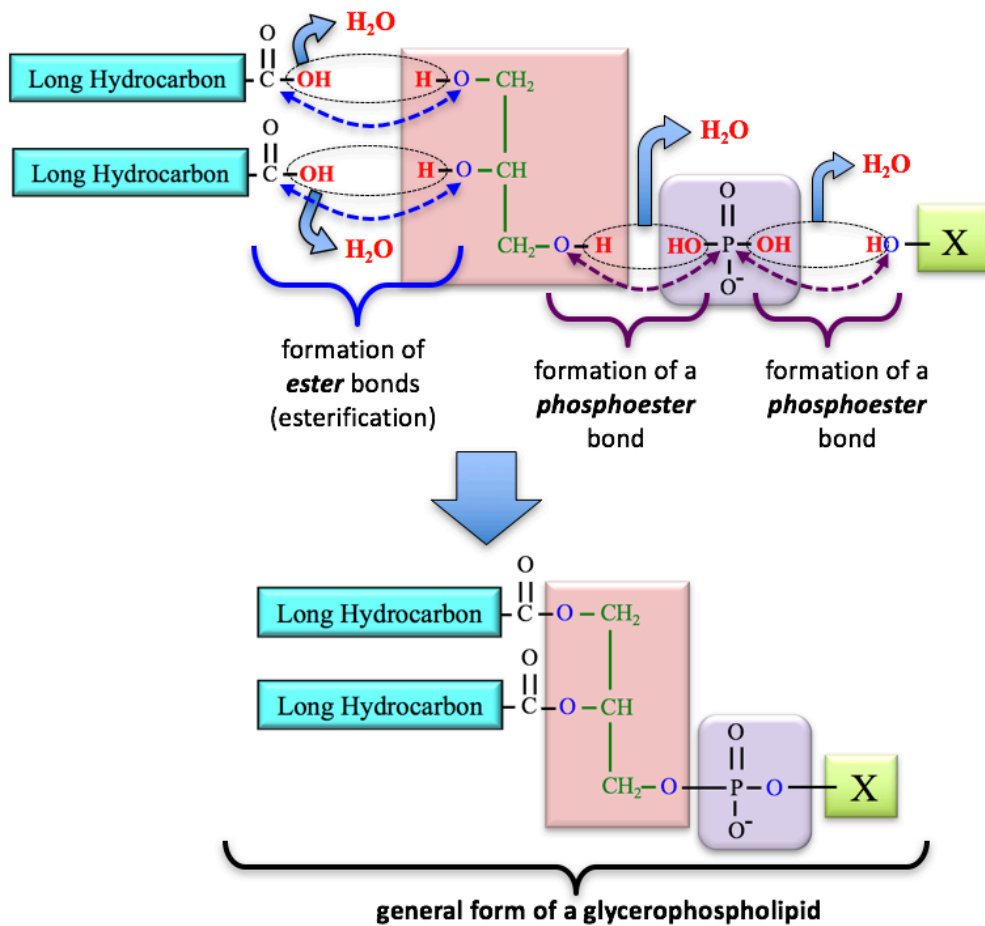
When **both** **OH**'s of a phosphate form phosphoester bonds, the bonding pattern is called a *phospho*_____ bond.

Note the similarity in the way that a carboxyl group (COOH) of a fatty acid reacts with an alcohol, and the way that a phosphate reacts with an alcohol.

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The **ester** and **phosphodiester** bonding patterns in a *glycerophospholipid* are highlighted and labeled in the structure shown below.

$$O$$
$$\|$$
Long Hydrocarbon $-C-O-CH_2$ ester bonding patterns

$$O$$
$$\|$$
Long Hydrocarbon $-C-O-CH$

$$O$$
$$\|$$
$$CH_2-O-P-O-X$$
$$|$$
$$O^-$$

phospho**di**ester bonding pattern
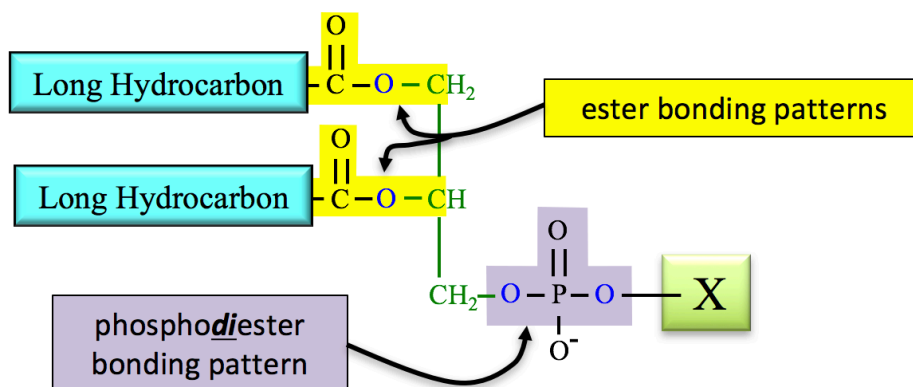
The various "residues" that make up a glycerophospholipid are labeled in the structure below.

fatty acid residues   glycerol backbone

$$O$$
$$\|$$
Long Hydrocarbon $-C-O-CH_2$

$$O$$
$$\|$$
Long Hydrocarbon $-C-O-CH$

X-group (organic group)

$$O$$
$$\|$$
$$CH_2-O-P-O-X$$
$$|$$
$$O^-$$

phosphate residue
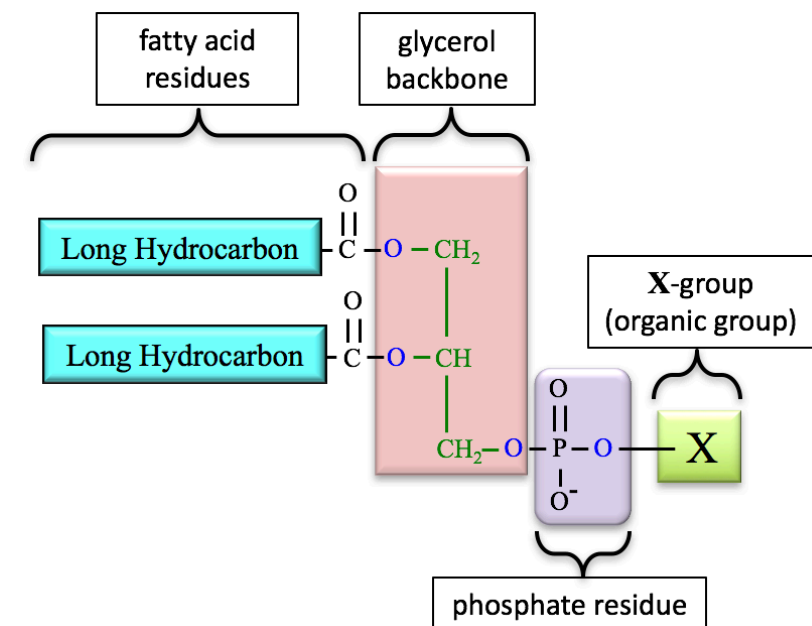
The atoms that came from glycerol are referred to the "***glycerol*** _____."

The identity of the organic "X-group" varies.

The subclasses of glycerophospholipids are determined by the identity of their X-groups.

The Three Most Common "X-Groups" found in Glycerophospholipids	
Organic "X group"	**Glycerophospholipid Class**
$-CH_2CH_2NH_3^+$	Phosphatidylethanolamine (present in *Cephalin*)
$-CH_2CH_2\overset{+}{\underset{CH_3}{\overset{CH_3}{N}}}-CH_3$	Phosphatidylcholine (present in *Lecithin*)
$-CH_2\underset{\overset{+}{NH_3}}{CH}\overset{O}{\overset{\|}{C}}-O^-$	Phosphatidylserine (present in *Cephalin*)
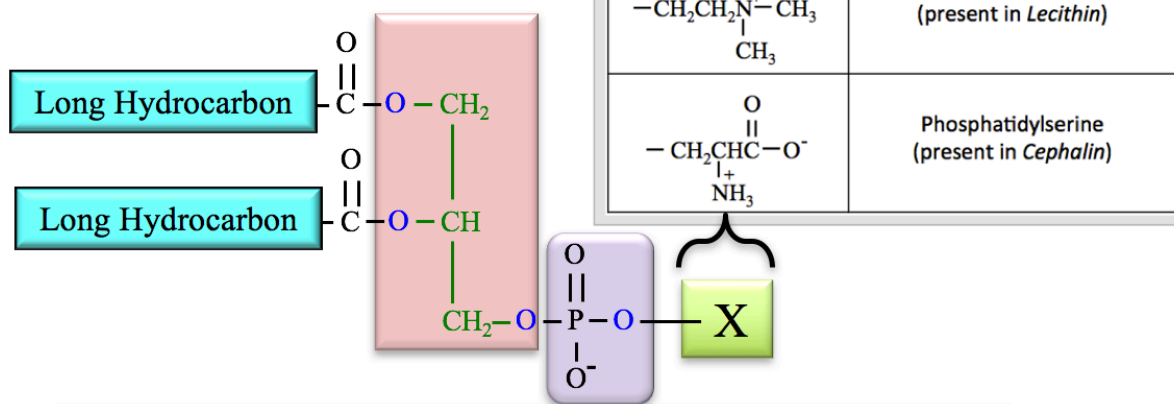
Phosphatidylethanolamines and **phosphatidylserines** are components of *cephalin*.

- Cephalin is found throughout the body, with especially large amounts present in the brain and nerve tissue.

Phosphatidylcholines are a component of *lecithin*.

- Lecithin is a term for the yellow-brown fatty substances present in animal and plant tissues.

A specific example of a *glycerophospholipid* is shown below.

Organic "X group"	**Glycerophospholipid Class**
$-CH_2CH_2NH_3^+$	Phosphatidylethanolamine (present in *Cephalin*)
$-CH_2CH_2\overset{+}{\underset{CH_3}{\overset{CH_3}{N}}}-CH_3$	Phosphatidylcholine (present in *Lecithin*)
$-CH_2\underset{\overset{+}{NH_3}}{CH}\overset{O}{\overset{\|}{C}}-O^-$	Phosphatidylserine (present in *Cephalin*)
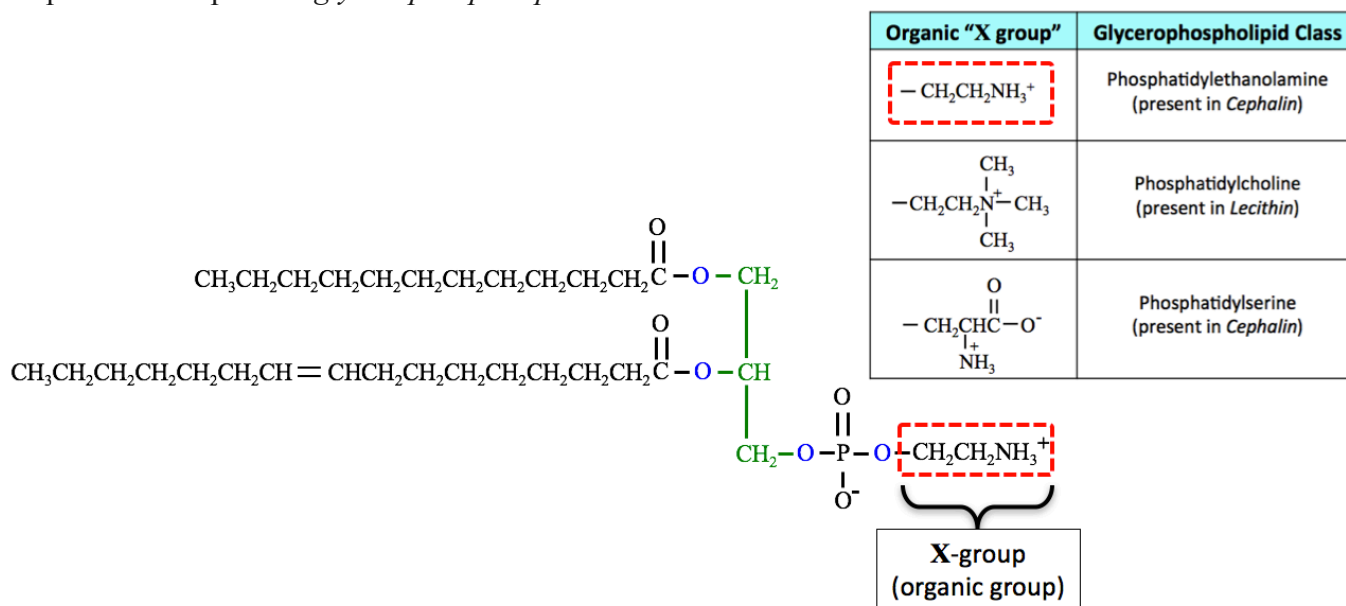
This particular glycerophospholipid is classified as a **phosphatidylethanolamine** because the X-group is - $CH_2CH_2NH_3^+$.

Glycerophospholipids have a *polar head* region and *nonpolar tails*, as depicted for the glycerophospholipid below.

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \overset{\overset{\displaystyle O}{\|}}{C} - O - CH_2$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH = CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2 \overset{\overset{\displaystyle O}{\|}}{C} - O - CH$$

$$CH_2 - O - \overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle O^-}{|}}{P}} - O - CH_2CH_2NH_3{}^+$$

Nonpolar Tails   **Polar Head**
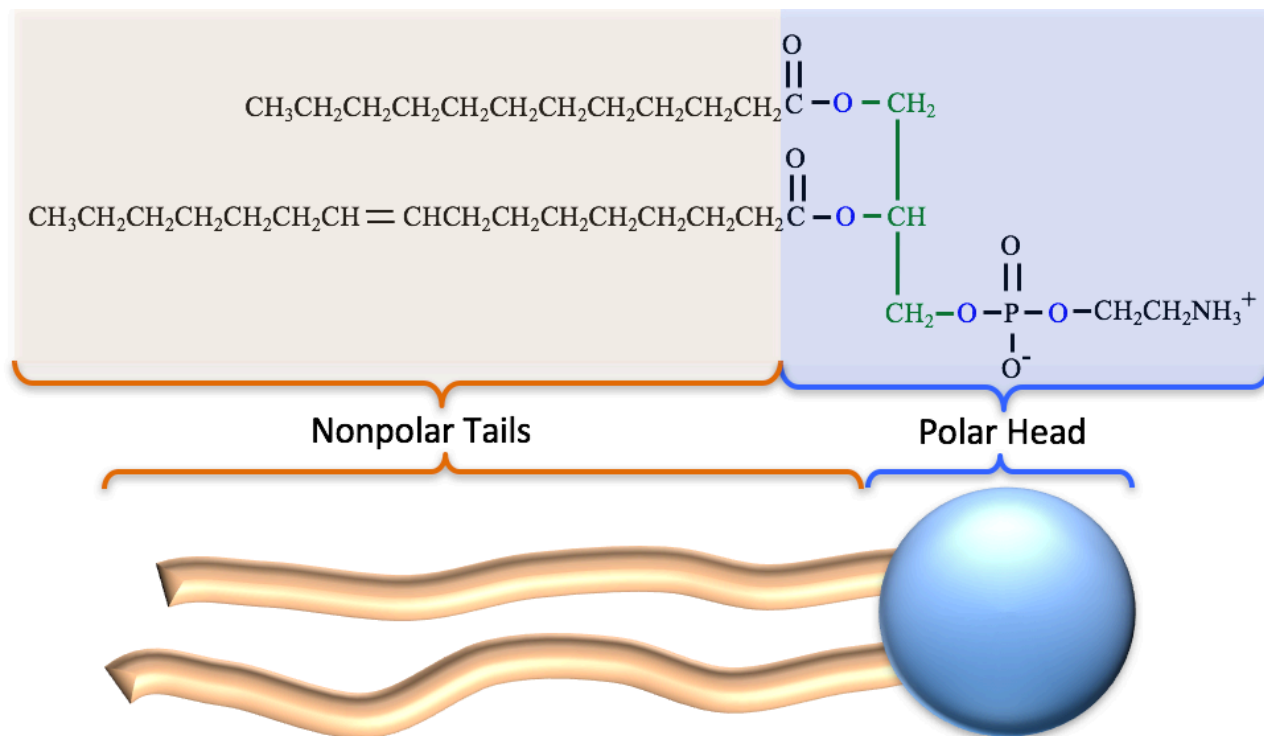
The *polar head* region is quite **hydrophilic**. This region is attracted to water through **dipole-dipole** interactions because it contains several "highly polar" bonds. It can **hydrogen bond** with water. The polar head is also attracted to water through **ion-dipole interactions** because of the *formal charge* on both an oxygen *and* a nitrogen. The hydrocarbon chains of the fatty acid residues make up the nonpolar tails.

2) Sphingophospholipids

The difference between the two classes of phospholipids - *glycerophospholipids* and *sphingophospholipids* - is that **sphingophospholipids** have a "_____ **backbone**" instead of a *glycerol backbone*.

Sphingophospholipids are made from the components shown below.

sphingosine

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH = CH - CH - OH$$

$$H - N - CH$$
$$| \quad |$$
$$H$$
$$CH_2 - O - H$$

| Long Hydrocarbon |
a fatty acid

$$\overset{\overset{\displaystyle O}{\|}}{C} - OH$$

$$\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle O^-}{|}}{HO - P - OH}}$$

a phosphate
(dihydrogen phosphate ion)

$$HO - X$$
an alcohol
(X = an organic group)

23
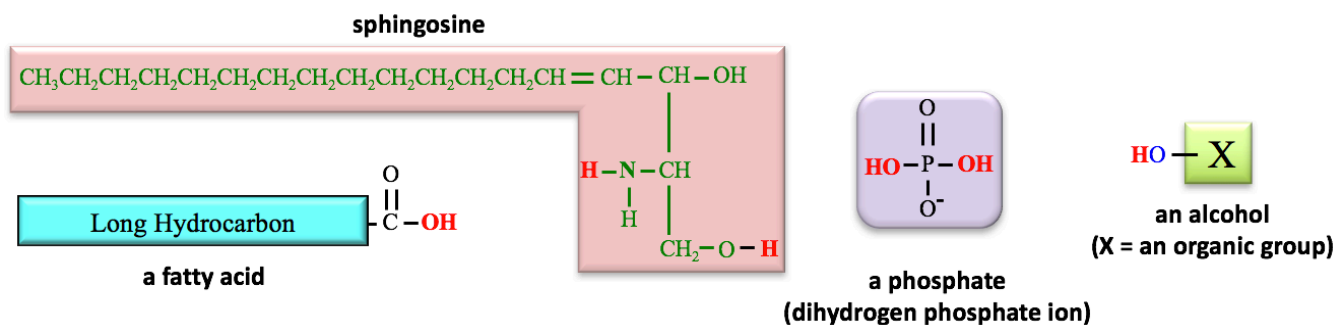
Let's take a look at the bonds that are made in the formation of a *sphingophospholipid*.

formation of an **amide** bond

formation of a **phosphoester** bond

formation of a **phosphoester** bond

sphingosine backbone

general form of a sphingophospholipid
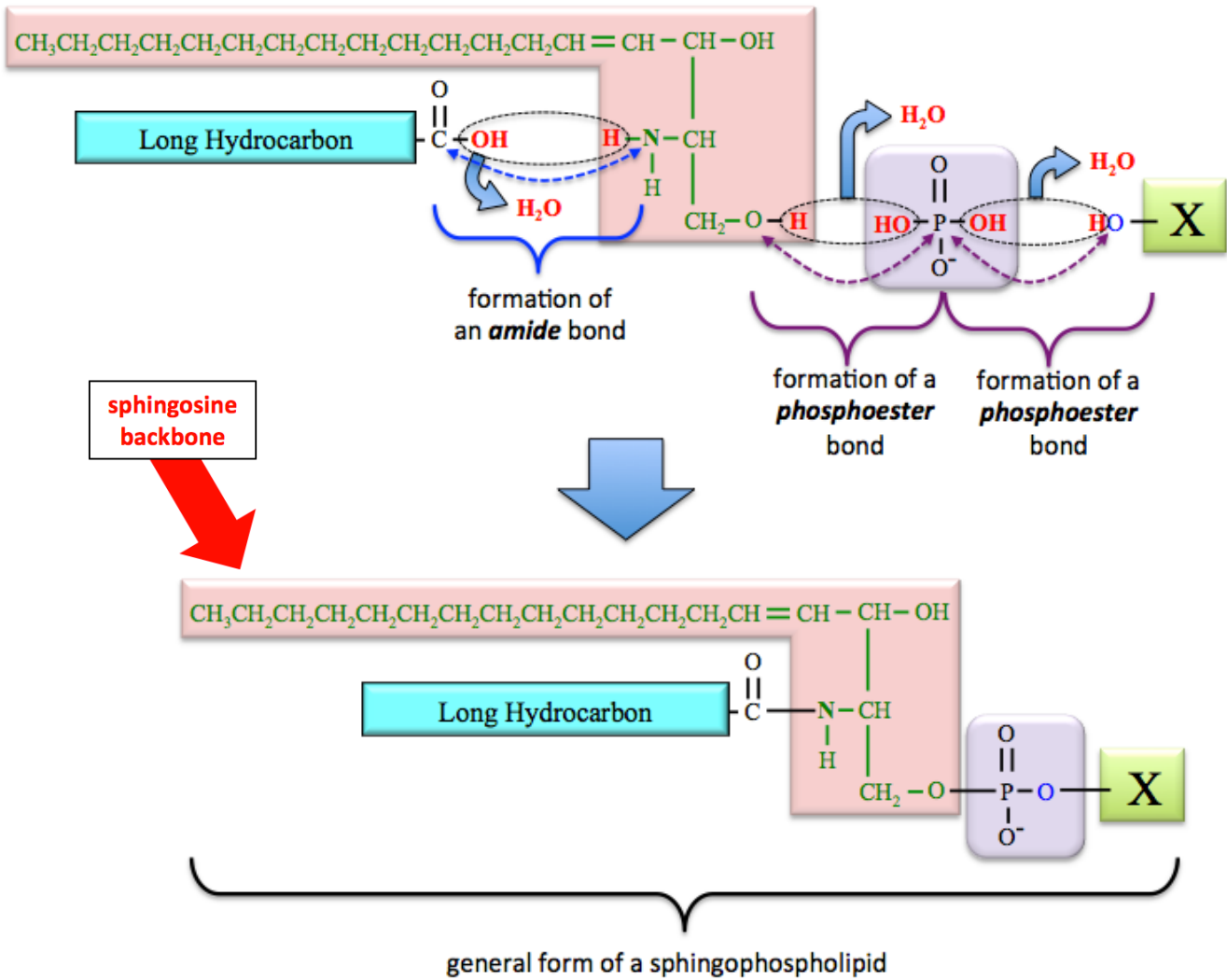
The **amide** and **phosphodiester** bonding patterns for a sphingophospholipid are indicated in the structure shown below.

amide bonding pattern

phospho**di**ester bonding pattern
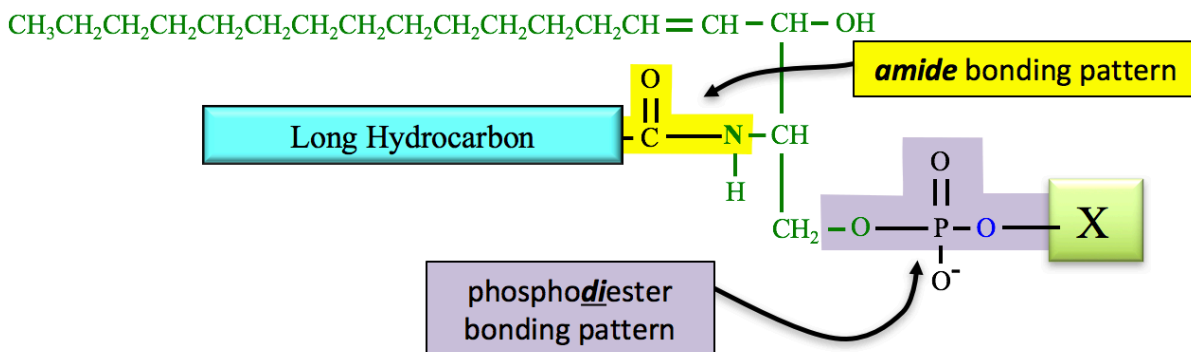
As was the case for glycerophospholipids, sphingophospholipids are classified based on their **X**-group.
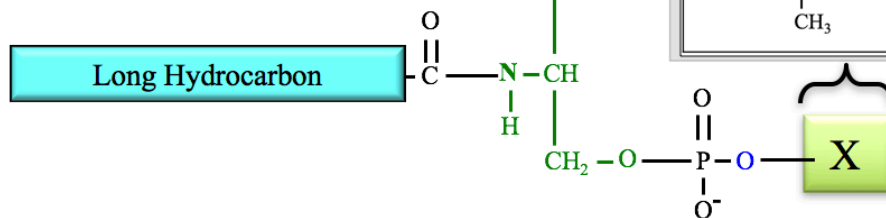
The Most Common "X-Groups" found in Sphingophospholipids	
"X-group"	**Sphingophospholipid Class**
$-H$	Ceramide
$- CH_2CH_2NH_3^+$ or $-CH_2CH_2\overset{+}{N}(CH_3)_3$	Sphingomyelin

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH = CH - CH - OH$$

Long Hydrocarbon

Sphingomyelins have this name because they are the most abundant class of *phospholipid* found in myelin (although they are the most abundant *phospho*lipids found in myelin, the most abundant *lipids* in myelin are *glycolipids*, which I will discuss soon). Myelin is a combination of lipids (85%) and proteins (~15%), assembled as a **bilayer** that wraps around nerve cell axons. The myelin sheath is an electrical insulator and its main function is to increase the speed at which nerve impulses are propagated along axons.
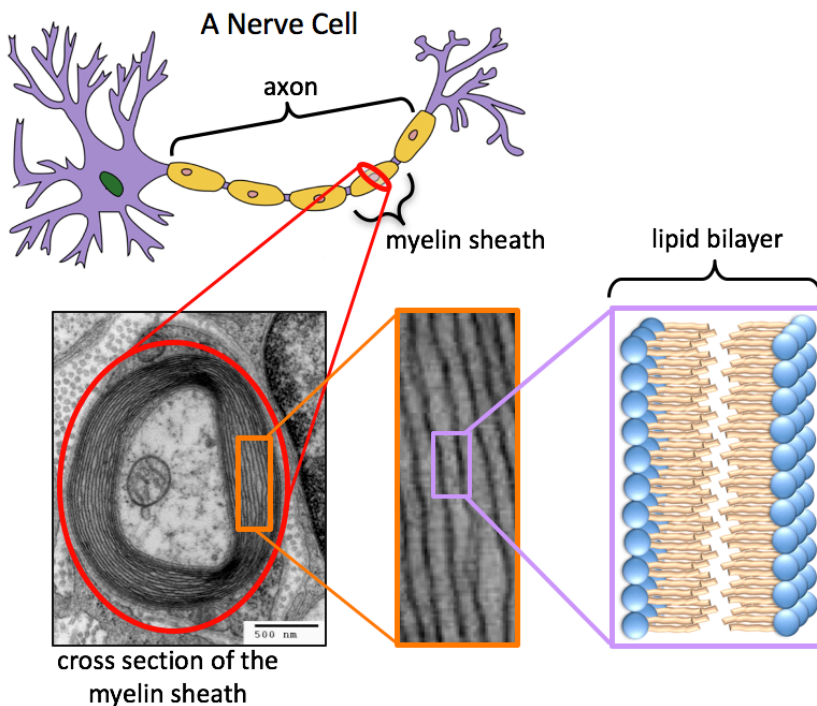
If the X-group of a sphingophospholipid is a hydrogen (instead of an organic group), then it is classified as a **ceramide**. *Ceramides* are found in cell membranes and in the myelin sheath of nerve cells.

A specific example of a sphingophospholipid (a sphingomyelin) is shown below.
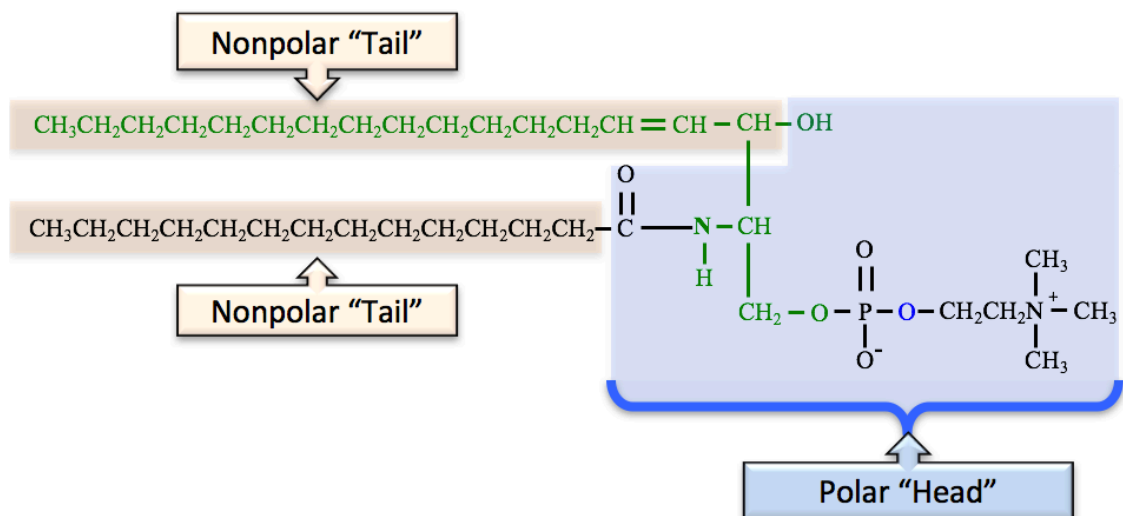
If you are looking at a color image, the atoms from sphingosine are in green font. I arbitrarily chose to use *myristic acid* as the fatty acid residue; any fatty acid could have been used.

This particular sphingophospholipid is classified as a *sphingomyelin* since the X-group is $CH_2CH_2N^+(CH_3)_3$.

Sphingophospholipids are amphipathic; they have a *polar head* region and *nonpolar tails*.

Note that most of the atoms from sphingosine are part of one of the lipid's nonpolar tails.

Review of Phospholipid Structure: Glycerophospholipids vs. Sphingophospholipids

If you are given the structure of a **phospholipid**, you should be able to determine if it is a *glycerophospholipid* or a *sphingophospholipid*.

The key to doing so is to identify either a *glycerol backbone* (for glycerophospholipids) or a *sphingosine backbone* (for sphingophospholipids).

An easy way to do so is to look for the **nitrogen** in the **amide bond** between the fatty acid residue and the *sphingosine backbone*. This *amide* bonding pattern is *present in sphingophospholipids, but not in glycerophospholipids*.
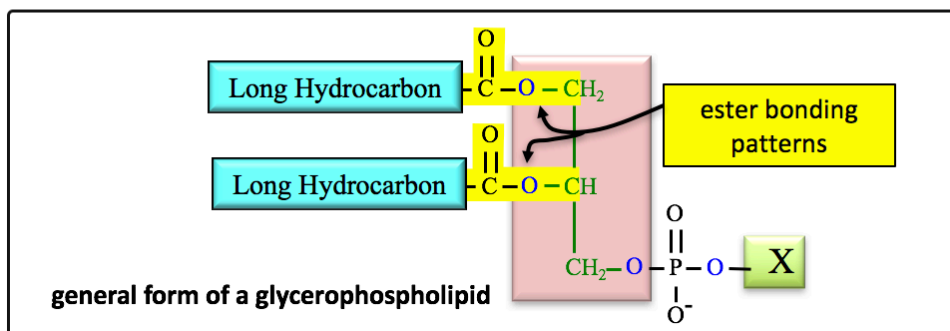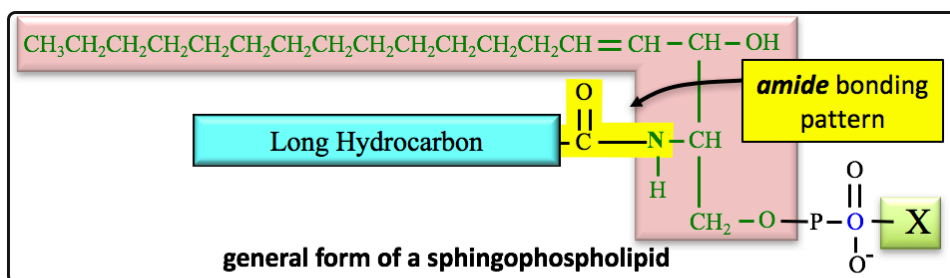
Understanding Check

Identify (circle) the ***nitrogen atom*** that is contained in the amide bonding pattern in the sphingophospholipid shown here.

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH = CH - CH - OH$

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle H}{|}}{C}}-N-CH$

$CH_2-O-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{N}}}-CH_3$
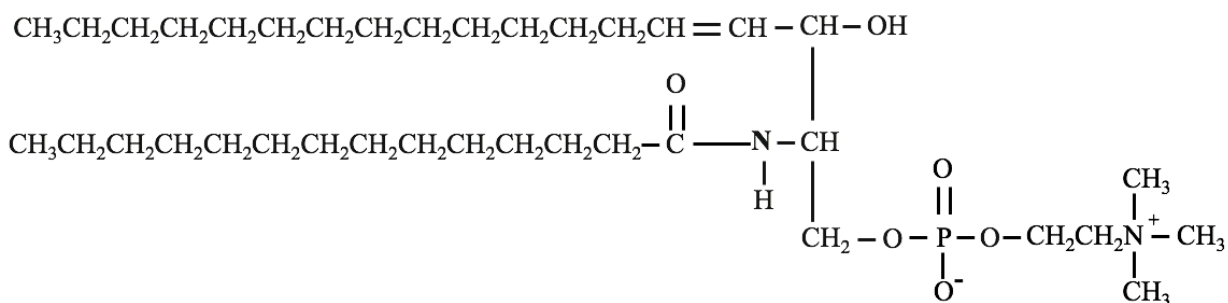
Understanding Check

Categorized each of the following compounds as being either a ***glycerophospholipid*** or a ***sphingophospholipid***.

a)

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-O-CH_2$

$CH_3CH_2CH_2CH_2CH_2CH_2CH = CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-O-CH$

$CH_2-O-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{N}}}-CH_3$

b)

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH = CH - CH - OH$

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle H}{|}}{C}}-N-CH$

$CH_2-O-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{N}H_3$

c)

$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-O-CH_2$

$CH_3CH_2CH_2CH_2CH_2CH_2CH = CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\displaystyle O}{||}}{C}-O-CH$

$CH_2-O-\overset{\overset{\displaystyle O}{||}}{\underset{\underset{\displaystyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{N}H_3$
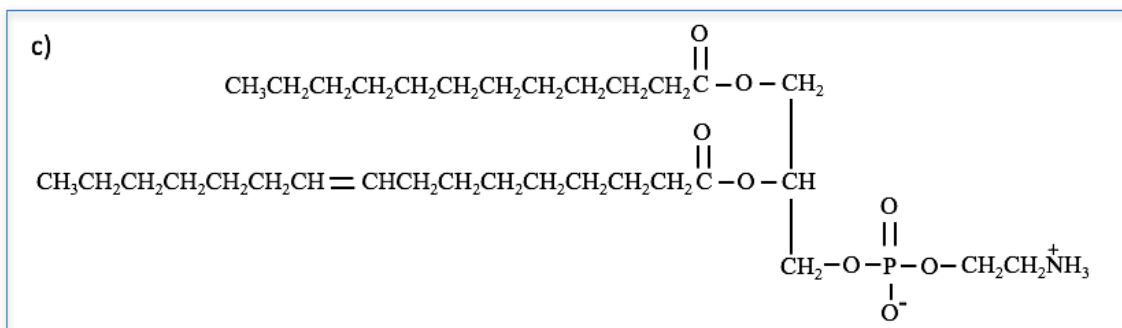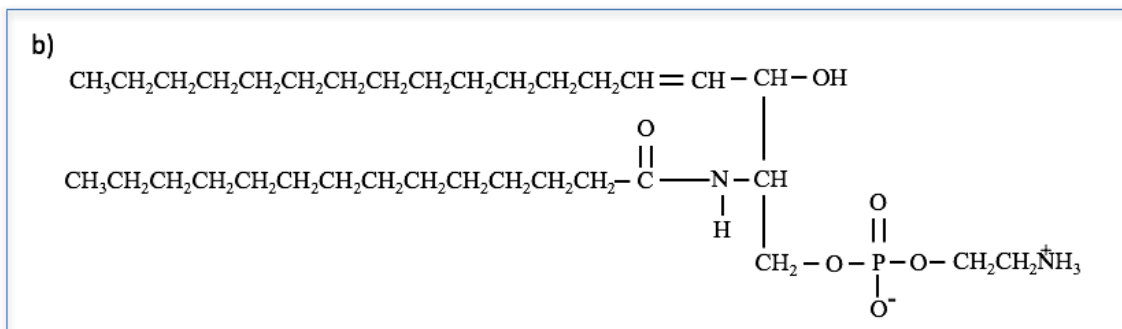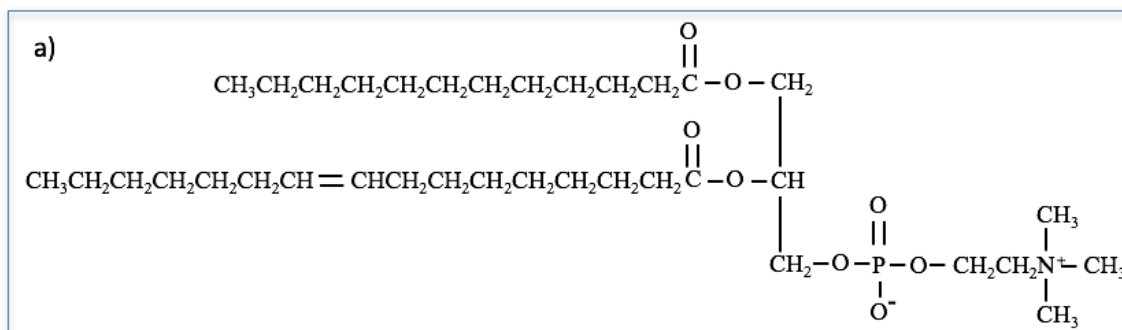
Understanding Check

Categorize each of the compounds shown here as being either a phosphatidylethanolamine, a phosphatidylcholine, a phosphatidylserine, a ceramide, or a sphingomyelin.

a)

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH=CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\textstyle O}{\|}}{C}-O-CH$$

$$CH_2-O-\overset{\overset{\textstyle O}{\|}}{\underset{\underset{\textstyle O^-}{|}}{P}}-O-CH_2CH_2\overset{\overset{\textstyle CH_3}{|}}{\underset{\underset{\textstyle CH_3}{|}}{N^+}}-CH_3$$

b)

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH=CH-CH-OH$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2-\overset{\overset{\textstyle O}{\|}}{C}\overset{}{\underset{\underset{\textstyle H}{|}}{-N-CH}}$$

$$CH_2-O-\overset{\overset{\textstyle O}{\|}}{\underset{\underset{\textstyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{N}H_3$$

c)

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH=CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2\overset{\overset{\textstyle O}{\|}}{C}-O-CH$$

$$CH_2-O-\overset{\overset{\textstyle O}{\|}}{\underset{\underset{\textstyle O^-}{|}}{P}}-O-CH_2CH_2\overset{+}{N}H_3$$

Glycolipids

Glycolipids are *lipids* that contain one or more _____ *residues*.

- A *glycolipid* is easily distinguished from a *phospholipid* by the *presence* of a monosaccharide residue and the _____ of a phosphate residue.

Glycolipids are found in the cell membranes of plants and animals.

- In all eukaryotic cells, the monosaccharide residues of the glycolipid extend from the outer surface of the cell membrane double layer into the aqueous region outside of the cell, as illustrated below.
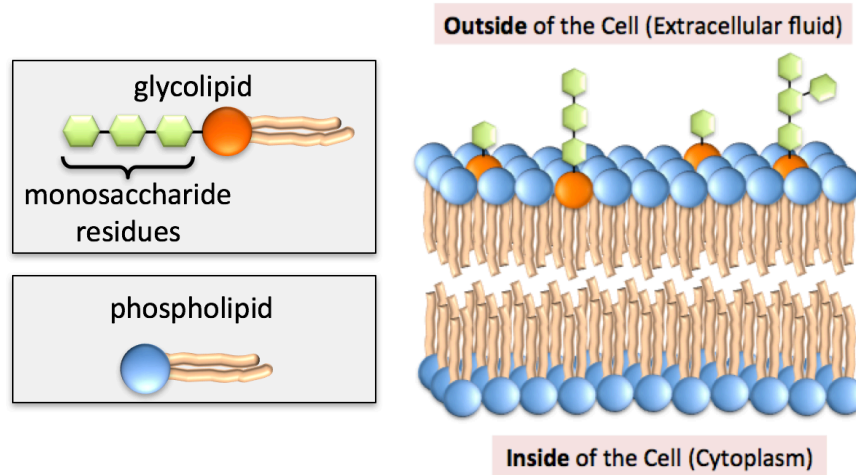
The specific monosaccharide residues that protrude from the membrane serve in maintaining membrane stability, attaching cells to one another to form tissues, and as a "recognition site" for "cell signaling" chemicals. Cell signaling chemicals make it possible for the cells to respond to their environment in order to enable functions such as tissue homeostasis, immunity, and the development of the organism. When signaling systems are not operating correctly to process the communication between cells and their environments, diseases such as cancer, diabetes, and autoimmune disorders occur.

An example of glycolipid recognition sites are the monosaccharides that protrude from red blood cells and form the basis of ABO blood typing. The illustration below shows the various bonding patterns of glycolipid/monosaccharides used for ABO blood typing and their classification.
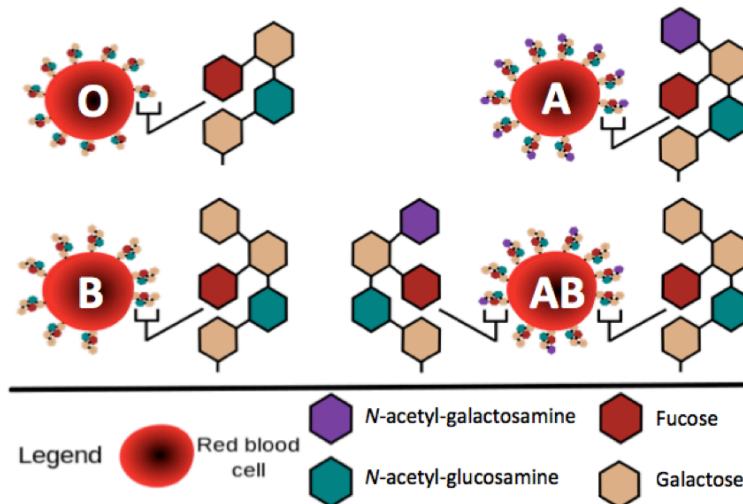
This image shows the glycolipid monosaccharides that define the four "ABO" blood types. Note that type AB red blood cells contain both type-A and type B glycolipids.

Glycolipids can be classified by their structures as **glyceroglycolipids** or **sphingoglycolipids.**

1) Glyceroglycolipids

Glycolipids with a *glycerol backbone* are called **glyceroglycolipids**.

general form of a glyceroglycolipid
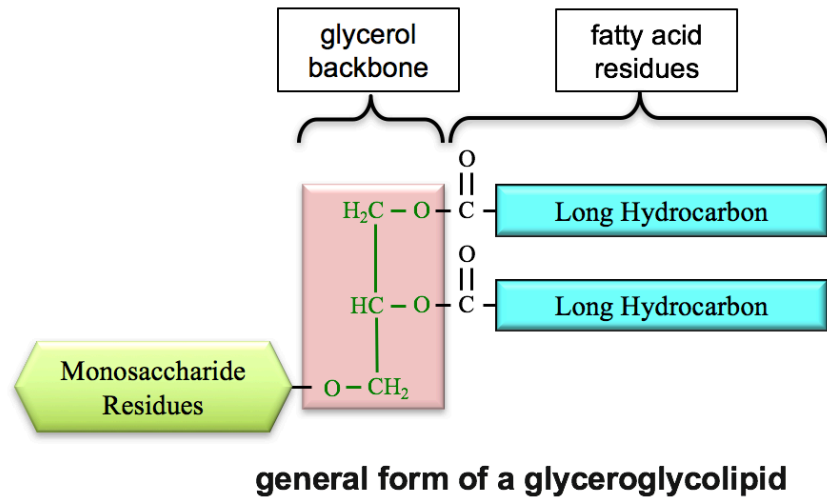
A specific example of a glyceroglycolipid is the monogalactosyldiglyceride (MGDG) shown below.

monogalactosyldiglyceride (a glyceroglycolipid)
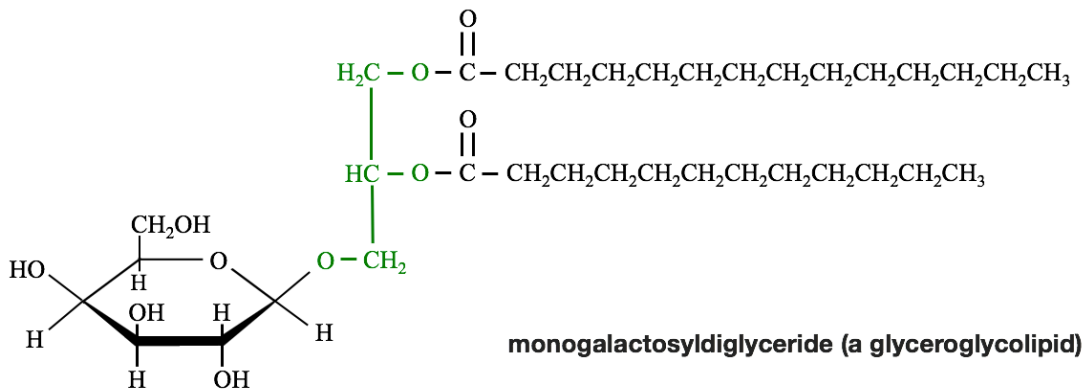
The monosaccharide residue in all monogalactosyldiglycerides is galactose. The fatty acid residues of monogalactosyldiglycerides vary; I arbitrarily chose the two fatty acid residues in the structure shown above. MGDG occurs in high quantity in the membranes that surround chloroplast organelles.

All glycolipids are *amphipathic*. They have a polar head region and nonpolar tails.

The multiple highly-polar **OH** groups from the monosaccharide make the polar head region quite hydrophilic.

Polar "Head"   **Nonpolar "Tails"**
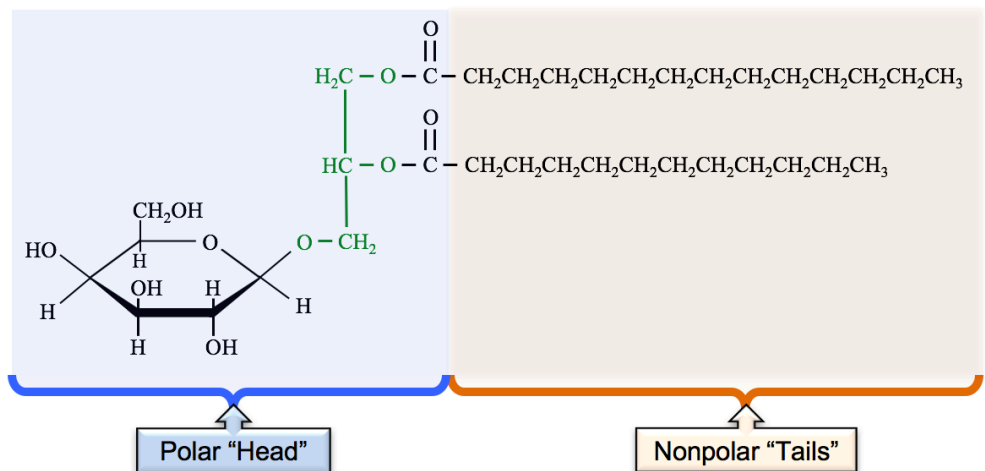
2) Sphingoglycolipids

Glycolipids with a *sphingosine backbone* are called **sphingoglycolipids**.

The general form of a sphingoglycolipid is shown below.
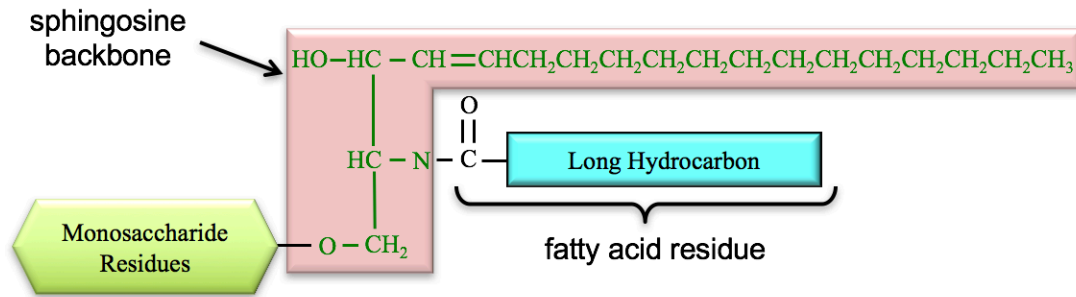
general form of a sphingoglycolipid

- Sphingoglycolipids are found predominantly in nerve and muscle cells.
- They are the major lipid component of the myelin sheath.

An example of a shpingoglycolipid is the glucosylceramide shown below:
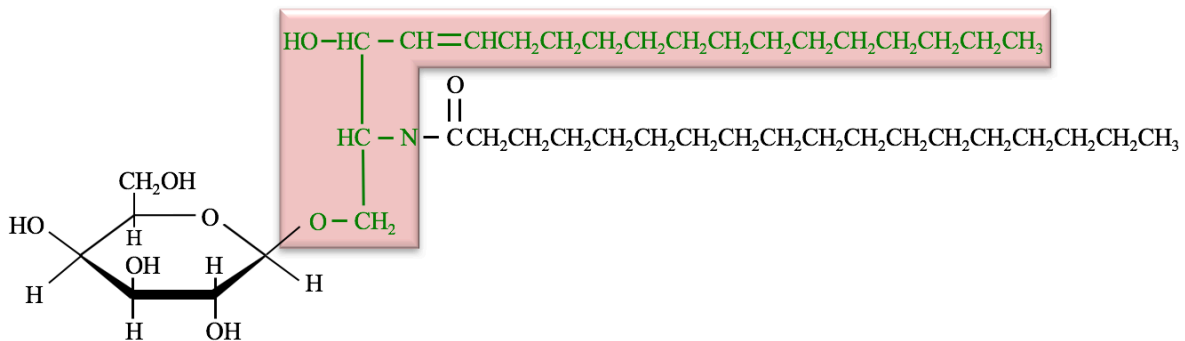
a glucosylceramide (a sphingoglycolipid)

The monosaccharide residue in all glucosylceramides is glucose. The fatty acid residue in glucosylceramides varies; I arbitrarily chose a stearic acid residue for the structure shown above.

The accumulation of large quantities of sphingolipids in cells and organs results from certain genetic diseases called *lipidosis*. The body normally controls the amount of sphingolipids that accumulate by using enzymes that catalyze reactions that break down sphingolipids. Genetic disorders result in a deficiency of an enzyme responsible for the breakdown of a sphingolipid. Gaucher's disease is caused by a deficiency in the enzyme that breaks down glucosylceramide. Krabbe disease is caused from a deficiency in the enzyme responsible for catalyzing the breakdown of galactosylceramine (a sphingolipid in which the monosaccharide residue is galactose). Tay-Sachs disease is a genetic disorder that causes a deficiency of the enzyme responsible for the breakdown of GM2-ganglioside (a sphingolipid in which the monosaccharide residues are a particular oligosaccharide). The other sphingolipidosis diseases are Fabry disease, Sandhoff disease, and metachromatic leukodystrophy. Some of these diseases can be treated by a very costly enzyme replacement therapy, however most sphingolipidosis cases result in death before five years of age.

Review of Phospholipid and Glycolipid Classification

Phospholipids and Glycolipids

Contains a *phosphate residue*:
Phospholipids

Glycerol Backbone:
Glycerophospholipids

Sphingosine Backbone:
Sphingophospholipids

Subclasses
- Phosphatidylethanolamines
- Phosphatidylserines
- Phosphatidylcholines

Subclasses
- Sphingomyelins
- Ceramides

Contains one or more *monosaccharide residues:*
Glycolipids

Glycerol Backbone:
Glyceroglycolipids

Sphingosine Backbone:
Sphingoglycolipids

Understanding Check

Categorized each of the following compounds as being either a ***phospholipid*** or a ***glycolipid***.

a)

$$H_2C-O-\underset{\underset{O}{\|}}{C}CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$$

$$HC-O-\underset{\underset{O}{\|}}{C}CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$$

CH₂OH ... HO ... H ... OH ... H ... H ... H ... OH ... O–CH₂

b)

$$H_2C-O-\underset{\underset{O}{\|}}{C}CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$$

$$HC-O-\underset{\underset{O}{\|}}{C}CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$$

$$\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{CH_3\overset{+}{N}}}-CH_2CH_2-O-\underset{\underset{O^-}{|}}{\overset{\overset{O}{\|}}{P}}-O-CH_2$$
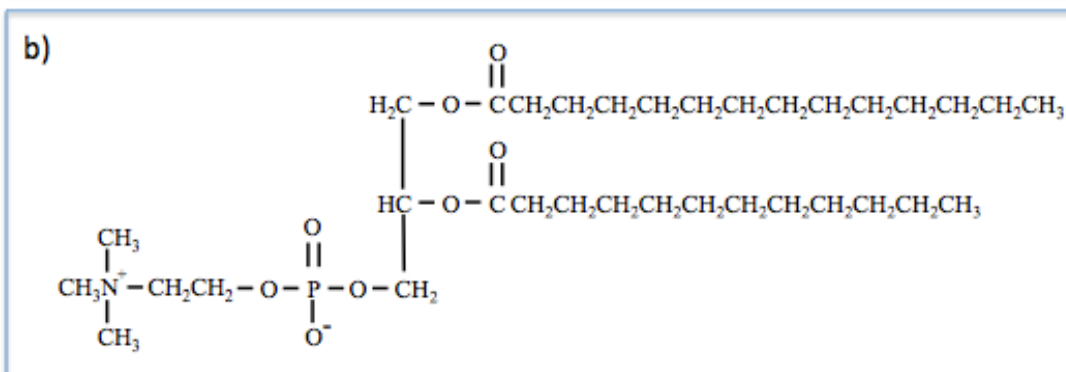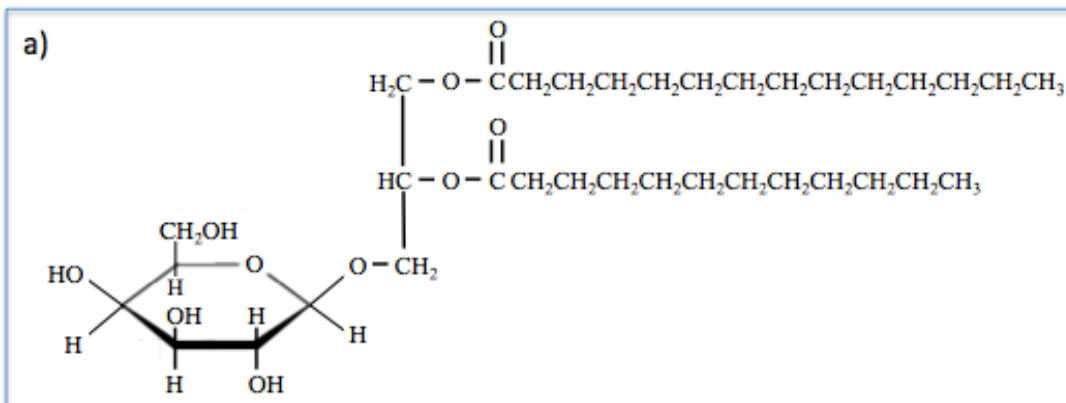
Steroids

Steroids are lipids that contain a particular _____, _____ structure.

- *Fused rings* are rings that *share* atoms.

The fused four-ring structure, which is common to all steroids, contains three six-member rings and one five-member ring, that are fused to each other in the pattern shown below.
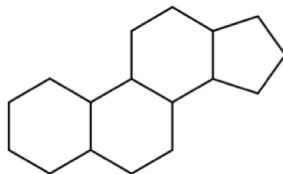
the fused, four-ring structure common to steroids

Outside of the health and scientific communities, the term "steroid" is often only associated with the performance enhancing drugs (*steroid hormones*) that are used by *some* athletes/bodybuilders. Those *steroid hormones* are just one type of steroid.

The *three types of steroids are*:
1. **cholesterol**
2. **steroid hormones**
3. **bile salts**

Cholesterol

Cholesterol is the name of the particular molecule shown below.
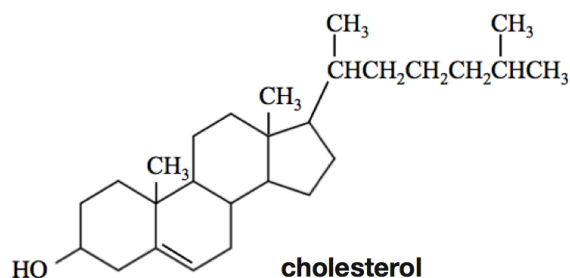
cholesterol

Cholesterol's primary biological roles are as a _____ *component* of animal biological membranes and as a starting material for the biosynthesis of _____ steroids (steroid hormones and bile salts).

Cholesterol is not found in significant quantities in plants. Animals can make cholesterol from other compounds; therefore, cholesterol is present in your body even if you don't ingest it.

Cholesterol maintains the structural integrity and rigidity of biological membrane double layers by embedding its hydrophobic fused-ring structure within the nonpolar tails of the double layer.

Cholesterol imparts rigidity to membranes because of the *lack of free rotation* within its fused-ring structure.

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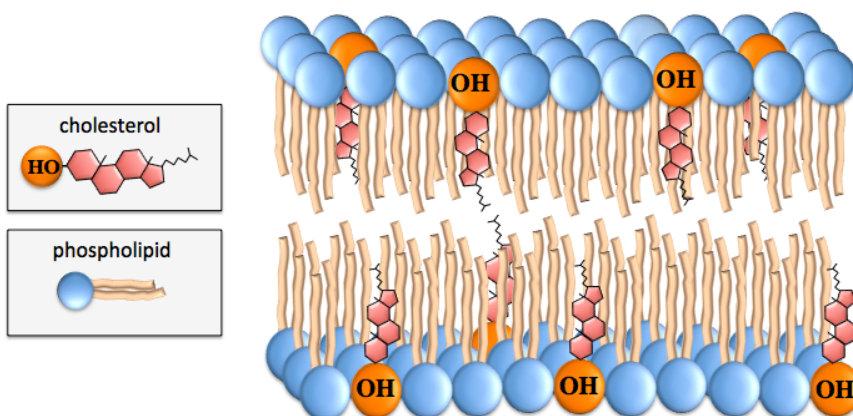
Animals produce other essential steroids (steroid hormones and bile salts) using cholesterol as a
_____ material.

- The production of steroids is called _____.
- **NOTE:** You **ARE NOT** required to memorize the steroidogenesis figure (below).
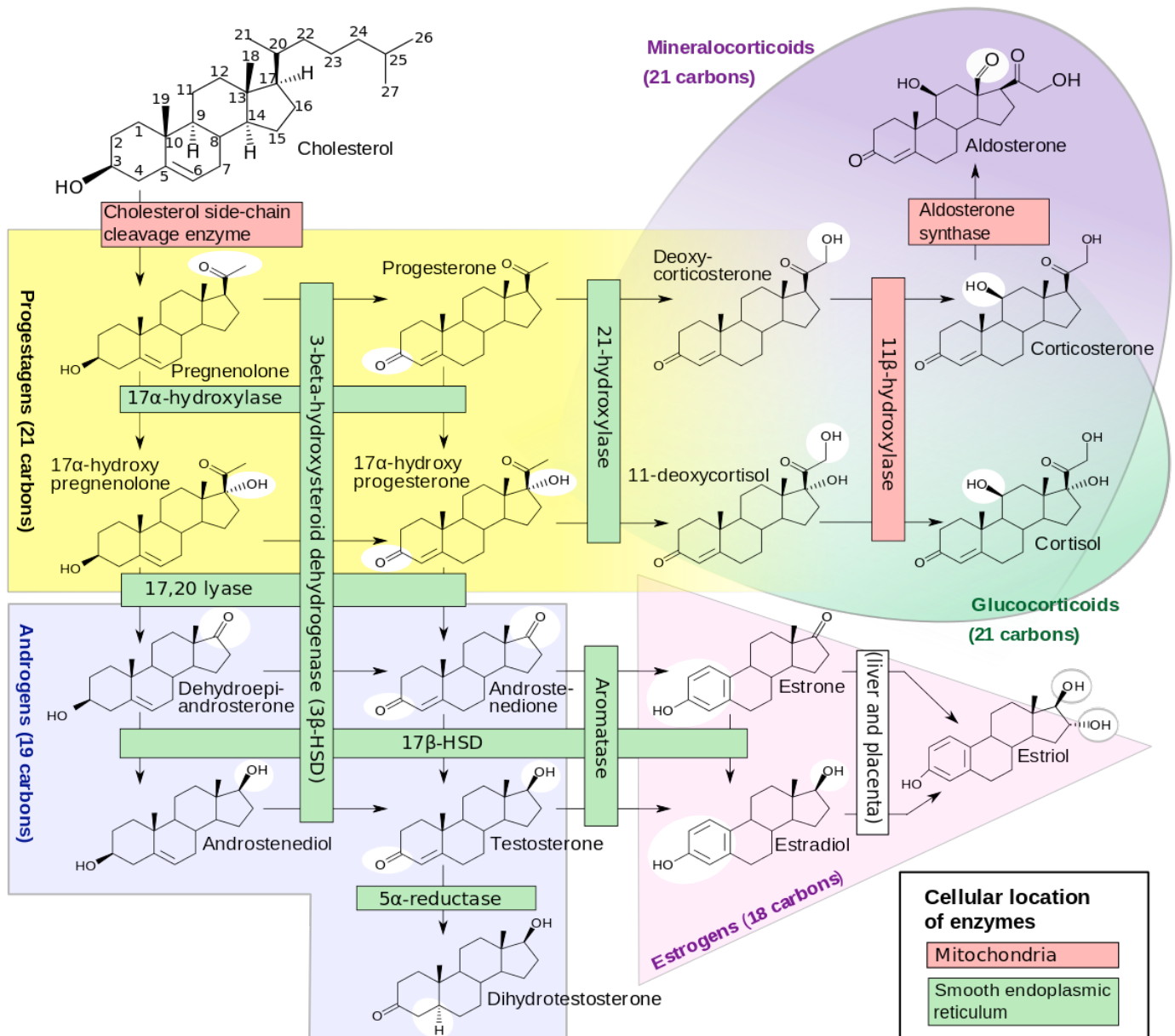
A diagram of the processes in which steroid hormones are produced from cholesterol is shown above. The enzymes that catalyze these reactions and their locations are indicated by the colored boxes drawn atop the reaction arrows. The white circles and ovals indicate the groups that were changed in the synthesis reactions. The cholesterol structure (upper left) has the *carbon positions* numbered. Wedges and dashes are used to indicate bonds that are oriented upward or downwards, respectively, relative to the ring structure. *α* and *β* designations have the same meaning as used for carbohydrates.

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Steroid Hormones

_____ are a class of ***signaling compounds*** that are produced by the glands of the endocrine or exocrine system, then released into the bloodstream (or sap in the case of plants).

Hormones vary in their chemical structure; those that are derived from cholesterol, as shown in the steroidogenesis diagram here, are called _____ ***hormones***.

An example of a ***steroid hormone*** is a "male sex hormone" called **testosterone**. Testosterone and other male sex hormones (androgens) are responsible for the development of male characteristics such as larger muscle growth, thick facial hair, male sex organs, and sperm production. Although testosterone is classified as one of the male sex hormones, it is also present, at lower levels, in females. The structure of testosterone and other androgens are shown in the *steroidogenesis diagram* (see the previous page).

- Testosterone acts to decrease body fat and increase muscle mass. Synthetic derivatives of testosterone, called **anabolic steroids**, will enhance these effects. You have probably heard much in the news about the use of anabolic steroids by athletes. Many professional sports organizations ban their use, and periodically test athletes to enforce the policy. Anabolic steroids are currently used in medical practice to increase muscle growth and appetite, induce male puberty, and to treat chronic wasting conditions including cancer and AIDS. It is considered unwise to use anabolic steroids in order to enhance athletic performance and for recreational bodybuilding because of the detrimental side effects; this is especially true for high doses and/or long-term use. Such side effects for males include pattern baldness, breast development, a reduction in testicle size, low sperm count, and infertility. The side effects for females include abnormal menstrual function, breast atrophy, increased facial hair, voice-deepening, and baldness. Other possible adverse side effects - for both men and women - include liver disease, heart disease, and depression.

Other examples of steroid hormones are **estrogens** and **progestogens**, the "female sex hormones." They are responsible for the development of female characteristics related to menstruation and reproductive cycles, such as broadening of the pelvis, fat deposited in breasts, and uterus size increase. An example of female sex hormone is ***progesterone***, which is responsible for many of the biological functions associated with pregnancy. For example, it causes the mucous membrane of the uterus to prepare for the implantation of eggs. If pregnancy does not occur, then progesterone levels decrease and cause menstruation. The structure of *progesterone* and other *progestogens* are shown in *the steroidogenesis diagram*.

Although the adrenal gland is best-known for its production of *adrenaline* (a ***non****steroidal* hormone), it does produce several *steroid hormones*. Steroid hormones produced by the adrenal gland are called **adrenal corticosteroids**. Examples of *adrenal corticosteroids* are ***cortisol*** and ***aldosterone***. One of the many roles of *cortisol* is to suppress immune responses. It is administered *as a therapeutic medication* under the name ***hydrocortisone***. *Aldosterone* plays an important role in regulating blood pressure and the concentration of some electrolytes. The structure of *cortisol* and *aldosterone* are shown in the *steroidogenesis diagram*.

Bile Salts

Bile salts are *amphipathic* compounds produced using _____ as a starting material.

They are produced in the liver and stored in the gallbladder.

The biological role of bile salts is to _____ and _____ dietary triglycerides (fats and vegetable oils) and _____ in their metabolism.

The structures of two bile salts are shown below; note the four *fused-ring* structures, which are present in *all steroids*.

glycocholate

taurocholate
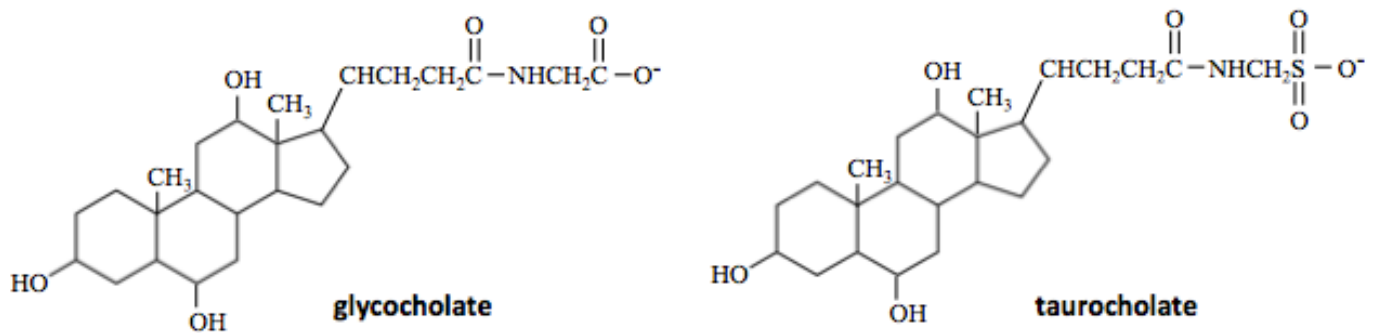
The amphipathic structure of a bile salt differs from the arrangement that you have seen for other amphipathic compounds. All of the amphipathic compounds that you have previously seen had polar "heads" connected to nonpolar "tails". *This is not the case for bile salts.*

Bile salts can be modeled as oblong disks that have a *polar* _____ and a *nonpolar* _____, as illustrated below.

glycocholate (a bile salt)

side view

polar side
(top)

nonpolar side
(bottom)
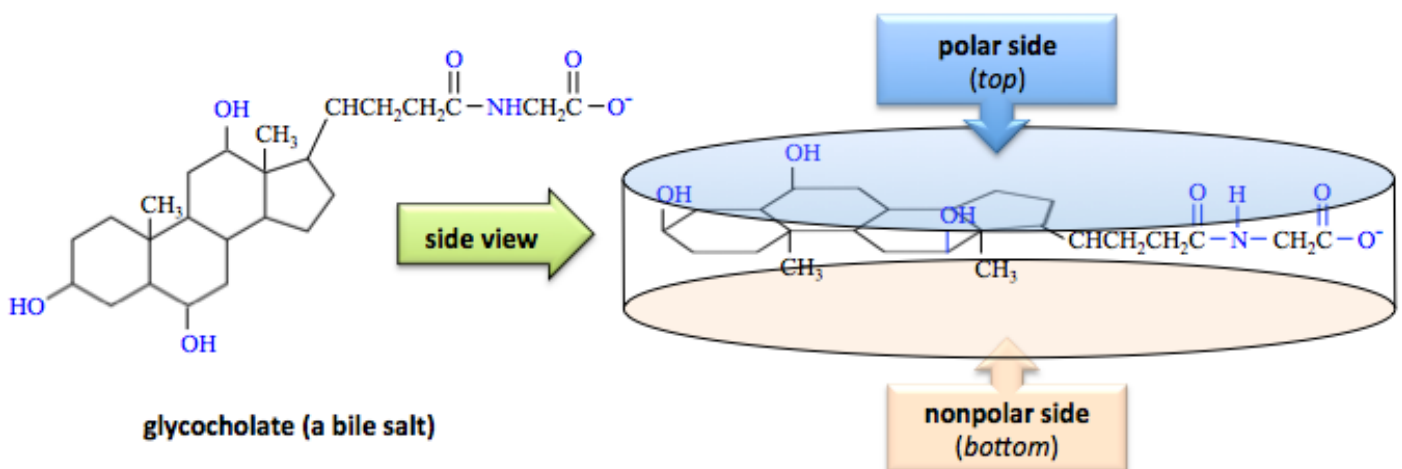
How do bile salts *emulsify* and *transport* dietary triglycerides and *assist* in their metabolism?

The triglycerides (fats and oils) that we eat are unable to pass through the intestine wall.

- In order for these nutrients to be used by the body, they must be broken down into smaller molecules, in a process called *digestion*.

Digestion of fats and oils involves the *partial hydrolysis* of triglycerides to produce fatty acid salts and _____, as shown for a typical triglyceride in the chemical equation below.

a triglyceride   a monoglyceride   two fatty acids (base forms)
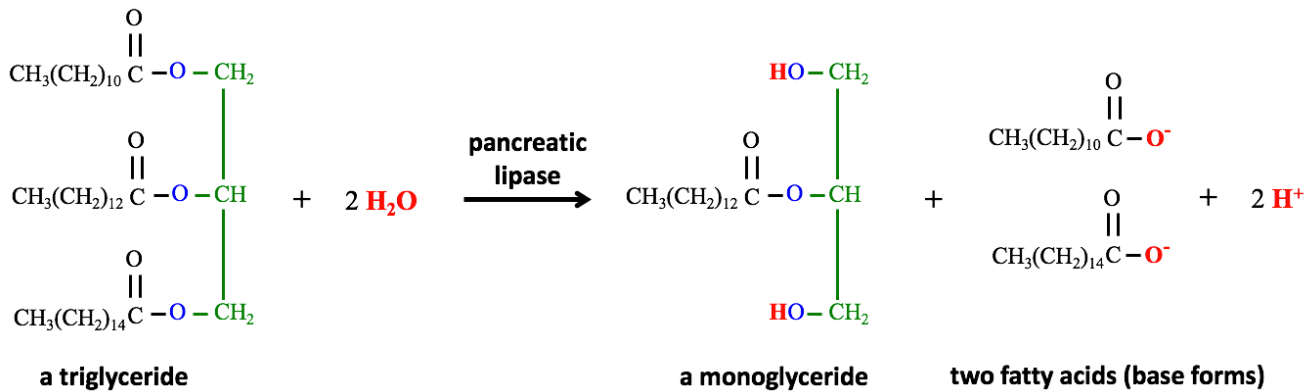
The enzyme responsible for catalyzing this reaction is called *pancreatic lipase*.

Bile salts disassemble the large globules of dietary triglycerides and cholesterol within the intestine into small droplets emulsified in micelles.

Pancreatic lipase enzymes are incorporated into the bile salt micelle monolayer, as illustrated in the cross sectional view shown below.
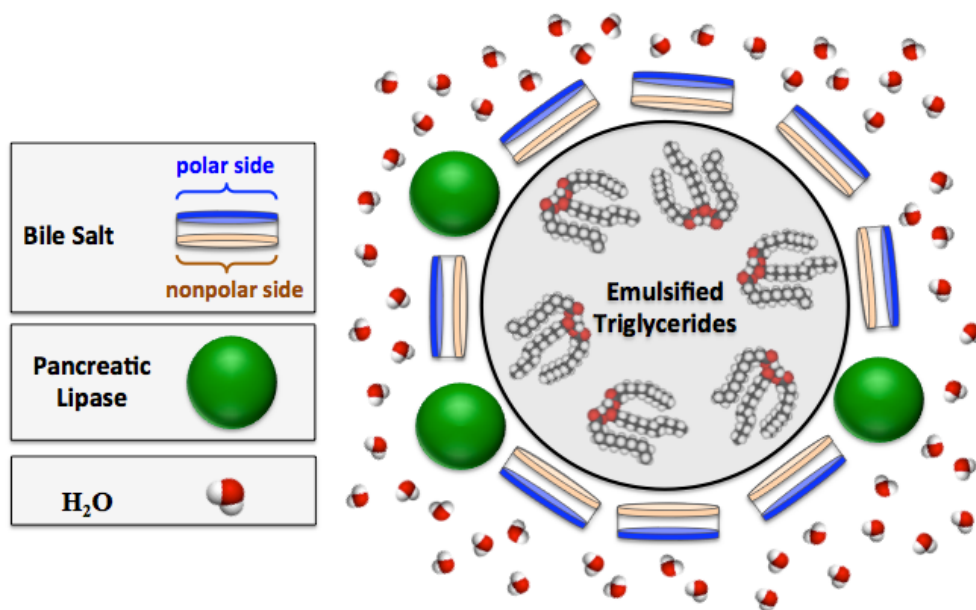
The fatty acids and monoglycerides that are formed by the digestion of fats and oils can pass through the walls of the intestine and then can be used by the body.

After being absorbed into the intestine walls, the fatty acids and monoglycerides are re-assembled back into triglycerides.

The triglycerides are then emulsified and transported, along with cholesterol, in a colloid called a _____.

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Transport of Cholesterol and Triglycerides

Since blood, lymph, and intercellular fluid are _____ *mixtures*, cholesterol and triglycerides must be _____ in order to be transported throughout the body.

- This is done by *lipoproteins*.

Lipoproteins are composed of a core that contains emulsified triglycerides and cholesterol, which is surrounded by a micelle monolayer made from proteins, phospholipids, and cholesterol.

Lipoproteins contain cholesterol in their micelle monolayers, *and* in their emulsified cores.

The cholesterol *in the emulsified core* of lipoproteins is in the form of *cholesterol esters,* formed by the esterification reaction of cholesterol with a fatty acid.

A cross-sectional illustration of a lipoprotein
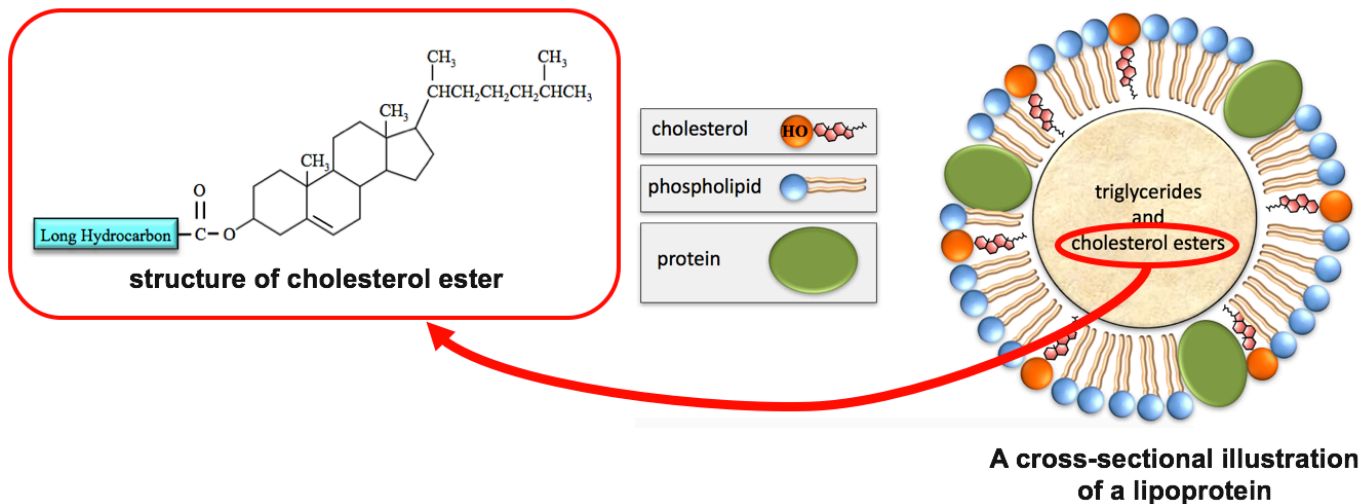
There are five classes of lipoproteins: *chylomicrons, very low-density lipoproteins* (VLDL)*, intermediate-density lipoproteins* (IDL), *low-density lipoproteins* (LDL), and *high-density lipoproteins* (HDL).

These classifications are based on the _____ of the lipoprotein particles.

- Since protein is more dense than lipid, the greater the percentage of protein, the higher the density of the lipoprotein.

Density Ranges and Percent (w/w) Compositions for Lipoprotein Classes					
Lipoprotein Classification	Density (g/cm³)	% Protein	% Cholesterol	% Phospholipids	% Triglycerides and Cholesterol Esters
chylomicrons	< 0.94	< 2	8	7	84
VLDL	< 1.006	10	22	18	50
IDL	1.006 - 1.019	18	29	22	31
LDL	1.019 - 1.063	25	50	21	8
HDL	1.063 - 1.21	33	30	29	4

The amounts of HDL and LDL in the blood have been correlated with the constriction (occlusion) of the coronary artery, which makes the heart work harder and can lead to myocardial infarction (heart attack). The thickening of the inner layer of the artery is caused by the accumulation of **plaque**, which is made from living white blood cells and remnants of dead cells, including **cholesterol** and **triglycerides**.

- A high LDL level is correlated with a greater risk of heart disease.

- A high HDL level is correlated with a lowered risk of heart disease.

For these reasons, it is recommended that adults have the lipid levels in their blood tested *at least* once every five years. The test is called a **lipoprotein panel**.   Although the concentration of cholesterol is not directly measured in these tests, the terms "total cholesterol," "bad cholesterol", and "good cholesterol" are often used by practitioners when describing or discussing the results of lipid panels.   Cholesterol is the name of a *particular molecule*, however, *in lipid panels*, the term "total cholesterol" is used for the concentration of HDL + LDL + 20% of the triglycerides. The term "bad cholesterol" is used for the concentration of LDL. The term "good cholesterol" is given to HDL since it transports cholesterol back to the liver (the liver can remove cholesterol from the body) and lowers the risk of heart disease.

Lipid Panel Level Concentration Categories			
Substance	**Desirable/Recommended Level**	**Borderline High Level**	**High Level**
"Total Cholesterol" (HDL + LDL + 20% of the triglycerides)	below 200 mg/dL	200-239 mg/dL	240 mg/dL and above
Triglycerides	below 150 mg/dL	150-199 mg/dL	200 mg/dL and above
LDL "Bad Cholesterol"	below 100 mg/dL (ideal)* 100-129 mg/dL (near ideal)	130-159 mg/dL	160-189 mg/dL (high) 190 and above mg/dL (very high)
	Considered *Protective* Against Heart Disease	**Intermediate Values (the higher, the better)**	**A Major *Risk Factor* for Heart Disease**
HDL "Good Cholesterol"	60 mg/dL and above	40-59 mg/dL	less than 40 mg/dL

Lipid and lipoprotein concentrations are measured in milligrams (mg) of substance per deciliter (dL) of blood.
*The LDL desirable values are lower than those shown in the table for persons at risk of heart attack.
Source: National Institutes of Health, *Medline Plus* (2012). Volume 7 Number 2 Page 6-7

Eicosanoids

The "*eicosa*" prefix in *eicosanoids* is from the Greek "*eicosa*," which means twenty.

The lipids called **eicosanoids** are _____ *molecules* that contain _____ carbon atoms.

- They are derived from one of three, twenty-carbon polyunsaturated fatty acids (arachidonic acid, eicosapentaenoic acid, or dihomo-gamma-linolenic acid).

Arachidonic acid, shown below, is the major precursor of eicosanoids.
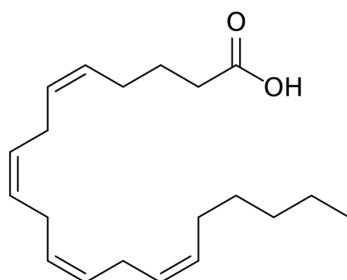
arachidonic acid

Arachidonic acid, eicosapentaenoic acid, or dihomo-gamma-linolenic acid undergo *reactions* that transform them into the various classes of *eicosanoids* - such as ***prostaglandins***, ***thromboxanes***, ***leukotrienes***, and ***prostacyclin***.

- For example, *arachidonic acid* can be converted to various eicosanoids as shown in the diagram below.
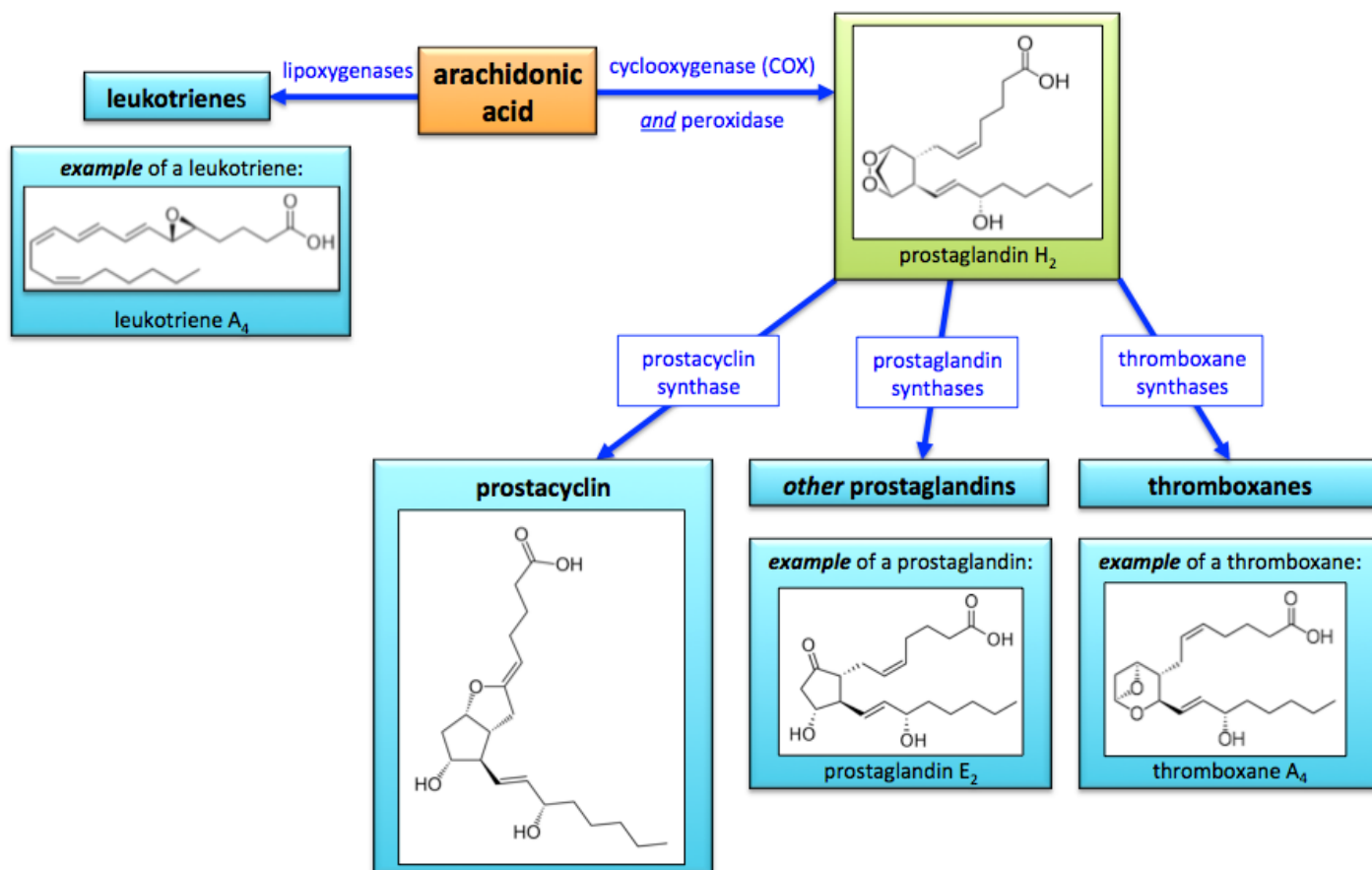
NOTE: You are **not** responsible for memorizing the enzymes for these reactions or the structures of the various eicosanoids.

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Prostaglandins

Prostaglandins have a wide range of biological effects, including causing pain, causing inflammation, causing fever, affecting blood pressure, inducing sleep, regulating blood flow to particular organs, controlling ion transport across membranes, and inducing labor.

Thromboxanes

Thromboxane A_2 is the major biologically-active form of thromboxanes. It acts as vasodilator and is involved in the facilitation of blood clotting.

Leukotrienes

Leukotrienes are involved in the regulation of immune responses and in induced muscle contractions in the lungs. The overproduction of a particular leukotriene (leukotriene D_4, ***not*** shown in the diagram on the previous page) is a major cause of inflammation in asthma. Some anti-asthma drugs block the production of leukotrienes.

Prostacyclin

Prostacyclin is involved in vasodilatation, *inhibition* of blood clotting, regulation of the contraction of smooth muscle, and inflammation.

Nonsteroidal Anti-inflammatory Drugs (NSAIDs)

NSAIDs such as aspirin, acetaminophen, and ibuprofen are taken to reduce pain, fever, and inflammation by blocking the action of the cyclooxygenase enzyme (COX) that catalyzes the conversion of arachidonic acid into prostaglandins and thromboxanes (see the eicosanoids formation diagram on the previous page).

Biological Membranes

Biological membranes are semipermeable physical barriers. Biological lipid double layer membranes not only function as cell membranes, but also exist within cells in order to form specialized compartments. For example, intracellular lipid double layer membranes surround a cell's nucleus, chloroplasts, and mitochondria. The lipid double layers in biological membranes contain components other than phospholipids and glycolipids. These other components, which include cholesterol and various proteins, are distributed throughout the lipid double layer, as illustrated *below* for a eukaryotic cell membrane.
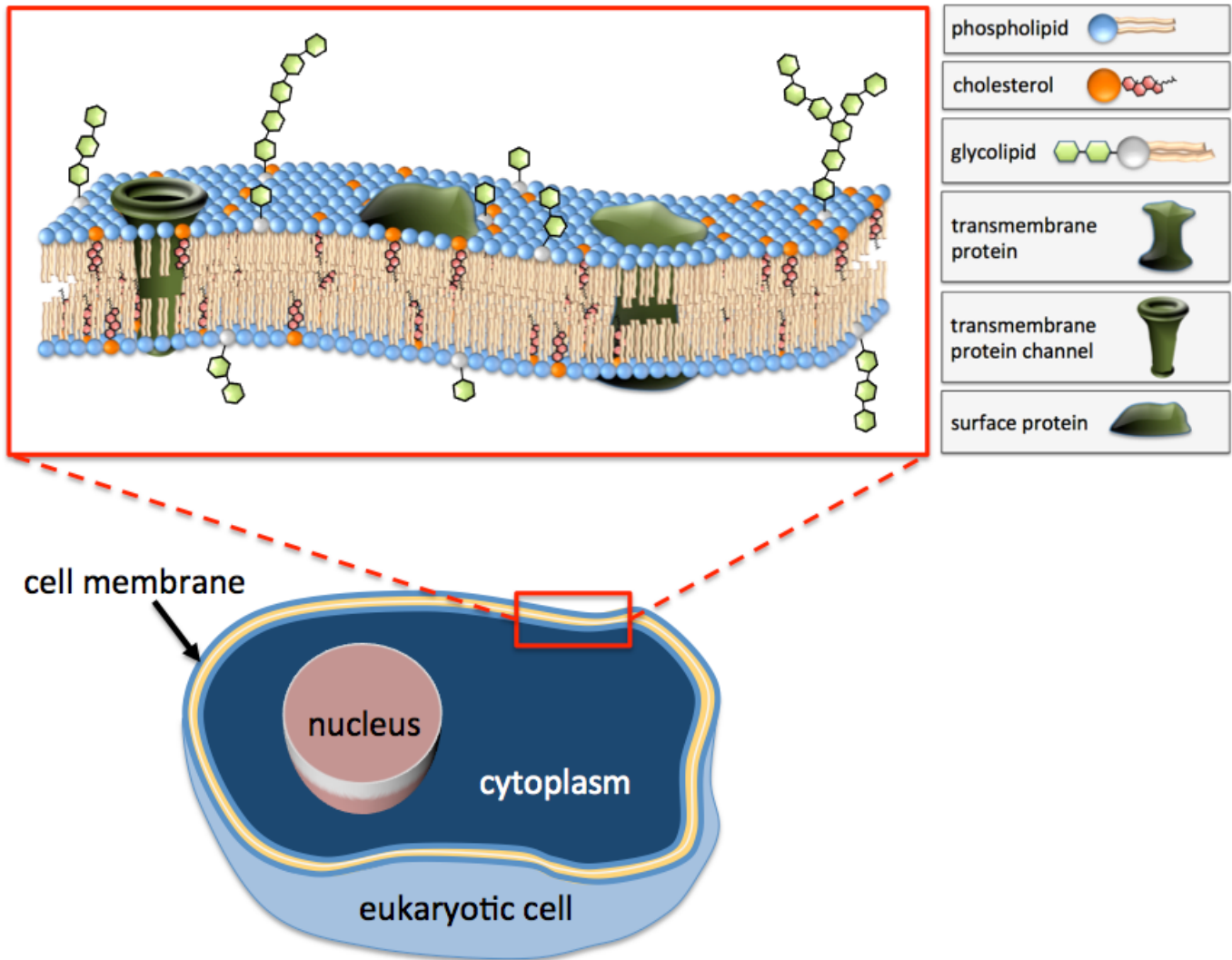
The forces holding the lipids and other components together in each of the two monolayer sheets are relatively weak. For this reason, membranes are flexible, and the membrane components are not locked in place; they are able to "slide" past each other. The flexibility of membranes **decreases** as the *chain lengths* and *degree of saturation* of the lipid nonpolar tails increase. This is the same trend as you saw for the melting points of fatty acids and triglycerides, because it results from increasing London forces.   In animals, the amount of membrane-cholesterol also regulates flexibility.

The Transport of Molecules and Ions Across Membranes

Certain compounds must be able to pass through cell membranes in order for cells to perform their biological functions.

The processes in which species are transported through membranes are classified as either

_____ *transport*

or

_____ *transport*.
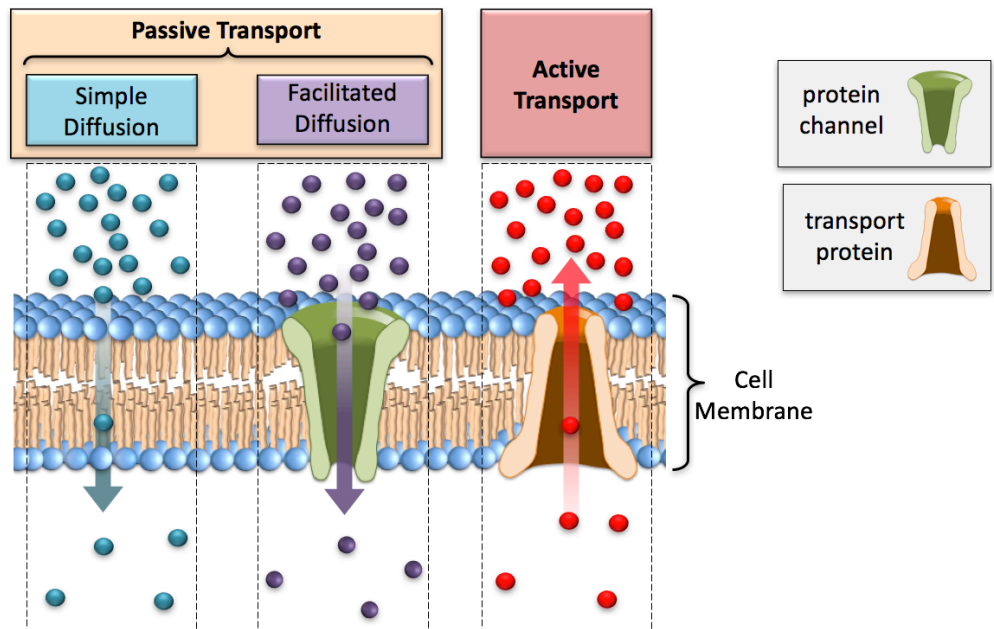
Some ***nonpolar*** and ***amphipathic*** compounds can pass through a membrane because of their attraction to the phospholipids in the membrane by noncovalent interactions.

- Species that are able to move through membranes in this way are called ***lipophilic compounds***.

The direction of the net transport of a *lipophilic* compound is determined by _____; there will be a net transport from the side of the membrane where its concentration is greater, to the side where its concentration is less.

- Recall, from chapter 7, that we described this type of transport as "with the concentration gradient." The energetic driving force for diffusion is the potential energy of the diffusing species' concentration gradient.

This diffusive movement of lipophilic compounds through a membrane is referred to as _____ **diffusion**.

Diffusion of small ions and polar molecules, which are *not* lipophilic, through membranes is facilitated by ***protein channels*** that pass through the cell membrane.

This diffusion of ions and polar molecules though protein channels is referred to as _____ **diffusion**.

- In *facilitated diffusion,* as with *simple diffusion*, a molecule or ion is transported from the side of the membrane where its concentration is greater to the side where its concentration is less, or "with the concentration gradient," and the energetic driving force is the potential energy of the diffusing species' concentration gradient.

Both ***simple diffusion*** and ***facilitated diffusion*** are called **passive transport** because they do not require an energetic input from sources other than the concentration gradient of the transported species.

- The transport of water molecules through membranes is a passive transport process, and is best described by ***osmosis*** (you learned about osmosis in chapter 7). The protein channels in which water molecules pass are called *aquaporins*.

In order for molecules or ions to be transported in the direction "against the concentration gradient" - from the side of the membrane where their concentration is less to the side where their concentration is greater - _____ **must be supplied**.

This type of transport is referred to as _____ *transport*.
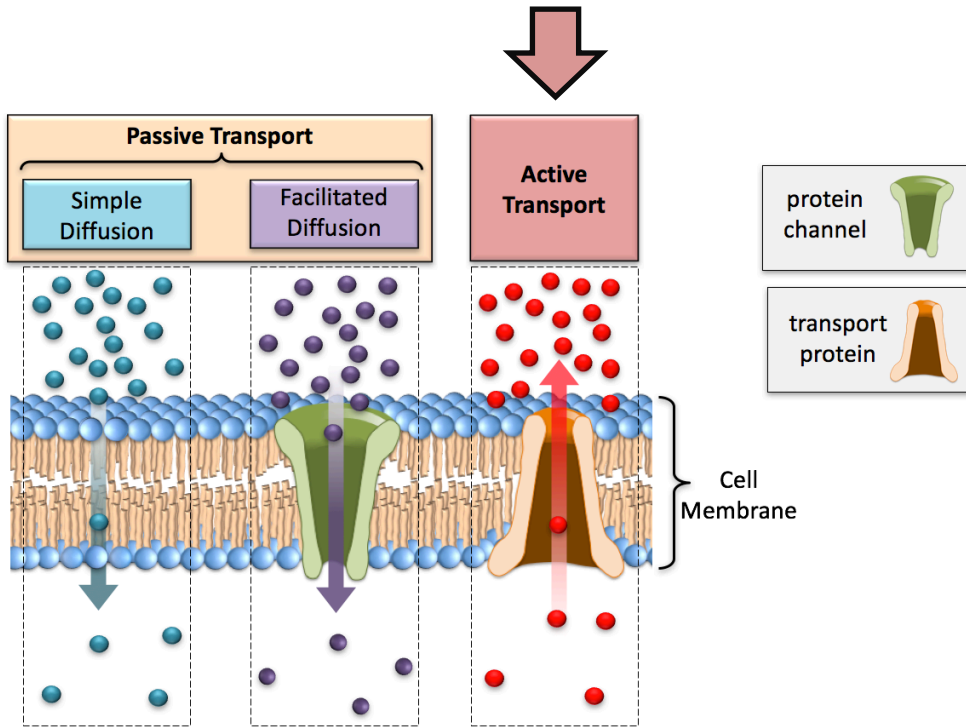
- Unlike the ***passive transport*** processes that are driven by the potential energy provided by the transported species' concentration gradient, in ***active transport***, energy must be supplied by ***some other source***.

In the *active transport* process, the ions or molecules cross the membrane with assistance from a _____ *protein*.

- An example of active transport is the transport of ions, amino acids, sugars, lipids, drugs, or other molecules "against their concentration gradient" through **ATP binding cassette transport proteins (ABC transporters)**. *ABC transporters* use chemical energy, supplied by **ATP**, to transport compounds through a membrane.

Understanding Check

a) Compare and contrast **simple diffusion** with **facilitated diffusion**.

b) Describe the *difference* between **passive transport** and **active transport**.

Fatty Acid and Triglyceride Worksheet and Key

1) Draw the condensed structural formula of any **saturated fatty acid**.

2)   a) Draw the condensed structural formula of any **monounsaturated fatty acid**.

   b) Draw the condensed structural formula of any **polyunsaturated fatty acid**.

3) Compare and contrast "fat" (triglycerides) and fatty acids.

4) Draw the condensed structural formula of any **saturated fat (triglyceride)**.

5) Draw the condensed structural formula of any **unsaturated fat (triglyceride)**.

KEY

1) Draw the condensed structural formula of any **saturated fatty acid**.

$$\overset{\displaystyle O}{\overset{\displaystyle \|}{}}$$

CH₃CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂ C—OH

Carbon chain should contain 12 or more carbons **and** should have **_all single bonds._**

2)
a) Draw the condensed structural formula of any **monounsaturated fatty acid**.

$$\overset{\displaystyle O}{\overset{\displaystyle \|}{}}$$

CH₃CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH═CHCH₂CH₂CH₂CH₂CH₂CH₂CH₂ C—OH
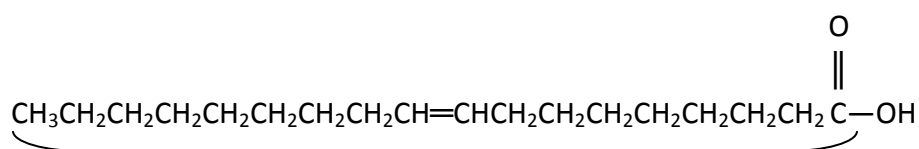
Carbon chain should contain 12 or more carbons **and** should have **_only one double bond._**

b) Draw the condensed structural formula of any **polyunsaturated fatty acid**.

$$\overset{\displaystyle O}{\overset{\displaystyle \|}{}}$$

CH₃CH₂CH₂CH₂CH₂CH₂CH═CHCH═CHCH₂CH₂CH₂CH₂CH₂CH₂CH₂ C—OH
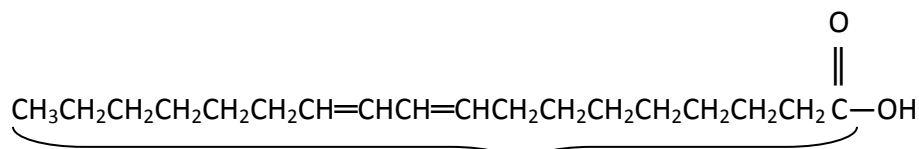
Carbon chain should contain 12 or more carbons **and** should have **_at least two double bonds._**

3) Compare and contrast "fat" (triglycerides) and fatty acids.

Fatty acids are long-chain _carboxylic acid_ molecules, typically 12-20 carbons in length. Triglycerides contain three fatty acid residues bonded to a glycerol backbone. Triglycerides can be formed by the esterification of three fatty acid molecules and one glycerol molecule.

4) Draw the condensed structural formula of any **saturated fat (triglyceride)**.

In a *saturated fat molecule* all *three hydrocarbon tails are saturated* (contain all single bonds). You can use any three *saturated* fatty acid residues in your structure.

Example of a correct structure:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

5) Draw the condensed structural formula of any **unsaturated fat (triglyceride)**.

In an *unsaturated fat molecule*, at least one of *hydrocarbon tails is unsaturated* (contains at least one double bond). You can use any three fatty acid residues in your structure, so long as at least one of them is unsaturated.

Example of a correct structure:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH=CHCH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

$$CH_3CH_2CH=CHCH_2CH_2CH_2CH_2CH_2CH_2CH=CHCH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH$$

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2 \; \overset{\overset{\textstyle O}{\|}}{C}-O-CH_2$$

Chapter 13 Lecture Notes: Peptides, Proteins, and Enzymes

Educational Goals

1. Describe the general bonding pattern of **α-amino acids** and understand how amino acids are classified by the *polarity* and *charge of their side-chains*.

2. Given the table of twenty common amino acids, determine the ***total charge*** of the dominant form of an amino acid (at physiological **pH**, at **pH** < 2, and at **pH** > 11).

3. Understand the three-dimensional information contained in the Fischer projection of an amino acid.

4. Given a Fischer projection of an amino acid, determine if it is an ***L*-amino acid** or ***D*-amino acid**.

5. Understand and define the term **peptide**.

6. Given the table of twenty common amino acids, be able to draw the structural formula of the peptide that is obtained when two or more particular amino acids are connected by **peptide bonds**.

7. Given the structural formula of a **peptide** be able to identify the **peptide bonds,** the **C-terminus,** the **N-terminus,** <u>*and*</u> the **peptide groups**.

8. Given the structural formula of a peptide and the table of twenty common amino acids, determine the ***total charge*** of the peptide's dominant form (at physiological **pH**, at **pH** < 2, and at **pH** > 11).

9. Given the structure of a peptide, and the table of twenty common amino acids name a particular peptide using amino acid residue *abbreviations*.

10. Compare and contrast **peptides** and **proteins**.

11. Understand and define **primary, secondary, tertiary, and quaternary protein structure**. Name the noncovalent interactions that are responsible for each level of structure.

12. Explain what is meant by the term **denaturation** and list the ways to denature a protein.

13. Understand the difference between **globular, fibrous, and membrane proteins**.

14. Compare and contrast **simple proteins** and **conjugated proteins**.

15. Understand the terms **cofactor** and **coenzyme**.

16. Understand how **enzymes** work and distinguish between **absolute specificity, relative specificity, and stereospecificity**.

17. Understand and define the terms: **essential amino acid, complete protein, incomplete protein, and complimentary protein**.

18. Understand how changes in **pH** and *temperature* can affect the reaction **rate** of an enzymatically-catalyzed reaction.

19. Understand how enzyme inhibitors and activators control enzymatic reactions, and compare and contrast **reversible** and **irreversible inhibitors**.

20. Understand how organisms regulate metabolic pathways using **feedback inhibition** and **positive feedback**.

Introduction

The _____ _____ of amino acids in a protein and the chemical nature of the

amino acid _____ _____ enable proteins to perform their functions.

- Typical protein functions:
    - Catalyze Reactions (enzymes)
    - Chemical Signaling (hormones)
    - Storage (e.g. myoglobin stores oxygen)
    - Structural (e.g. collagen in skin and tendons)
    - Protective (e.g. antibodies)
    - Contractile (e.g. myosin in muscle)
    - Transport (e.g. hemoglobin)

Amino Acids

Structure of Amino Acids

Amino acids are organic compounds that contain a _____ *and* a

_____.
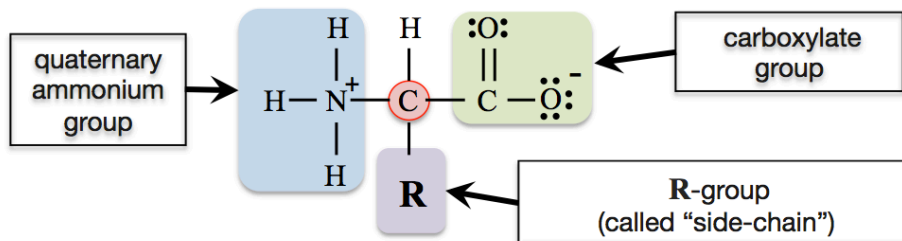
For amino acids, the **R-group** is often called the "**side-chain**" or "**variant group**."

The *side-chain* can be a hydrogen atom, hydrocarbon, or various other groups of bonded atoms.

Amino acids are named based on the identity of their _____.

- For example, if the side-chain is a hydrogen atom (H), then the amino acid is called *glycine*; if the side-chain is a methyl group (CH_3), then the amino acid is called *alanine*.
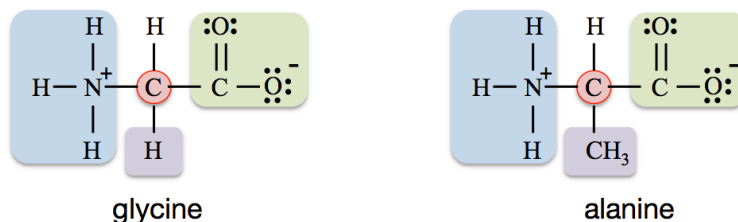
There are 23 amino acids that make up the proteins in plants and animals, 20 of them are directly specified by the genetic code in DNA.

These twenty amino acids are called the _____ *amino acids.*

- All twenty *common amino acids* are _____ amino acids.
- They are called **α**-amino acids because their *side-chains* are attached to **α**-carbons.
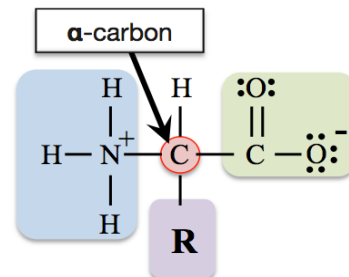
REMINDER: The **α**-carbon is the carbon that is bonded to the carboxyl group's carbonyl carbon.

The *twenty common amino acids* are often referred to using three-letter abbreviations. The structures, names, and abbreviations for the twenty common amino acids are shown below. Note that they are all **α-amino acids**.

Name (abbreviation)	Structural Formula	Name (abbreviation)	Structural Formula	Name (abbreviation)	Structural Formula
Glycine (Gly)		Methionine (Met)		Lysine (Lys)	
Alanine (Ala)		Phenylalanine (Phe)		Arginine (Arg)	
Valine (Val)		Tryptophan (Trp)		Histidine (His)	
Leucine (Leu)		Aspartic Acid (Asp)		Tyrosine (Tyr)	
Isoleucine (Ile)		Glutamic Acid (Glu)		Serine (Ser)	
Proline (Pro)		Asparagine (Asn)		Threonine (Thr)	
Glutamine (Gln)					
Cysteine (Cys)					

3

Charges on Amino Acids

The structural formulas of the common amino acids all contain at least one *carboxylate group* and one *quaternary ammonium group*.
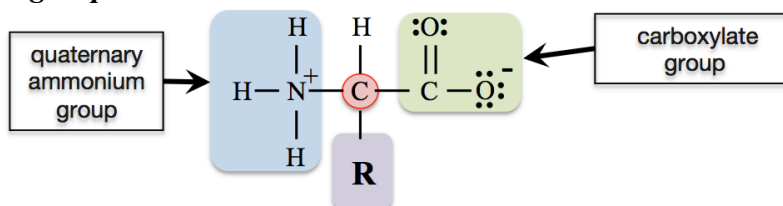
In previous chapters you learned that in aqueous solutions, the *carboxylate group* is in equilibrium with its _____, the *carboxyl group*:

carboxylic acid
(acid form)

carboxylate ion
(base form)

pKₐ = **2 to 5**, depends on **R** group
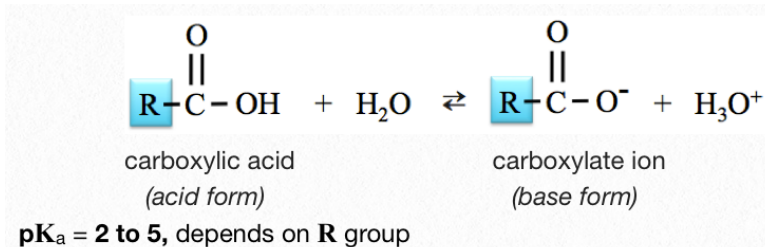
From the _____ relation, we know that when the **pH** is less than the **pKₐ** of a carboxyl group, then the carboxylic acid form (**R-COOH**) is predominant, and when the **pH** is greater than the **pKₐ**, then the carboxylate ion form (**R-COO⁻**) is predominant.

Likewise, the *quaternary ammonium group* is in equilibrium with its conjugate, the *amine group*:

quaternary ammonium ion
(acid form, **pKₐ ~9.5**)
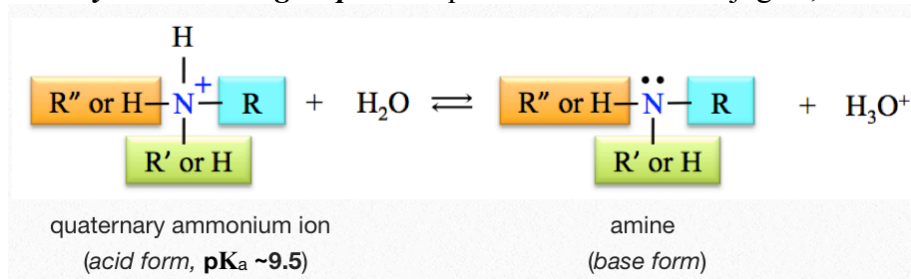
amine
(base form)

When the **pH** of a solution is less than the **pKₐ (~ 9.5)**, then the *quaternary ammonium group* (acid form) is predominant, and when the **pH** is greater than the **pKₐ**, then the amine group (base form) is predominant.

Since amino acids involve the **carboxyl group/carboxylate group conjugate pair** *and* the **quaternary ammonium group/amine group conjugate pair**, then the _____ _____ *of the predominant form of an amino acid* will depend on the_____ .

EXAMPLE: Consider the predominant form of *alanine* at physiological **pH** (**pH** ~7.4):
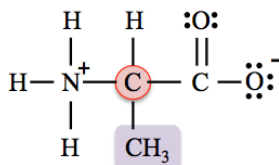
- The **pKₐ** values of amino acid carboxyl groups are between **2** and **5** (depending on which amino acid), therefore, at **pH** = **7.4**, the base form (carboxylate ion) is predominant.

- *Quaternary ammonium groups* that are attached to the *α*-carbons of amino acids have **pKₐ** values of about **9.5**, therefore, at **pH** = **7.4**, the quaternary ammonium group (acid form) is predominant.

4

The predominant form of *alanine* has a negative (1-) formal charge on the *carboxylate group* and a positive (1+) formal charge on the *quaternary ammonium group*, which gives it a *total charge* of _____.
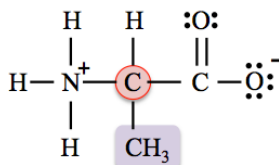
predominant form of *alanine* at **pH = 7.4**

When an amino acid has a total charge equal to zero, it is called a _____.
- (*zwitter* is German for *hermaphrodite* or *hybrid*).

The amino acid structures in the table (provided earlier) are the predominant forms at physiological pH.

In sufficiently acidic or basic solutions, the _____ _____ of the predominant form of an amino acid *will change* from its physiological value.

EXAMPLE: Consider the *total charge* of the predominant form of *alanine* in an extremely **acidic** solution.

At **pH = 1.0** (an extremely *acidic solution*) the **pH** is _____ than the **pK$_a$** of *both* the carboxyl group and the quaternary ammonium group, therefore both groups exist in their **acid form**, as shown below.
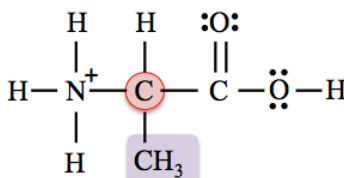
predominant form of *alanine* at **pH = 1.0**

The predominant form of *alanine at* **pH = 1.0** has an *uncharged* carboxyl group (**COOH**) and has a positive (1+) formal charge on the nitrogen of the quaternary ammonium group, which results in a _____ **(1+) total charge**.

EXAMPLE: Consider the *total charge* of the predominant form of *alanine* in an extremely **basic** solution.

At **pH = 12.0** (an extremely *basic solution*) the **pH** is _____ than the **pK$_a$** of *both* the carboxyl group and the quaternary ammonium group, therefore both groups exist in their **base form**, as shown below.
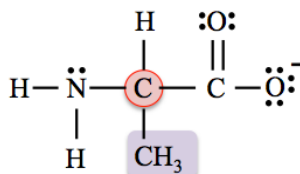
predominant form of *alanine* at **pH = 12.0**

The predominant form of *alanine at* **pH = 12.0** has a negative (1-) formal charge on the single-bonded oxygen of the carboxylate group and an *uncharged* nitrogen in the amine group, which results in a _____ **(1-) total charge**.

Practice Problems: The amino acid structures in the table provided earlier are the predominant forms at physiological **pH**.

   a. Draw the predominant form of valine when the **pH = 7.4**
   b. Draw the predominant form of valine when the **pH = 1.0**
   c. Draw the predominant form of valine when the **pH = 12.0**
   d. What is the *total charge* of the predominant form of valine when the **pH = 7.4?**
   e. What is the *total charge* of the predominant form of valine when the **pH = 1.0?**
   f. What is the *total charge* of the predominant form of valine when the **pH = 12.0?**

Classification of Amino Acids

Amino acids are classified by the _____ *of their side-chain* and the ***ability of their side-chain***

to acquire _____ _____ (at physiological **pH**).

Amino Acid Class	Side Chain Polarity	Side-Chain Charge at Physiological pH
Nonpolar	nonpolar (hydrophobic side-chain)	zero
Polar neutral	polar (hydrophilic side-chain)	zero
Polar acidic	polar (hydrophilic side-chain)	negative
Polar basic	polar (hydrophilic side-chain)	positive

1) Nonpolar Amino Acids

Nonpolar amino acids have ***nonpolar (hydrophobic) side-chains*** <u>and</u> their predominant forms have *uncharged* side-chains at physiological pH.

- The *nonpolar amino acids* (their predominant forms at physiological **pH**) are:

glycine   alanine   valine   proline   phenylalanine

leucine   isoleucine   methionine   tryptophan
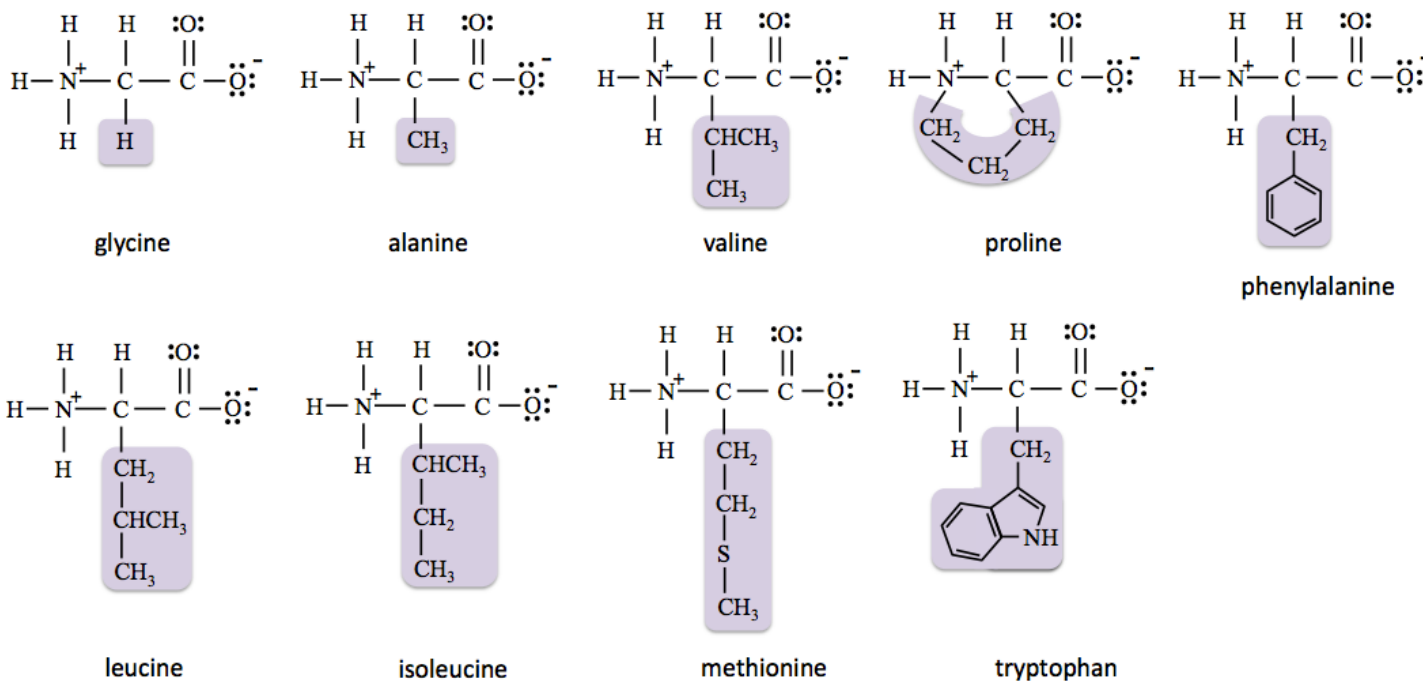
Note that although the side-chain of *tryptophan* contains a few highly-polar bonds, the hydrocarbon part is so large that it dominates the interactions, making the side-chain *hydrophobic*. For this reason, tryptophan is put into the *nonpolar* class.

2) Polar Neutral Amino Acids

Polar neutral amino acids have ***polar (hydrophilic) side-chains*** <u>and</u> their predominant forms have *uncharged* side-chains at physiological pH.

- The *polar neutral amino acids* (their predominant forms at physiological **pH**) are:

glutamine   asparagine   tyrosine

cysteine   serine   threonine

7
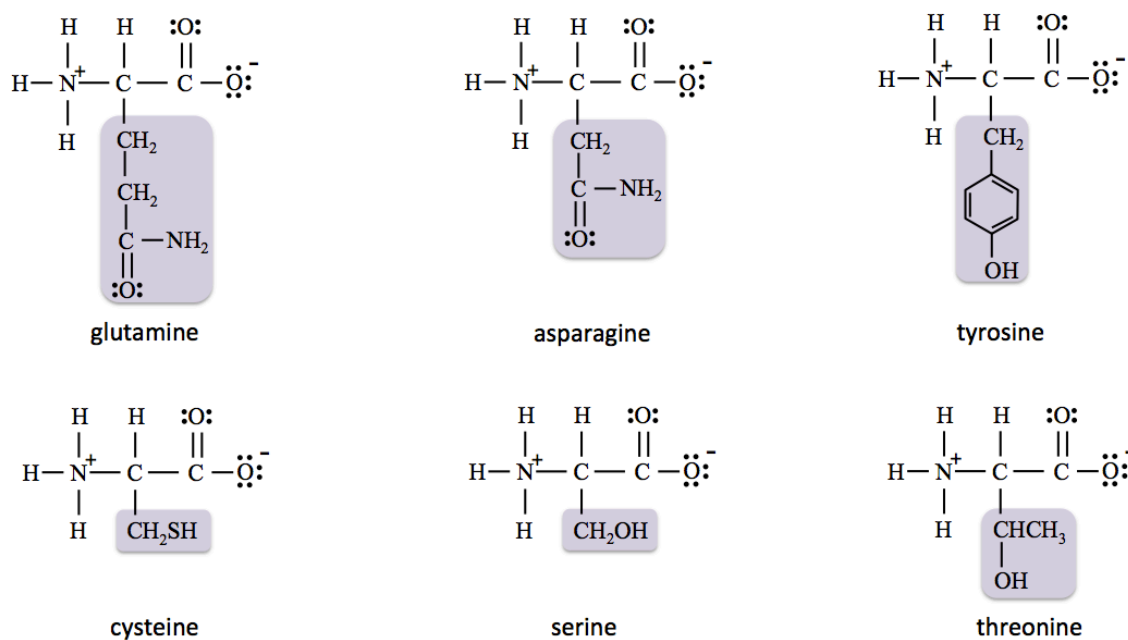
3) Polar Acidic Amino Acids

Polar acidic amino acids have *polar (hydrophilic) side-chains* <u>and</u>, their predominant forms have side-chains with **negative (1-)** *formal charge* at physiological **pH**.

- This formal charge is from a _____ *group*.

The *polar acidic amino acids* (their predominant forms at physiological **pH**) are:
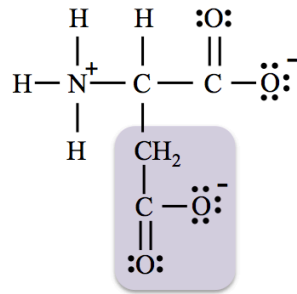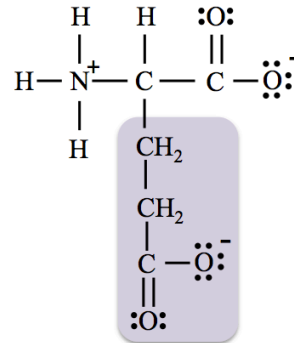
aspartic acid   glutamic acid

Polar *acidic* amino acids are given the "*acidic*" term in their classification because their acid forms are stronger acids than those of the polar "*basic*" amino acids (discussed next).

4) Polar Basic Amino Acids

Polar basic amino acids have *polar (hydrophilic) side-chains* <u>and</u>, except for *histidine*, their predominant forms have side-chains with **positive (1+)** *formal charge* at physiological **pH**.

- This formal charge is from a *quaternary ammonium group*.

- The *polar basic amino acids* (their predominant forms at physiological **pH**) are:
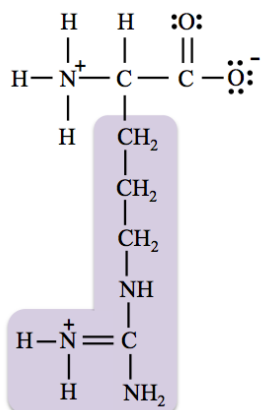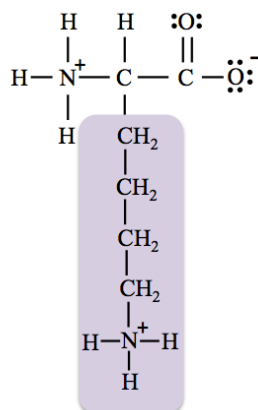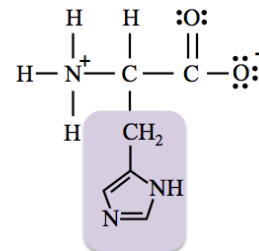
arginine   lysine   histidine

Properties of Amino Acids

Although some amino acids contain hydrophobic side-chains, overall they are _____ - _____.

All amino acids are _____ due both to the presence of polar covalent bonds that are capable of forming hydrogen bonds with water, and to the fact that they can carry charges (-COO⁻ and/or -NH₃⁺).
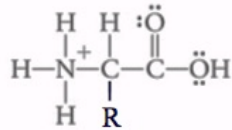
Acidic
pH 1
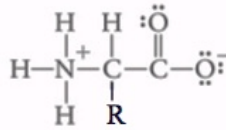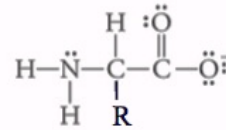
Basic
pH 14

Stereoisomerism of Amino Acids

With the exception of glycine, all of the α-amino acids are _____ because the α-carbon atom in each is attached to four different groups.
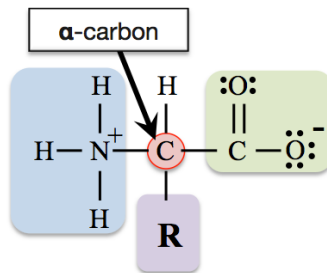
The presence of chiral carbons produces stereoisomers with mirror images: _____.

Fischer projections of amino acids have the *carboxylate group* on **top** and the *side-chain* on the **bottom**.

- **L-amino acids** have the NH_3^+ on the _____.

- **D-amino acids** have the NH_3^+ on the _____.

Organisms use only L-amino acids to produce proteins.

| **You try one:** Draw Fischer projections of the D-isomer and the L-isomer of ***alanine***. |
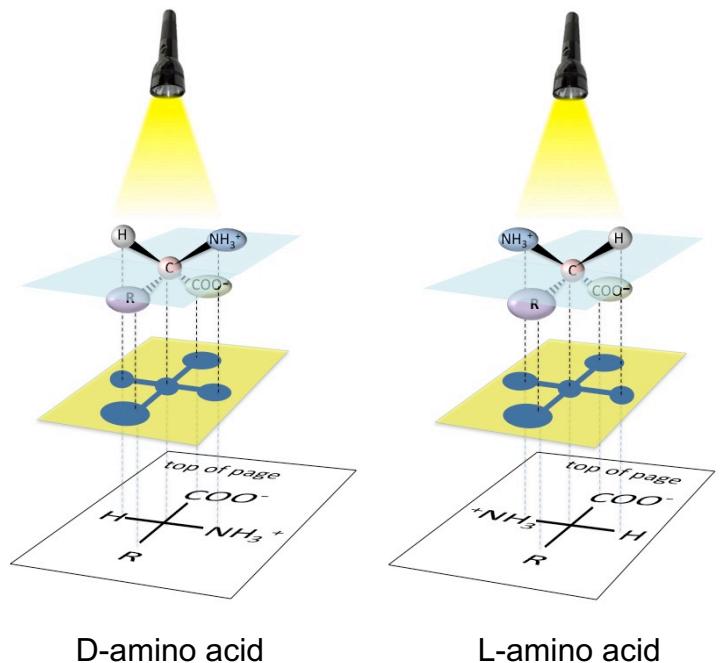
D-amino acid   L-amino acid

Peptides and Proteins

The Peptide Bond

Peptides and proteins consist of amino acid residues joined by _____ (amide) bonds.

Formation of a Peptide Bond

Step 1: The two amino acids are drawn side-by-side. The single-bonded *oxygen atom* is removed from the *carboxylate group* on the *left-most* amino acid. *Two* hydrogen atoms are removed from the *quaternary ammonium group* on the *right-most* amino acid. The oxygen atom and the two hydrogen atoms combine to form a water molecule.
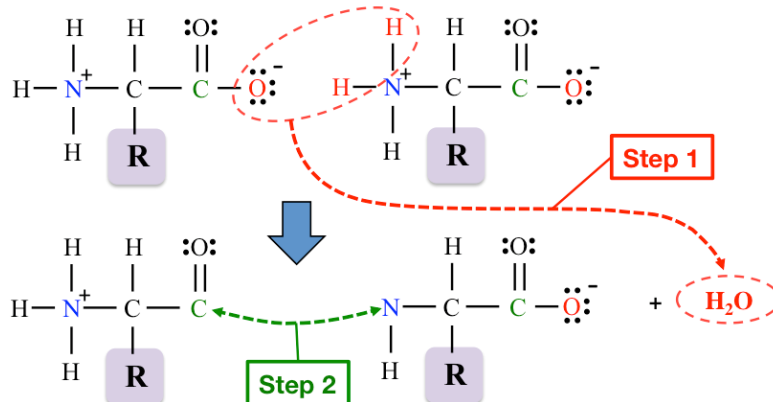
Step 2: A *new bond* is made between the carbonyl carbon and the nitrogen.
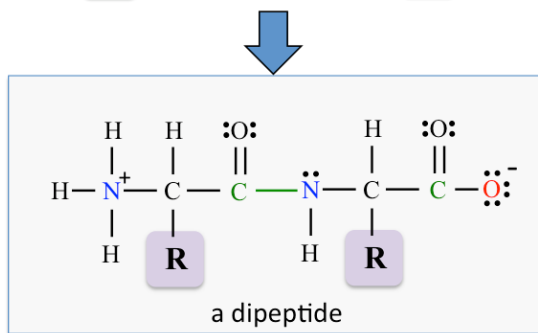
The peptide formed in this example is called a _____ because it contains *two* amino acid residues.

The *new bond* between the two amino acid residues is called a **peptide bond**.
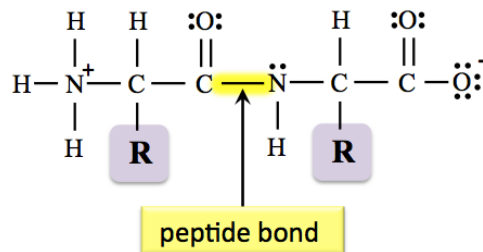
You try one: Draw the structural formula of the *dipeptide* that contains *two **valine*** amino acid residues. Label the peptide bond

.

Formation of Larger Peptides

Larger peptides are formed by adding more amino acids, one by one, to a growing peptide.

Example: Formation of a Tripeptide

- Begin with the general form of a *dipeptide* and then add a *new amino acid residue*.

- The new *peptide bond* can be made using the same **two steps** as we used when we made a *dipeptide*.
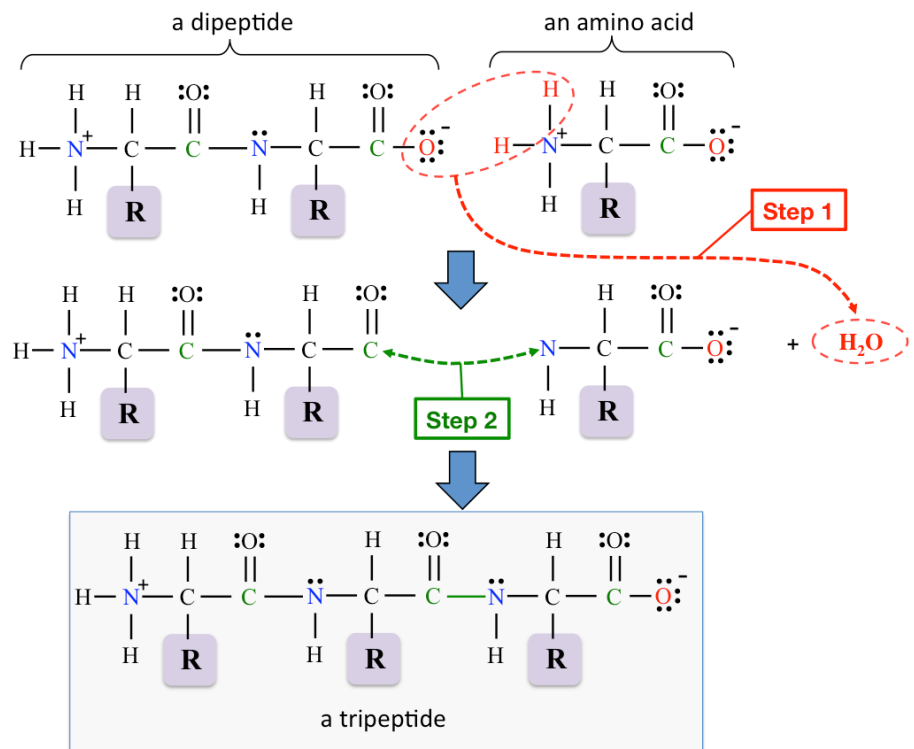
This process can continue and larger peptides can be formed by adding more amino acids, one by one, to a growing peptide.

Peptide Terminology

The **end** of the peptide structural formula that has a **quaternary ammonium group** is called the

_____-terminus, and the **end** that has a **carboxylate group** is called the _____-terminus.
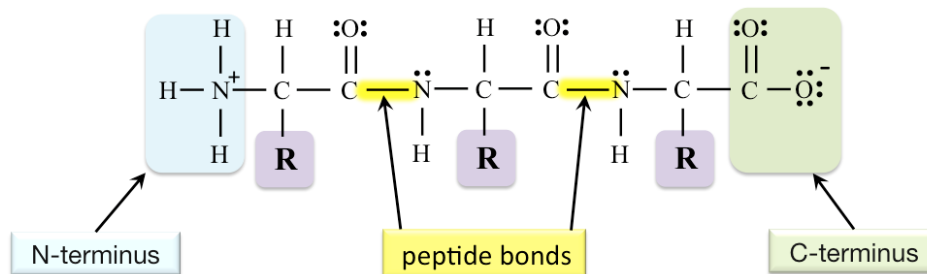
The bonding pattern around a *peptide bond* is called the **peptide** _____.
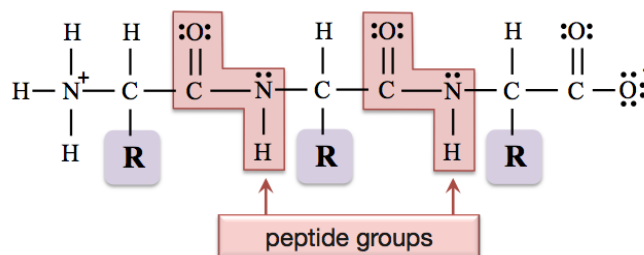
Note that **nitrogen in a peptide group does not** have a (1+) formal charge, as does the *nitrogen in the quaternary ammonium group at the N-terminus.*

Peptides are identified by the use of a common name *or*, by listing its amino acid residues' *three-letter abbreviations* in order from N-terminus to C-terminus.

Example of identifying a peptide from its amino acid residue's *abbreviations*: **Val-Asp-Ala-Arg-Gly**.

a *pentapeptide*

Val-Asp-Ala-Arg-Gly
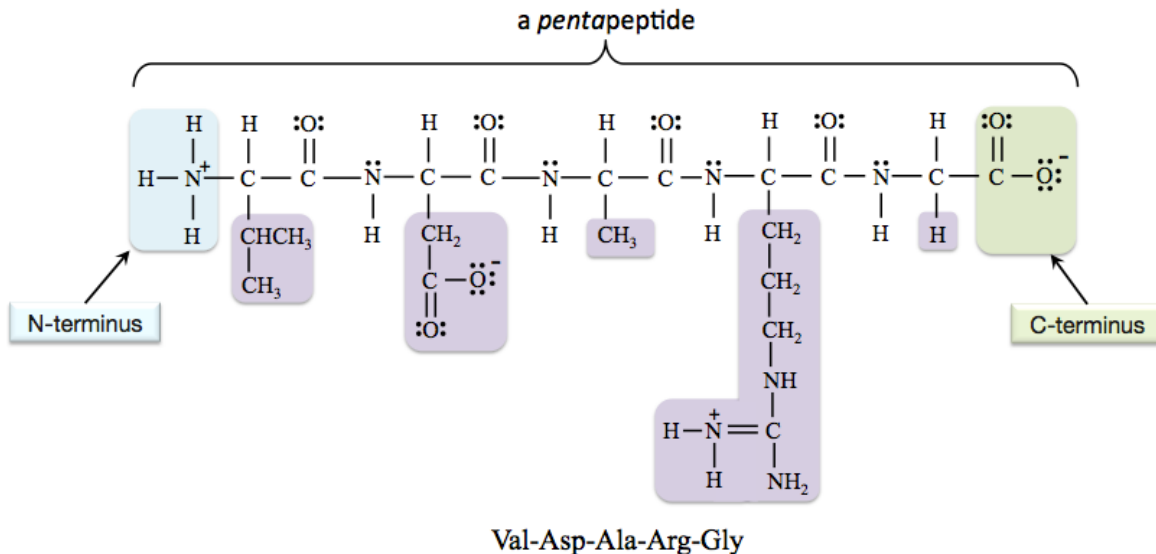
I drew this pentapeptide by forming peptide bonds between the predominant forms of the amino acids at physiological **pH**, therefore the resulting pentapeptide is also in the form that is predominant at physiological **pH**. Note that *two of the side-chains* in this peptide carry a formal charge. This peptide has a total charge equal to **zero** because the *two negative charges* and *two positive charges* add up to **zero**.

You try one:

a. Draw the *structural formula* for the predominant form of Gly-Lys-Tyr-Ala at physiological **pH**.
b. Label the **peptide bonds** and *circle* the **peptide groups**.

   NOTE: If you correctly connect the amino acid structural formulas from the amino acid table, then the peptide that you draw will be the predominant form at physiological **pH**.

Also: What is the ***total charge*** of the peptide that you drew for in the previous problem?

Examples of Biologically-Relevant Peptides

A **protein** consists of one or more *large peptides* and has *a specific biological function*. Although shorter peptide chains (less than about *fifty* amino acid residues) have specific biological functions, they are generally not classified as proteins. Short peptide chains function as chemical signaling compounds; over one hundred of them have been identified.

Endorphins are examples of chemical signaling peptides. They are natural painkillers that are produced in the body. They interact with receptors in the brain to inhibit the transmission of pain signals. Five endorphins have been found (so far). An example of an endorphin peptide is *α-endorphin*. It contains sixteen amino acid residues, which are connected in the sequence (N-terminus to C-terminus) shown below:

<div align="center">

Tyr-Gly-Gly-Phe-Met-Thr-Ser-Glu-Lys-Ser-Gln-Thr-Pro-Leu-Val-Thr

</div>

Another example of a peptide is *oxytocin*. It is produced by the pituitary gland, and stimulates uterine contractions in labor. *Oxytocin* contains *nine* amino acid residue, which are connected in the sequence shown below:

<div align="center">

Cys-Tyr-Ile-Gln-Asn-Cys-Pro-Leu-Gly

</div>

Oxytocin was the first naturally-occurring hormone to be produced in a laboratory.

Protein Structure

The structure of proteins is understood in terms of four levels of organization:

1) _____
2) _____
3) _____
4) _____

Primary Protein Structure

The _____ of amino acid residues in a peptide or protein is referred to as its *primary structure*.

- Example: The primary structure of the pentapeptide is shown below:

<div align="center">
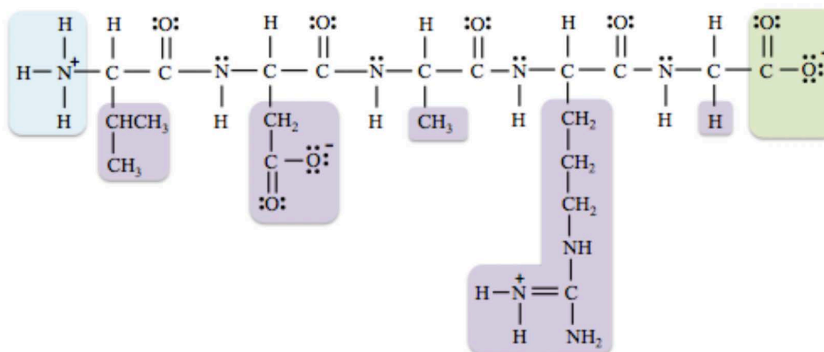
Primary Structure:
valine   aspartic acid   alanine   arginine   glycine
(Val-Asp-Ala-Arg-Gly)

</div>

The primary structure of peptides and proteins is analogous to the arrangement of letters in a word.

edit ≠ diet ≠ tide ≠ tied

Primary structure of a protein is the linear sequence of amino acids connected by peptide bonds.

- Different proteins typically contain from about 40 to over 4000 amino acids
- There are 400 distinct dipeptides (20^2).
- There are 8000 distinct tripeptides (20^3).
- When there are 100 amino acids in the chain, there are $20^{100} = 1.27 \times 10^{130}$ distinct peptides!

Understanding Check: Write the names (using the three letter abbreviation method) of all of the tripeptides that can be made by combining one glycine (gly), one alanine (ala), and one aspartic acid (asp) residue. For example, one of the tripeptides is gly-ala-asp.

Secondary Protein Structure

The properties of proteins depend not only on their sequence of amino acid residues, but also on how they are folded, twisted, and bent.

Secondary protein structure describes the geometric patterns that occur when individual peptide chains "fold" back on themselves.

Secondary structure results from _____ _____ between **peptide groups** within an individual peptide.

There are **two common types** of secondary structures, the _____ _____ (**α helix**) and the

_____ _____ (**β sheet**).

The Alpha Helix

The *alpha helix* geometric pattern resembles a

_____.
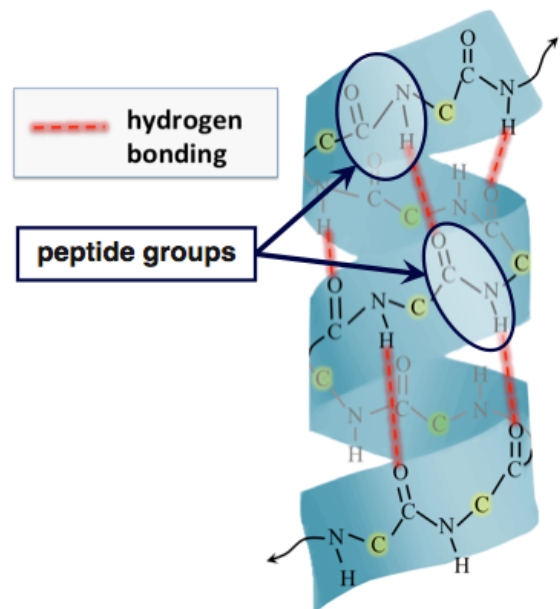
The Beta Sheet

The **beta sheet** geometry occurs when a peptide folds back on itself in a _____ arrangement.

Illustrative Model of a Beta Sheet

hydrogen bonding   beta sheet
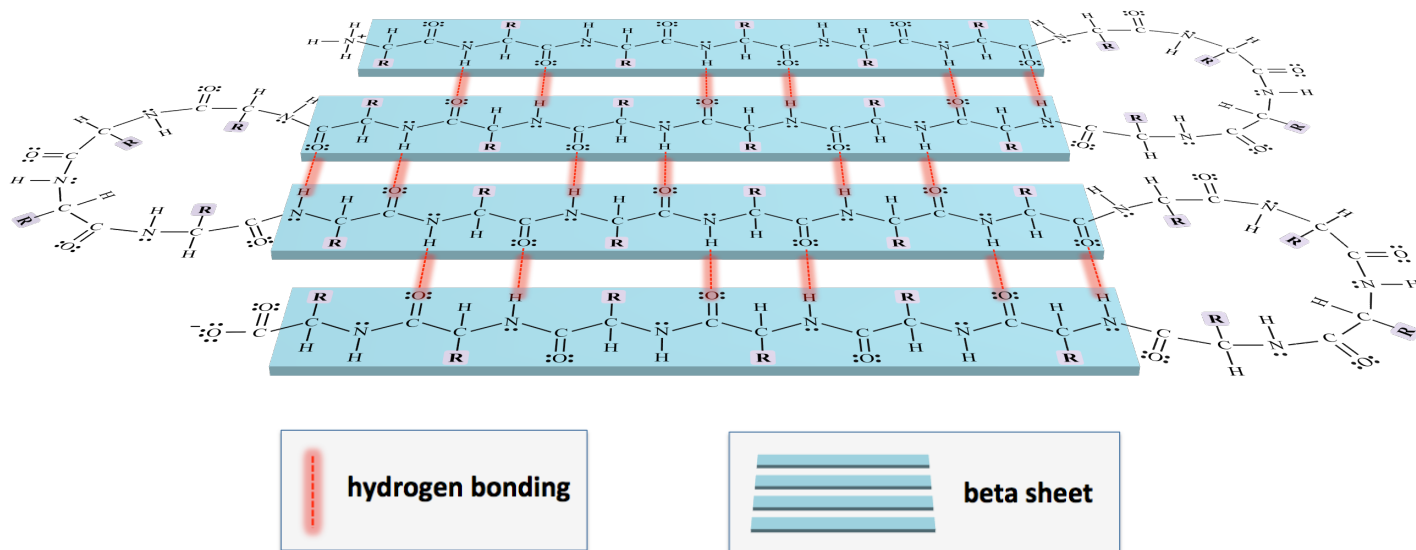
In addition to *alpha helices* and *beta sheets*, there are a few other, much less frequently seen geometries that are also categorized as secondary structures. Since these other secondary structures are relatively rare, I will not discuss their particularities.

A key feature of *secondary protein structure* is that it **only** involves *hydrogen bonding between peptide groups within an individual peptide chain*.

Tertiary Protein Structure

Alpha helices and/or beta sheets, along with the *unorganized sections* of a peptide chain, "*fold*" into a more compact shape.

- The _____ shape of a peptide is called the **tertiary structure**.

"***Ribbon models***" are often used in order to visualize tertiary protein structure. These illustrative models use ribbon-like shapes to represent the geometry of secondary structures. The spring-like ribbons represent alpha helices and the flat side-by side ribbons represent beta sheets. Sometimes arrows are used at the ends of ribbons to indicate the direction (from N-terminus to C-terminus). Lines or thin tubes are used for *unorganized sections* of a peptide chain. The ribbon model for *ribonuclease A* protein (RNase A), an enzyme used to break down RNA, is shown on the right.

Ribbon Model of an *RNase A* Protein

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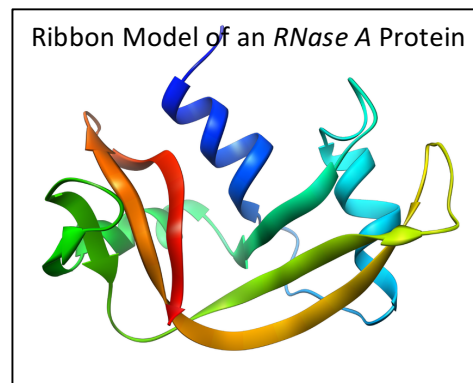
Of the many folding patterns (conformations) possible for a protein, there is usually only one that leads to a _____(biologically active) molecule.

The sequence of amino acids (primary structure) ultimately determines which folding pattern is selected, so both secondary and tertiary structure _____on primary structure.

Some of the interactions that are involved in **tertiary structure** are illustrated below.
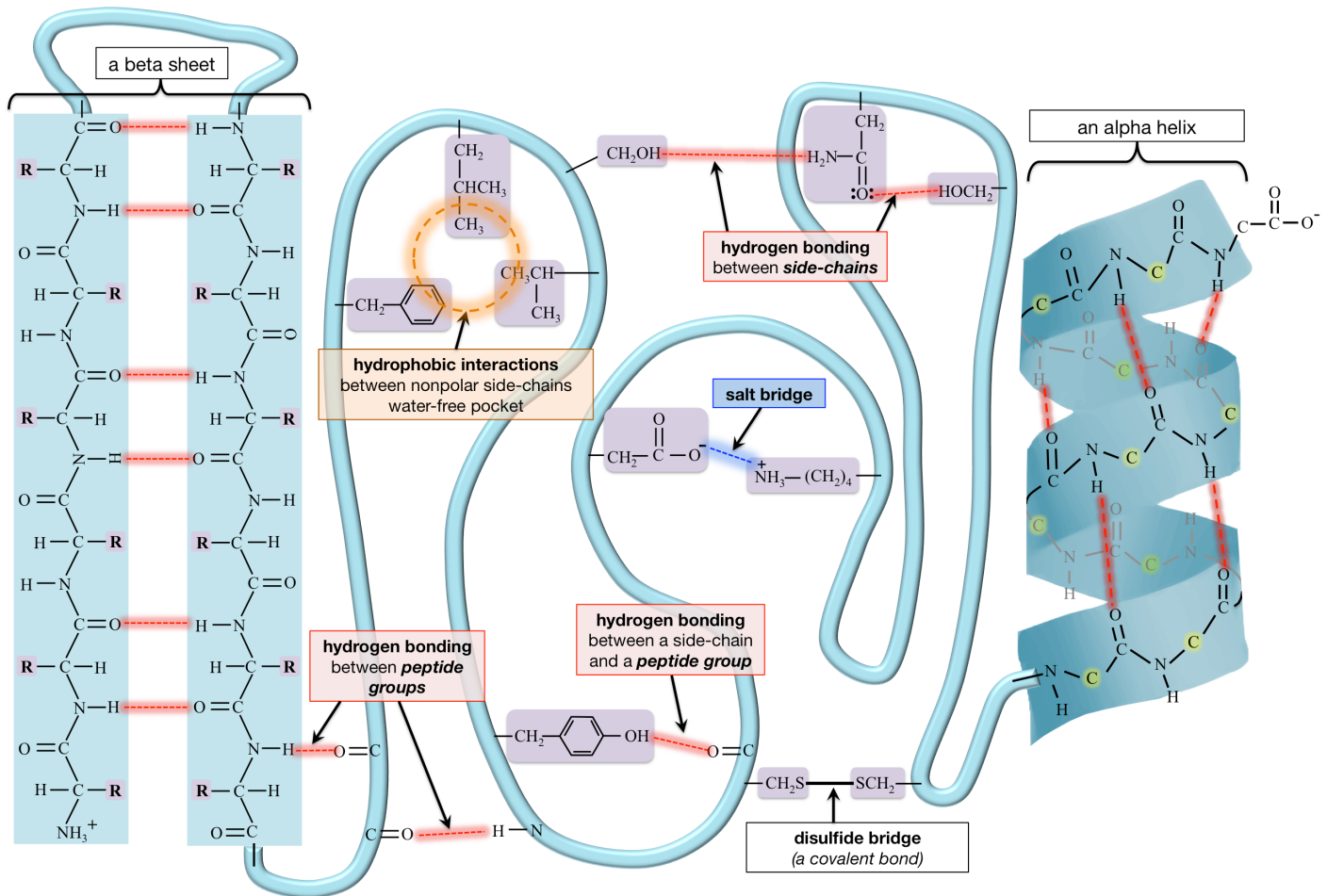
Description of Tertiary Structure Interactions:

1) Hydrophobic Interactions

Nonpolar side-chains are attracted to **other** *nonpolar side-chains* through *London forces,* and form "**water-free pockets**" in the interior region of the folded and compacted peptide (see the illustration above).

2) Hydrogen Bonding

Hydrogen bonding in *tertiary structures* can occur between polar side chains (that contain the features necessary for hydrogen bonding) and/or peptide groups. See the illustration above.

3) Salt Bridges

I introduced **salt bridges** to you, in chapter 4, as one of the *five noncovalent interactions*. A *salt bridge* is an attractive force between the **positive** formal charge on *polar basic* amino acid residue and a **negative** formal charge on a *polar acidic* residue (see the example in the illustration above).

4) Disulfide Bridges

In a previous chapter, you learned that *disulfide (covalent) bonds* can be formed by the oxidation of two thiol (**SH**) groups. *Disulfide bonds* in proteins are called *disulfide bridges*. Each *cysteine* residue contains a thiol group in its side-chain that is capable of forming a disulfide bridge with *another* cysteine residue, as shown above.
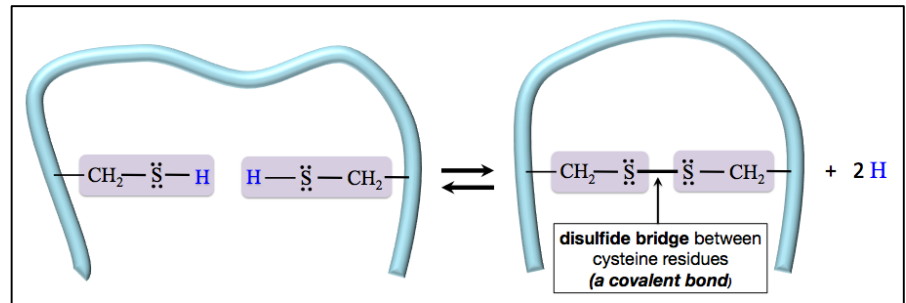
5) Dipole-Dipole and Ion-Dipole Forces

Dipole-dipole attractive forces can occur between polar side-chains and/or peptide groups. These interactions are not included in the illustration on the previous page. If needed, you can review dipole-dipole and ion-dipole interactions in section 6 of chapter 4.

Quaternary Structure

A large number of native proteins are a combination of

_____   _____   _____ polypeptide chain.
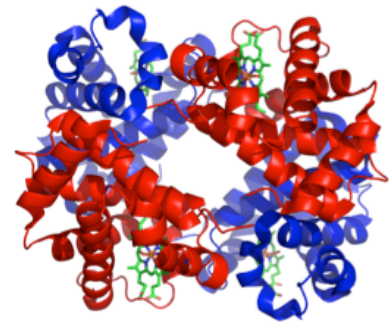
- **Example:** *Hemoglobin*

Image source: Wikimedia Commons, Author: Richard Wheeler, CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcode

Quaternary protein structure is the overall shape that occurs when **two or more _____** *peptide chains* assemble to make a protein.

In proteins composed of *two or more* peptide chains, the individual peptide chains are referred to as "**subunits**."

The quaternary structures of large proteins are sometimes depicted using *space-filling models*. In these models, the various subunits are often shaded with different colors or grey-scale tones.

- **Example:** *ATP synthase*

The forces that hold the subunits together in *quaternary structures* are **the same** as those involved in *tertiary structures*.
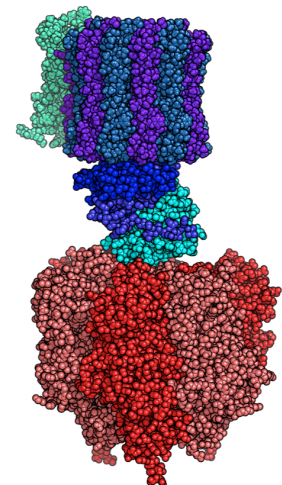
Image source: Wikimedia Commons, Author: Alex.X CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcod

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Understanding Check: In which of the following levels of protein structure can hydrogen bonding play a role?
- a) primary structure
- b) secondary structure
- c) tertiary structure
- d) quaternary structure

Globular, Fibrous, and Membrane Proteins

Proteins generally fall into one of three categories:

1) _____ proteins

2) _____ proteins

3) _____ proteins

Globular Proteins

Globular proteins have a highly- _____ and compact shape.

- The overall shapes of these proteins are more "sphere-like" than "string-like."

- The globular shape allows for *hydrophobic* side-chains to be directed to the protein's interior (forming "water-free pockets"), while *polar* side-chains are oriented outward to form a *hydrophilic* exterior. The hydrophilic exterior allows globular proteins to be more easily dispersed in solutions (intercellular and extracellular).

Globular proteins function as enzymes, chemical signaling compounds, transporters of other compounds, and antibodies.

Hemoglobin (shown on the right) is an example of a globular protein

Image source: Wikimedia Commons, Author: Richard Wheeler, CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcode
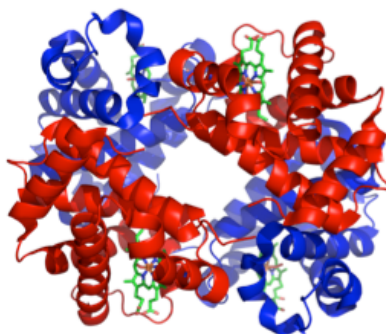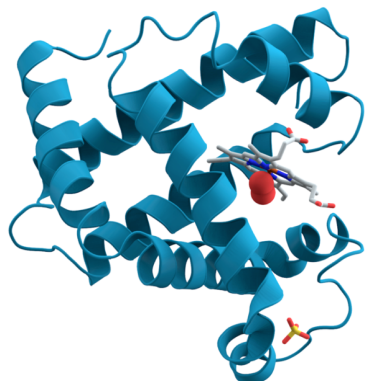
Myoglobin (shown on the left) is another example of a globular protein. It is used to store oxygen (O_2) in muscle tissue, thereby allowing organisms to function while holding their breath. *Myoglobin* is responsible for the red color of meat. It is found in especially high concentration in diving animals, such as seals and whales. It is composed of just one peptide chain. Human myoglobin contains 153 amino acid residues and eight alpha helices. It contains a *heme* prosthetic group (shown in grey) that binds oxygen (shown as red spheres next to the heme group).

Albumin is another example of a globular protein.

Human *albumin* is the most abundant protein in human blood plasma. Its biological functions include transporting hormones, fatty acids, and other compounds, acting as a buffer, and maintaining osmotic pressure.
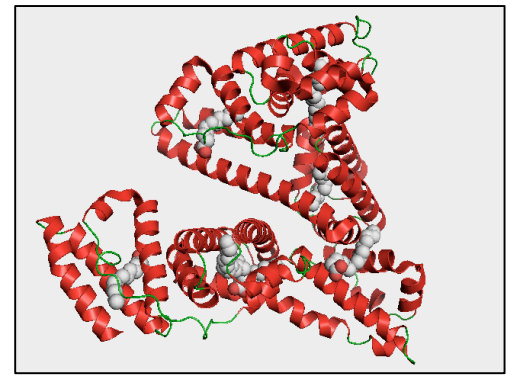
Antibodies, also referred to as **immunoglobulins** (Ig), are *globular proteins*.
Antibodies are able to act as protective agents by binding to specific, usually harmful, objects - called *antigens*. Antigens are often foreign (nonself) objects such as harmful bacteria or viruses. When an antibody binds to an antigen, it either directly neutralizes the antigen, or marks it so that the antigen can be subsequently neutralized by other components of the immune system.

The smallest antibodies are composed of a *single* immunoglobulin unit, called an **immunoglobulin monomer**. An immunoglobulin monomer is shaped a bit like the letter "Y," and is often illustrated using a Y-shape, as shown on the *right-hand side* of the illustration.

antigen binding sites (paratopes)

antigen binding sites (paratopes)

Ribbon model of an immunoglobulin monomer

"Y-shape" model of of an immunoglobulin monomer
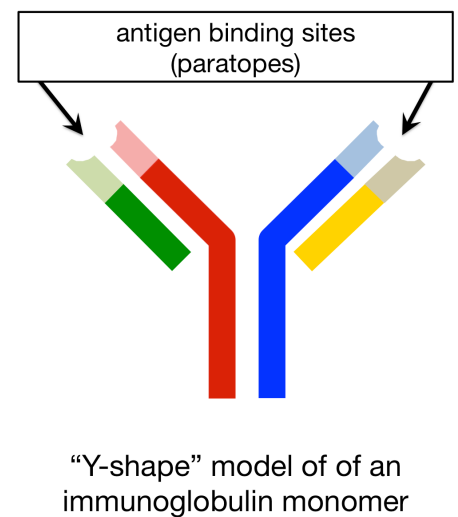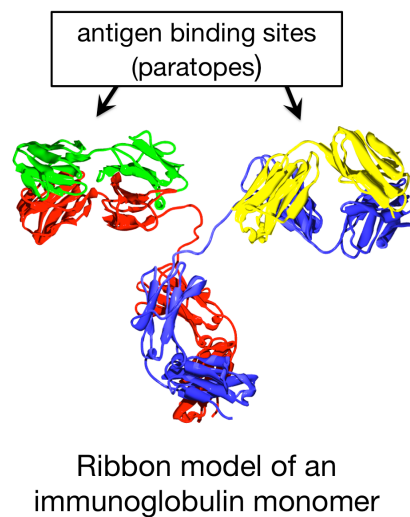
An antigen binding site, called the **paratope**, binds to a particular part of an antigen called the **epitope**.

- The binding between antigen and antibody occurs because of **noncovalent attractive forces**, *which are maximized due to the* _____ *shapes of the paratope and epitope.*

epitopes

Antigen

Antigen

The epitope matches the paratope, so the antibody binds to the antigen.

The epitope does not match the paratope, so the antibody does not bind to the antigen.
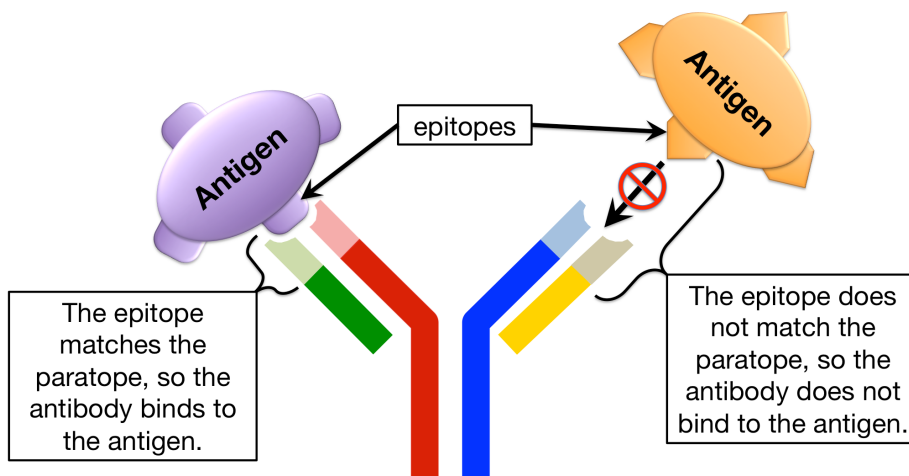
Note that in the Y-shape antibody model shown on the left, the *paratope* will only bind with one of the two antigens - the antigen that has a complementary epitope. We say that the paratope (or antibody binding site) is "_____" for a particular epitope.

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The immune system can produce an almost infinite variety of paratope shapes by varying the paratope region's amino acid sequence (and therefore its shape). By doing so, antibodies are produced to be *specific* for one particular antigen, much like a lock is *specific* for one key.

Some antibodies contain **more than one** *immunoglobulin unit.* Placental mammals, which includes humans, have immunoglobulin monomer, immunoglobulin dimer, and immunoglobulin pentamer antibodies. Immunoglobulin *dimers* are made from **two** immunoglobulin monomers, and immunoglobulin *pentamers* are made from **five** immunoglobulin monomers. These three types of antibody structures are illustrated below.

immunoglobulin monomer
(single immunoglobulin unit)

immunoglobulin dimer

immunoglobulin pentamer
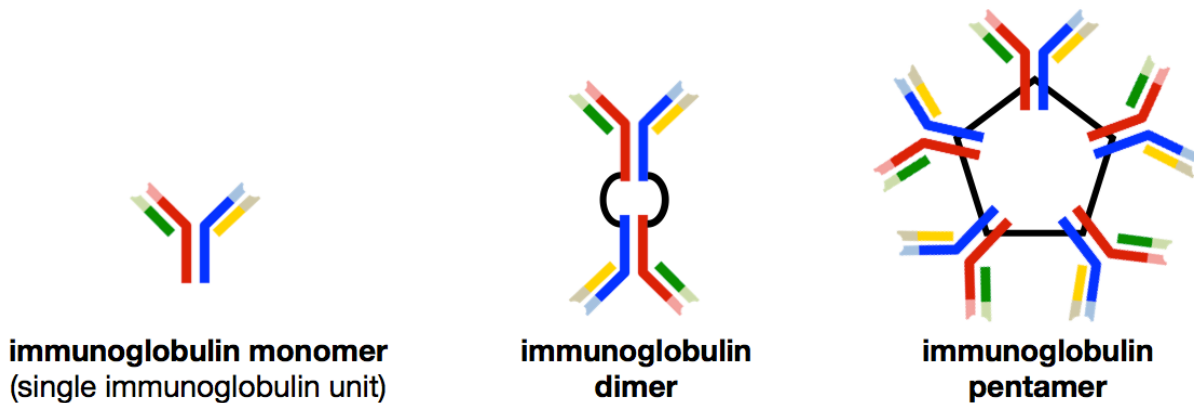
One last note on antibodies:

Antibodies have _____ (oligosaccharides) that are covalently bound to **some** of their amino acid residue *side-chains*.

- Proteins, such as antibodies, that contain carbohydrates are called _____.

Fibrous Proteins

Fibrous proteins have long and narrow "_____ -like" shapes.

- They are *much less compact* than *globular* proteins.

The narrower shape makes it difficult for hydrophobic side-chains to be oriented toward the interior region of a fibrous protein, and results in a *hydrophobic* exterior. For this reason, fibrous proteins tend to be water-<u>in</u>soluble.

Fibrous proteins play important roles in providing structural rigidity and in contractile movement (muscles).

An example of a *fibrous protein* is **collagen**. *Collagen* is the most abundant protein in the body. Its function is to provide structural rigidity and stiffness. It is found in skin, ligaments, tendons, and other parts of the body. An illustration of the components of *collagen* are shown below.
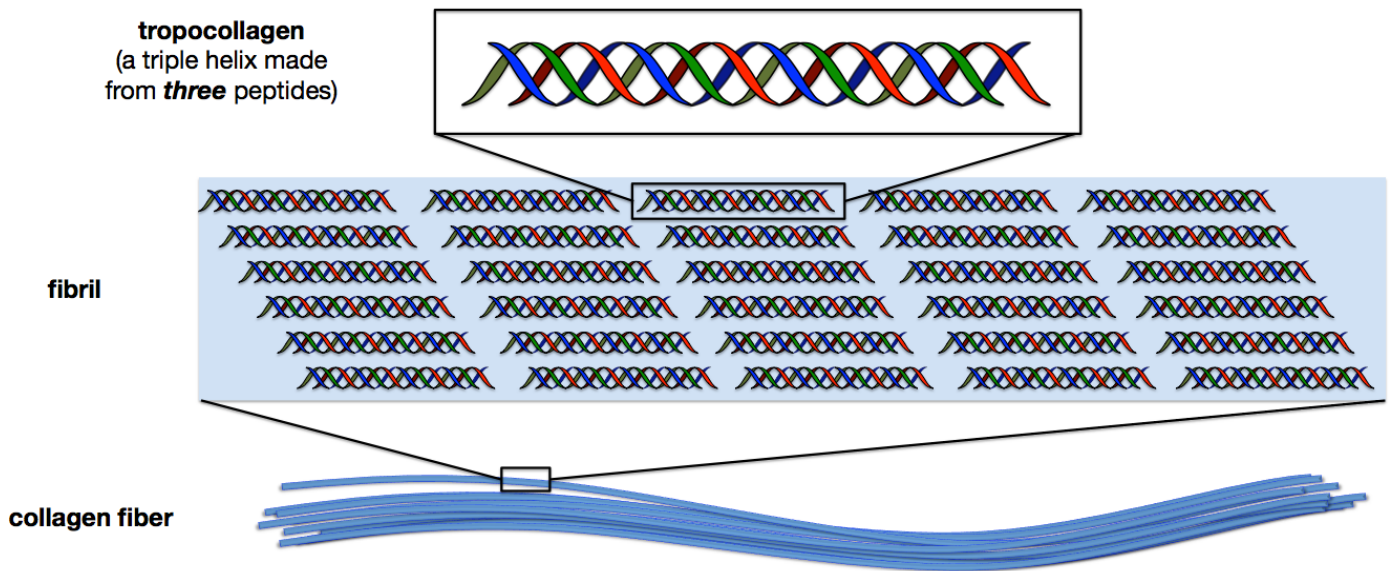
Other examples of fibrous proteins are **keratins**. Their primary role is to provide structural rigidity and stiffness. *Keratins* are some of the strongest natural materials.

- K*eratins can be* classified as **alpha-keratins** or **beta-keratins**.

Alpha-keratins are found in places such as hair, wool, horns, hooves, claws, and nails.

In hair, *two* peptide *double* helices are twisted around each other to form a **protofibril**, as shown below.

a protofibril
two peptide *double helices* that are twisted around each other
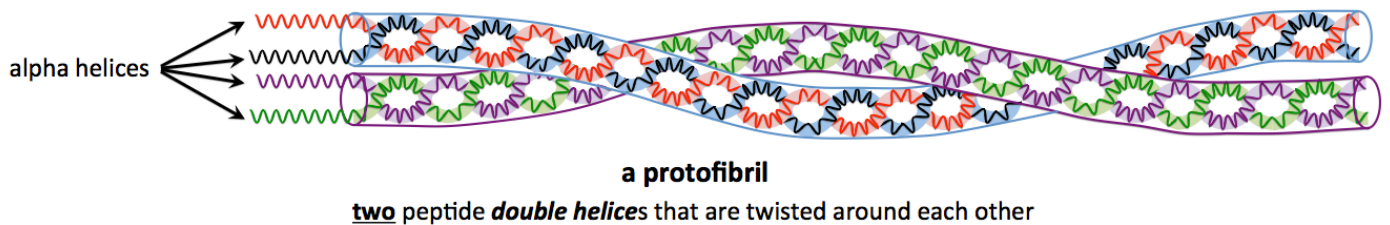
Protofibrils bundle together to form **microfibrils**. *Microfibrils* bundle together to form **macrofibrils**. Each **hair cell** is primarily composed of bundled *macrofibrils*.

A **single hair** consists of bundled hair _____.
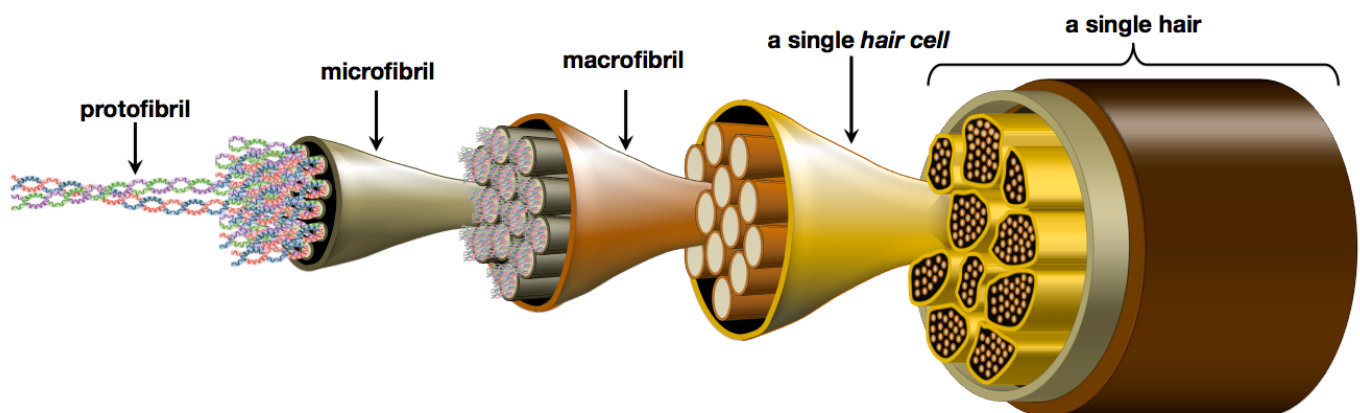
Beta-keratins

Beta-keratins, which are also fibrous proteins, are found in places such as reptilian skin, the outer layer of human skin, bird feathers and beaks, turtle shells, silk, and the tongue.

- Beta-keratins are composed of fibers that primarily contain **beta sheet** *secondary* structures.

- The *beta sheets* are stacked in _____ *tertiary* structures.

An example of a beta-keratin structure can be seen in **silk**. The stacked beta sheets, which are held together by disulfide bridges and noncovalent interactions, entwine to form a **fibroin microfibril**. *Fibroin microfibrils* assemble to form **fibrils.** *Fibrils* assemble to form **fibroin filaments**. Two *fibroin filaments* are held together by *sericin protein*, which acts like a glue to hold the two fibroin filaments together in a single silk fiber, as shown below.
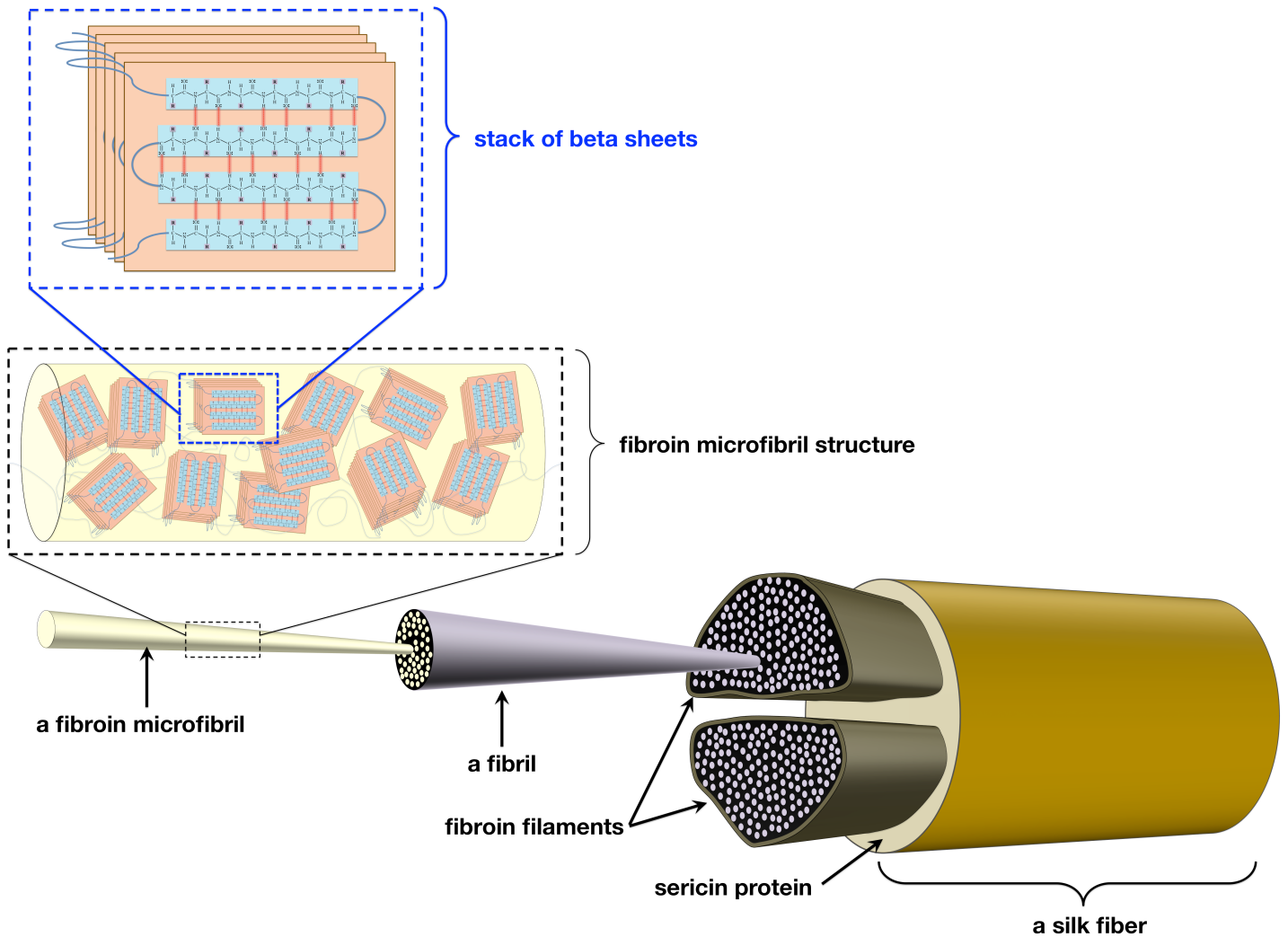
Fibroin microfibril keratin fibers are also found in spider webs. The structure of *spider's silk* is illustrated below.

22
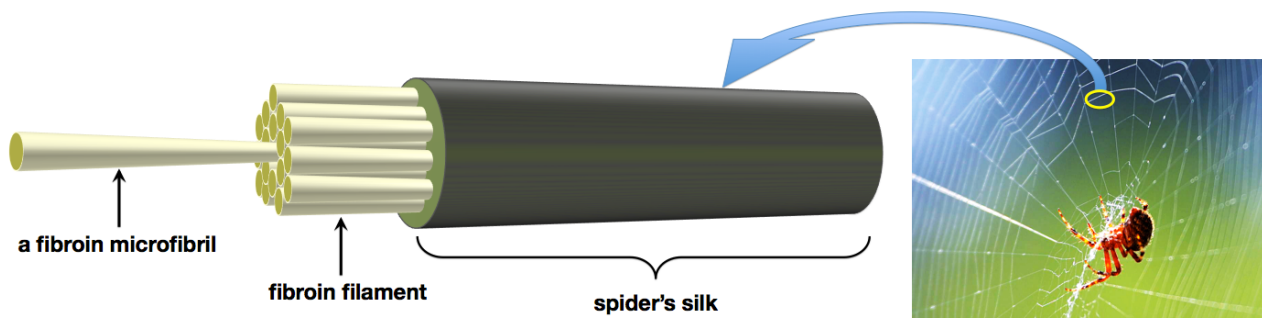
Fibrous Proteins in Muscles

Muscle contraction involves the interaction of *fibrous proteins*.

Muscles are composed of bundled muscle_____.

section of a single muscle cell

a myofibril

a sarcomere

nuclei

thin filament

troponin   actin   tropomyosin

thick filament

myosin

tail

head
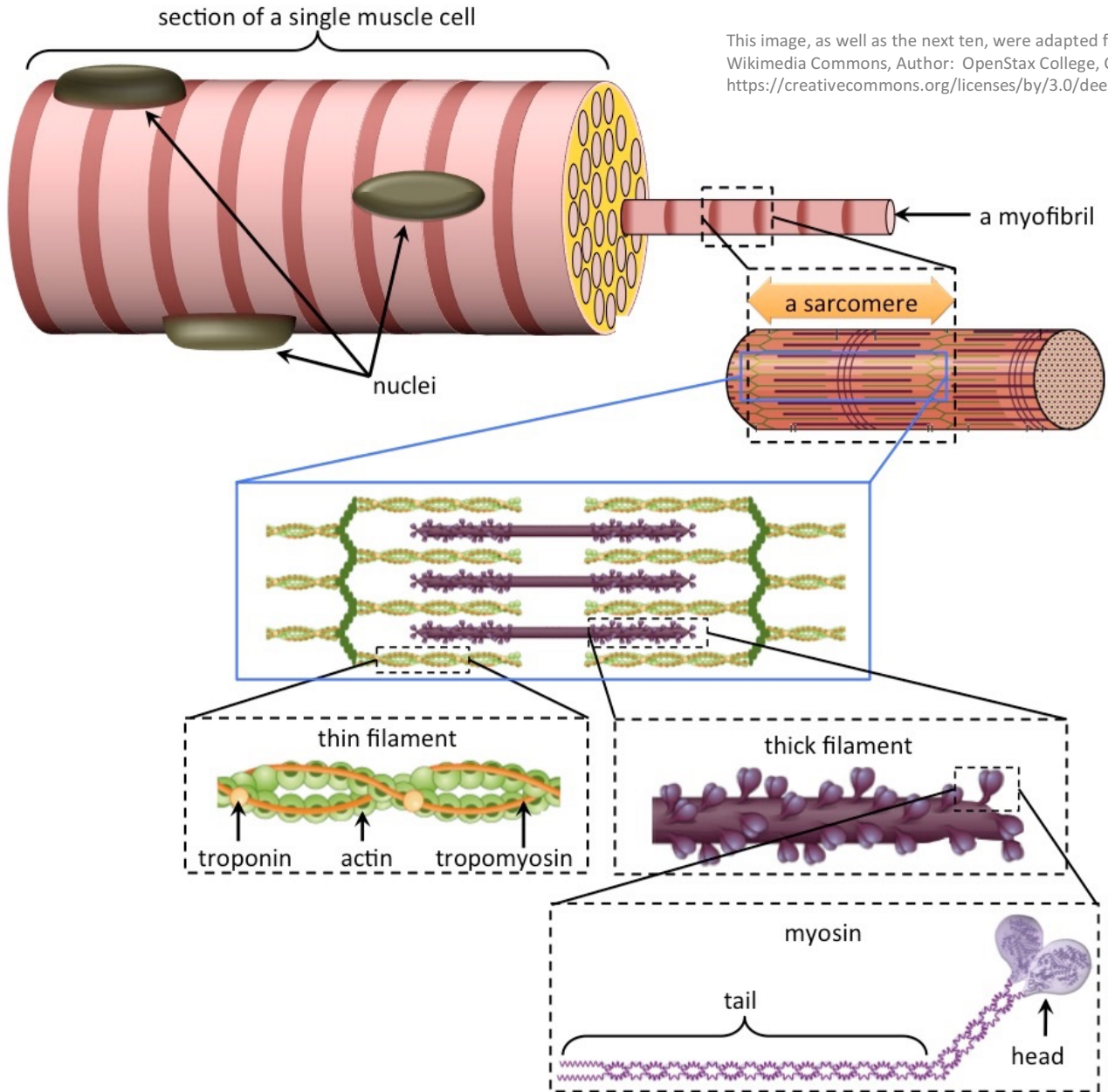
A muscle cell is a polynuclear (many nuclei) cell that contains long protein fibers called **myofibrils**.

Myofibrils are composed of individual contractile units called **sarcomeres**.

Sarcomeres contain fibrous proteins called "_____ **filaments**" and "_____ **filaments**."

Thick filaments are composed of **myosin** fibrous protein.

- The ***myosin tail region*** is composed of two alpha helices that are twisted around each other.
- In the ***myosin head region***, the individual alpha helices split apart from each other and fold into more compacted tertiary structures.

Thin filaments are composed of three proteins: actin, troponin, and tropomyosin.

How Muscles Work: The Sliding Filament Model

Before contraction, the thick
and thin filaments are in a
relaxed state (non contracted),
as shown in the top of the
figure on the right.
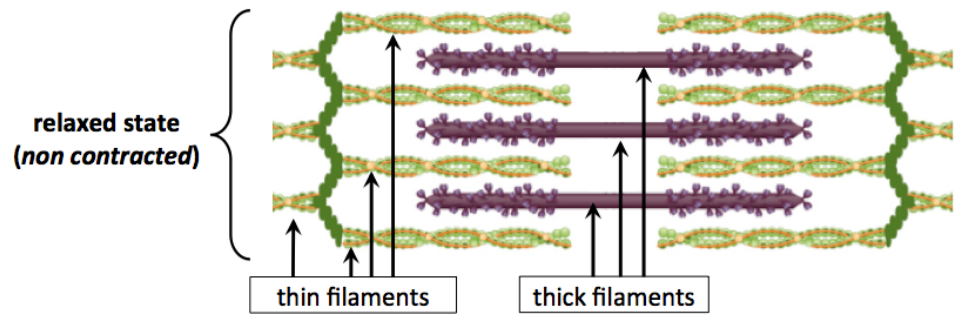
During muscle contraction,
the *thick filaments* and *thin
filaments* "slide" past each
other to shorten (contract) the
overall structure, as shown in
the contracted state in the
bottom of the figure.
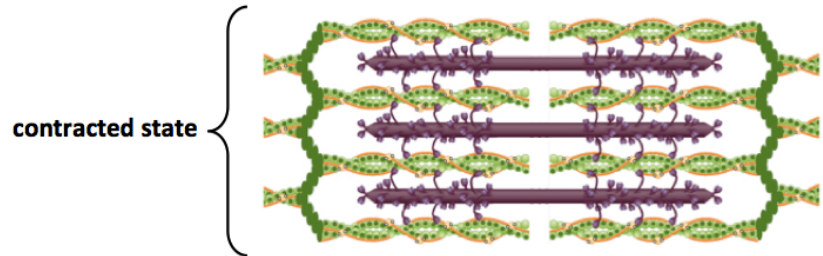
Let's now consider how and when the filaments "slide" past each other. We will begin with a small
section of a thick and a thin filament in the state illustrated below.
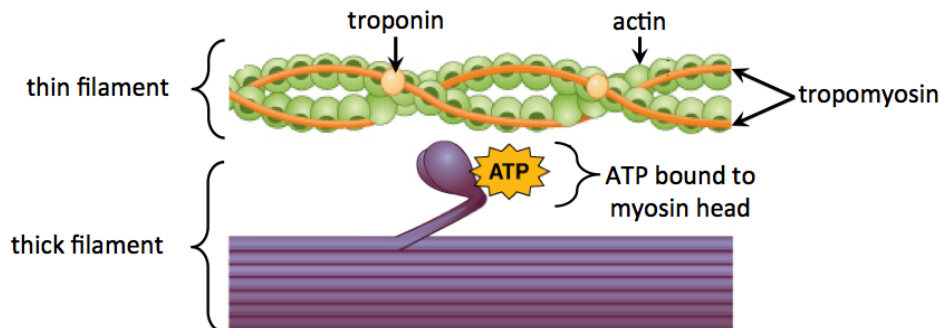
In this initial state, adenosine triphosphate (ATP) is attached to the head region of myosin.

The chemical energy stored in _____ is used to make the muscle contract.

- The hydrolysis of ATP reaction is capable of releasing energy:

$$\text{ATP } (aq) + \text{H}_2\text{O } (l) \rightleftarrows \text{ADP } (aq) + \text{P}_i (aq) \quad \Delta G = -7{,}300 \text{ Joules per mole of ATP}$$
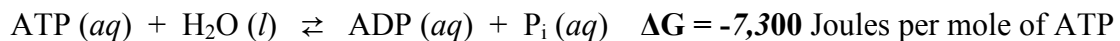
P_i is an abbreviation for a phosphate group, and ADP is *adenosine diphosphate.*

The energy released by this reaction can be used to slide the thin and thick filaments past each other.

1) *Actin* contains sites to which *myosin* heads can bind.
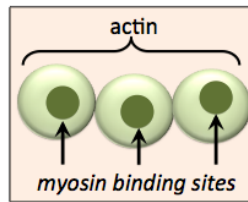
In our initial state, *tropomyosin fibers* block *actin's* myosin binding sites so that the myosin heads are unable to attach to the *thin filament,* as shown in the illustration on the right.
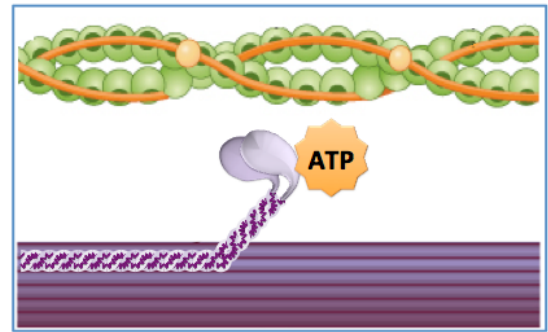
2) Muscle contraction begins in response to an action potential (nerve impulse) that originates in the central nervous system.

- The electrical signal is transferred to a particular muscle and causes an organelle called the sarcoplasmic reticulum to release calcium ions.
- When calcium ions are released, they bind to *troponin,* which causes the *tropomyosin fibers* to move and thereby exposes the *myosin binding sites*.
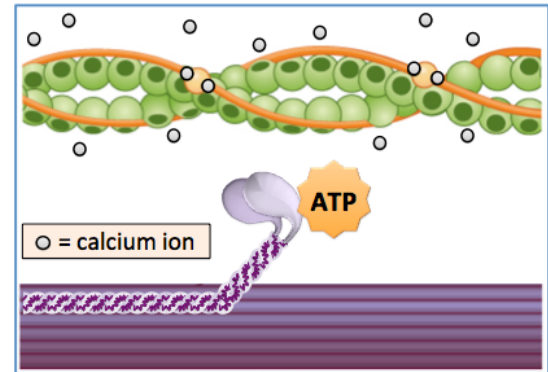
3) ATP is hydrolyzed to ADP and P_i. Energy released from the hydrolysis of ATP reaction ***is used to change the conformation (shape) of myosin***. This results in a "cocked" myosin head.

- This is analogous to "cocking the hammer" of a pistol, or pulling back on the string of a bow-and-arrow. In this step, the ADP and Pi that are produced remain attached to the "cocked" myosin head, as shown on the right.
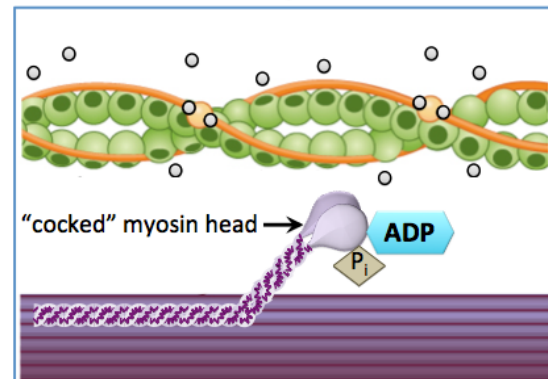
4) The "cocked" myosin head attaches to a myosin binding site on the thin filament. This attachment is a noncovalent interaction.

25
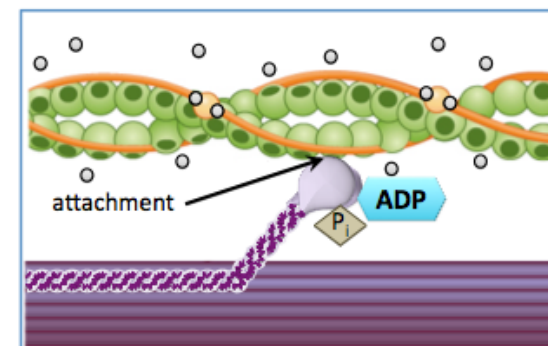
5) ADP and P$_i$ are released from the myosin head. This allows the myosin to bend back to its original "un-cocked" position.

- In our "cocked" pistol analogy, this step represents what happens when the trigger of a pistol is pulled: the pistol's "hammer" springs forward (to strike the bullet's cartridge).

- In our *bow-and-arrow analogy*, this step represents what happens when the string is released: it moves forward and accelerates the arrow.

Because the myosin head is attached to the thin filament, as the myosin bends, the thin filament "slides" past the thick filament.
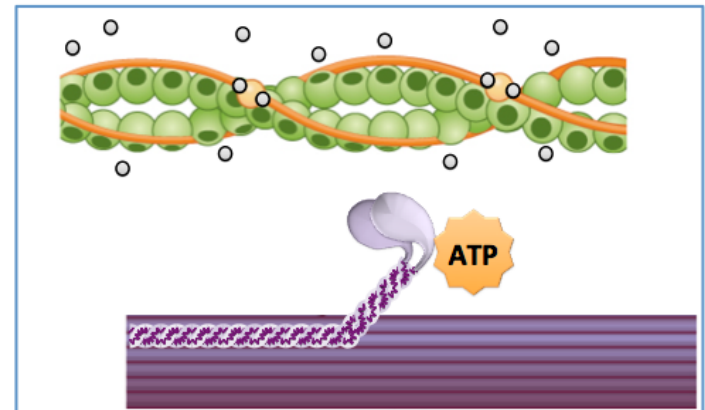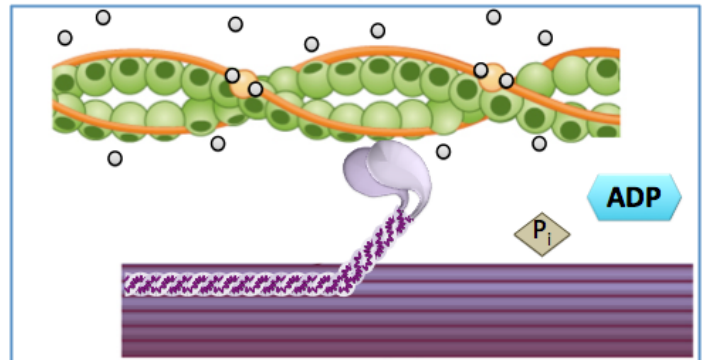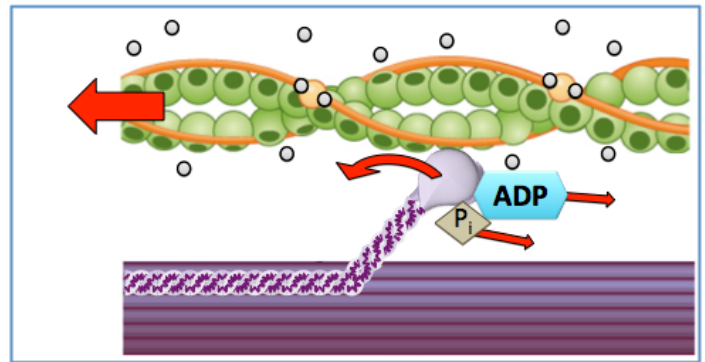
6) ATP binds to the myosin head, which causes the head to detach from the thin filament. ***This completes the cycle***; the system is now back to its original configuration and the cycle can repeat so long as calcium and ATP are present. As this cycle repeats, the muscle can continue to shorten. Since calcium ions are constantly being transported ***back*** *into the sarcoplasmic reticulum*, their release must be continuously induced by central nervous system impulses in order for muscle contraction to continue.

If ATP is not present, the myosin remains bound to the thin filament. This state is observed after death, since ATP is no longer produced, and is called *rigor mortis*.

Membrane Proteins

Membrane proteins are proteins that are _____ to biological membranes.

Membrane proteins function as enzymes, cell recognition markers, receptors (allowing chemical signals to be relayed between the interior and exterior of cells), and transporters of compounds in and out of cells.

Some membrane proteins extend through the _____ membrane and are called **transmembrane proteins**.

Examples of **transmembrane proteins** include the *aquaporins*.

- *Aquaporins* function as *transporter proteins;* they facilitate the transport of water molecules (only) in and out of cells. There are several types of aquaporins, one of them, *aquaporin-1*, is illustrated on the right.

phospholipid bilayer

aquaporin-1
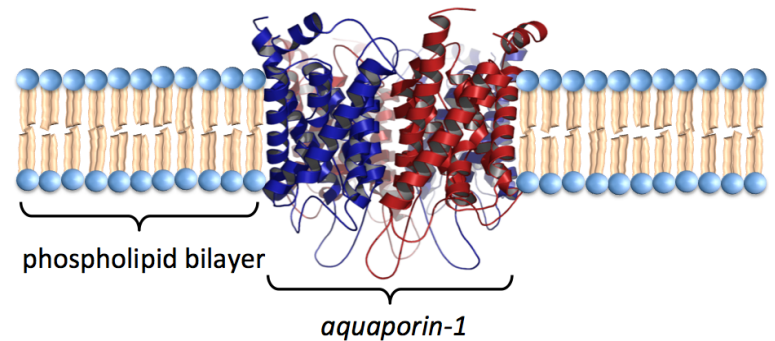
Source: The protein structure is from Wikimedia Commons, Author: Vossman CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcode

Some membrane proteins **do not** *completely extend through* the membrane; these are called

_____ **proteins**.

An example of a **monotopic protein** is *cyclooxygenase-2*.

- *Cyclooxygenase-2* is responsible for converting eicosanoic acid into prostoglandins, prostoscyclin, and thromboxane (you learned about this enzyme and these reactions in a previous chapter). An illustration of cyclooxygenase-2 attached to a membrane is shown on the right.
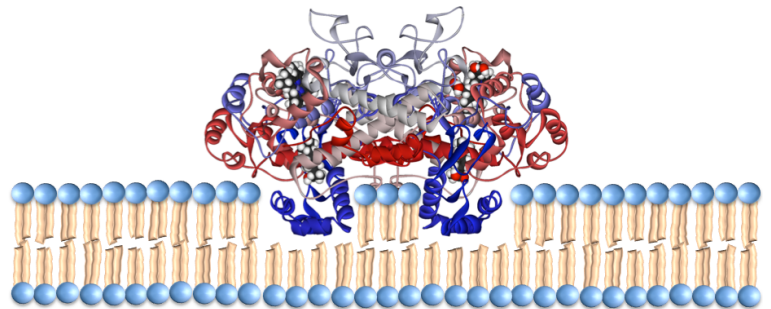
Understanding Check: Globular vs. Fibrous vs. Membrane Proteins

Do a bit of online research to determine if *succinate dehydrogenase* is a **globular**, **fibrous**, or **membrane** protein.

Prosthetic Groups: Simple vs. Conjugated Proteins

Some proteins contain only amino acid residues, these are called _____ **proteins**.

Other proteins contain amino acid residues **and** _____ amino acid components.

Proteins that contain non amino acid components are called _____ **proteins**.

- The *non* amino acid components of these proteins are called _____ **groups**.

- An example of a *prosthetic group* is the *heme* group, which is present in *hemoglobin*. The main role of *hemoglobin* is to transport oxygen (O_2) molecules. Heme groups contain an iron ion, to which an oxygen molecule can be quite strongly attached.

A ribbon model of human hemoglobin, with a magnification insert showing the bonding pattern in one of its four heme groups, is shown below.
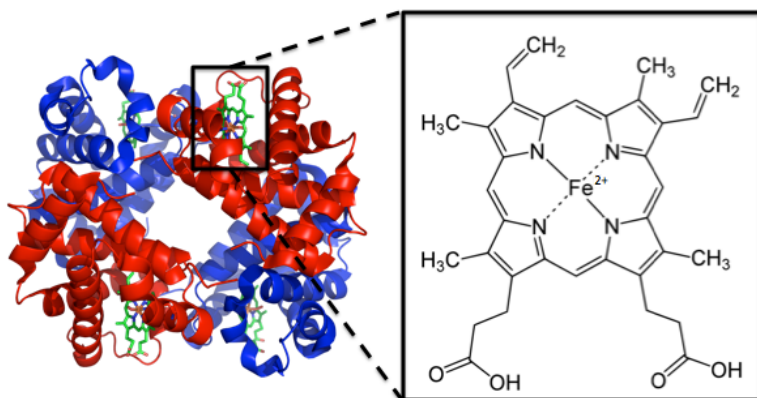
Hemoglobin contains *four* heme groups (shaded green in the figure above). Each heme group is capable of binding one oxygen molecule. Heme prosthetic groups are also found in *myoglobin*, *catalase*, and other proteins.

Denaturation of Proteins

The shape of a protein is the key factor in its ability to perform its biological role. ***Protein shape is maintained by the attractive forces involved in secondary, tertiary, and quaternary structures***. When these attractive forces are disrupted, the native shape of proteins can be changed enough that a partial or complete loss of bioactivity (function) occurs.

When a protein loses some or all of its biological activity in such a manner, this is referred to as

"**protein** _____."

In most cases, unless the shape change is very minor, the denaturation is ***irreversible***.

Any mechanical or chemical agent that causes the denaturation of a protein is called a _____ _____.

Some of the most common ***denaturing agents*** are listed and described below:

1) _____ The noncovalent attractive forces involved in ***secondary, tertiary, and quaternary structures*** in proteins are easily disrupted by heating. The cooking of an egg is an example of heat denaturation.

2) _____ _____ , which can disrupt the noncovalent attractive forces involved in secondary, tertiary, and quaternary structures. An example of denaturation of protein by mechanical agitation is the foaming that occurs during beating of raw egg (yolks removed). Chefs use this process to make *meringue*.

3) _____ _____ Some amphipathic compounds can cause denaturation by inserting their nonpolar ends into an association of hydrophobic side chains and thereby displacing some of the side chains. For example, *detergents* are capable of denaturing proteins.

4) _____ _____ Some polar solvents, such as acetone or ethanol, can interfere with hydrogen bonding, dipole-dipole, and ion-dipole interactions by competing for a protein's existing interactions.

5) _____ _____, which can disrupt a protein's **salt bridges** and **ion-dipole interactions.** Near physiological pH, the predominant form of *polar acidic* side-chains and *polar basic* side-chains (except for histidine) have a *formal charge*. These charged side-chains help proteins maintain their tertiary and/or quaternary structure because they participate in *salt bridges* and *ion-dipole* interactions.

The Disruption of a Salt Bridge by pH Changes

pH = 1 At pH = 1, the predominant form of the polar acidic side-chain has **no formal charge** and **cannot form a salt bridge.**

pH = 7 At pH = 7, the predominant form of the polar acidic side-chain **and** the polar basic side-chain have **formal charges** and **form a salt bridge.**

pH = 14 At pH = 14, the predominant form of the polar basic side-chain has **no formal charge** and **cannot form a salt bridge.**

Middle: Illustration of a salt bridge that can form between a *polar acid* and polar basic *side-chain* at pH = 7.
Right: When the pH is changed to a value greater than the pK$_a$ of a polar basic side-chain then its *uncharged* base form becomes predominant. This uncharged side-chain cannot participate in salt bridge interactions.
Left: When the pH is changed to a value less than the pK$_a$ of a polar acid side-chain, then its *uncharged* acid form becomes predominant. This uncharged side-chain cannot participate in salt bridge interactions.

- An example of the denaturation of proteins by a pH change is the use of citric acid in the marination (soaking) of fish and shellfish in a dish called ceviche. The citric acid comes from citric juices such as lemon, lime, orange, or grapefruit juice.

Essential Amino Acids: Complete, Incomplete, and Complementary Proteins

Organisms produce (synthesize) protein from dietary amino acids.

Our bodies are capable of producing _____ of the twenty common amino acids (from other amino acids or certain other compounds.

- Therefore we do not necessarily need to obtain these eleven amino acids in our diet.

The other _____ amino acids *can only be obtained by eating proteins that contain them*.

- These nine amino acids are called _____ **amino acids**, and are listed below.

Histidine (His)	Methionine (Met)	Lysine (Lys)
Leucine (Leu)	Threonine (Thr)	Valine (Val)
Isoleucine (Ile)	Tryptophan (Typ)	Phenylalanine (Phe)

Foods that contain **all** of the essential amino acids are called _____ **proteins.**

- Most animal products are *complete proteins*. Examples: eggs, meat, milk, fish, and poultry.

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Foods that contain proteins but do not contain *all of the essential amino acids* are called _____ **proteins**.

- These include most plant proteins.

  o Examples of *incomplete proteins* and their missing essential amino acids are listed in on the right:

Food	Amino Acid Deficiency
rice, wheat, oats	lysine
beans	methionine, tryptophan
peas	methionine
soy	low in methionine
corn	lysine, tryptophan
almonds, walnuts	lysine, tryptophan

Combining of two or more *incomplete proteins* that are deficient in *different* amino acids is a dietary strategy used to ensure the intake of all nine essential amino acids.

- For example, if you eat beans and rice, you obtain all of the essential amino acids since rice contains the amino acids that beans lack, and vice versa.

- When proteins are combined in this way, they are called _____ **proteins**.

Understanding Check

Which two foods (from the table above) could *each* be eaten with *corn* as a *complementary protein*?

Enzymes

Catalysts are substances that increase the rates of chemical reactions. Life requires that many chemical reactions occur within organisms. The human body employs over a thousand chemical reactions. Many of these reactions would occur *too slowly* to be useful in the absence of a catalyst. Nature provides humans and other biological organisms with proteins that are capable of catalyzing reactions.

Protein catalysts are called _____.

- Among all plants and animal species, over 5,000 chemical reactions are catalyzed by enzymes.

- Enzymes are capable of increasing the rate of a chemical reaction by up to a factor of one thousand.

Scientists who specialize in studying enzymes are called *enzymologists*.

Enzymologists refer to the *reactants* of catalyzed reactions as _____.

- Most enzymes are composed of hundreds or thousands of amino acid residues, however only a small region of the enzyme makes contact with the *substrates*.

Let's take a look at a model that describes *enzymatic catalysis*.

The part of the enzyme that makes contact with substrates is called the

" _____ _____ ."
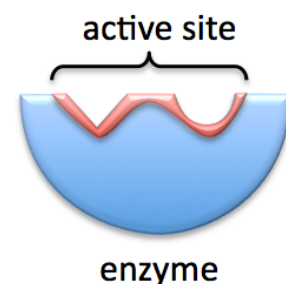
In this model, we will represent an enzyme and its active site as illustrated on the right.

We will consider a reaction where ***two*** substrates (reactants) are converted to ***one*** product, as illustrated below.

Reaction to be catalyzed:
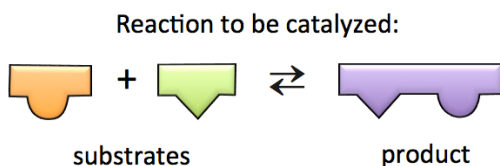
In this example, *two* substrates react to form *one* product, however this model *will also apply to other cases* such as *one* substrate compound forming *two* products, or *two* substrate compounds forming *two* products.

The *enzymatic catalysis model* is illustrated below.
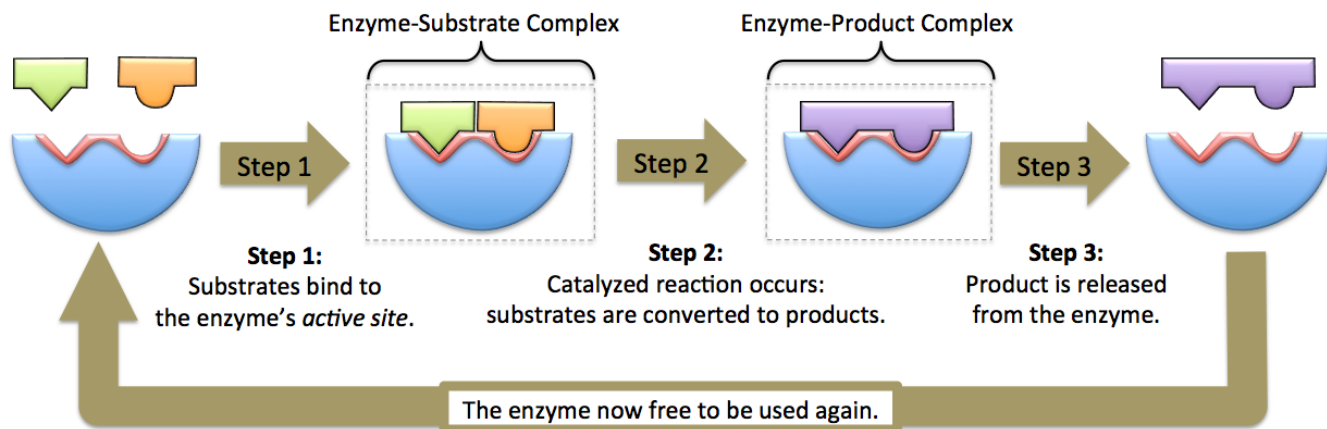
In **Step 1**, the substrates bind to the ***active site*** of an enzyme.
- The substrates are held tightly in the active site by ***noncovalent attractive forces, which are maximized due to the complementary shapes of the substrates and active site*.**
- The particle that is formed when the *substrates* are bound to the enzyme is called the **enzyme-substrate complex**.

In **Step 2**, the chemical reaction occurs.
- Substrates are converted to products when covalent bonds within the substrates are broken **and/or** new bonds are made.
- The particle that is formed when the *product* is bound to the enzyme is called the **enzyme-product complex**.

In **Step 3**, the newly formed product is released.
- Note that after products are released from enzymes, the enzymes are free to accept new substrates and the cycle can repeat.

Enzymes ____ _____ ***affect*** the *equilibrium concentrations* of products and reactants (substrates), they only increase the reaction rates, and therefore equilibrium is reached more quickly.

All catalysts, including enzymes, _____ the ***activation energy*** of a reaction and thereby *increase the reaction rate*.

Compare the reaction energy diagram of an ***enzymatically catalyzed*** reaction with that of an ***un-catalyzed*** reaction:
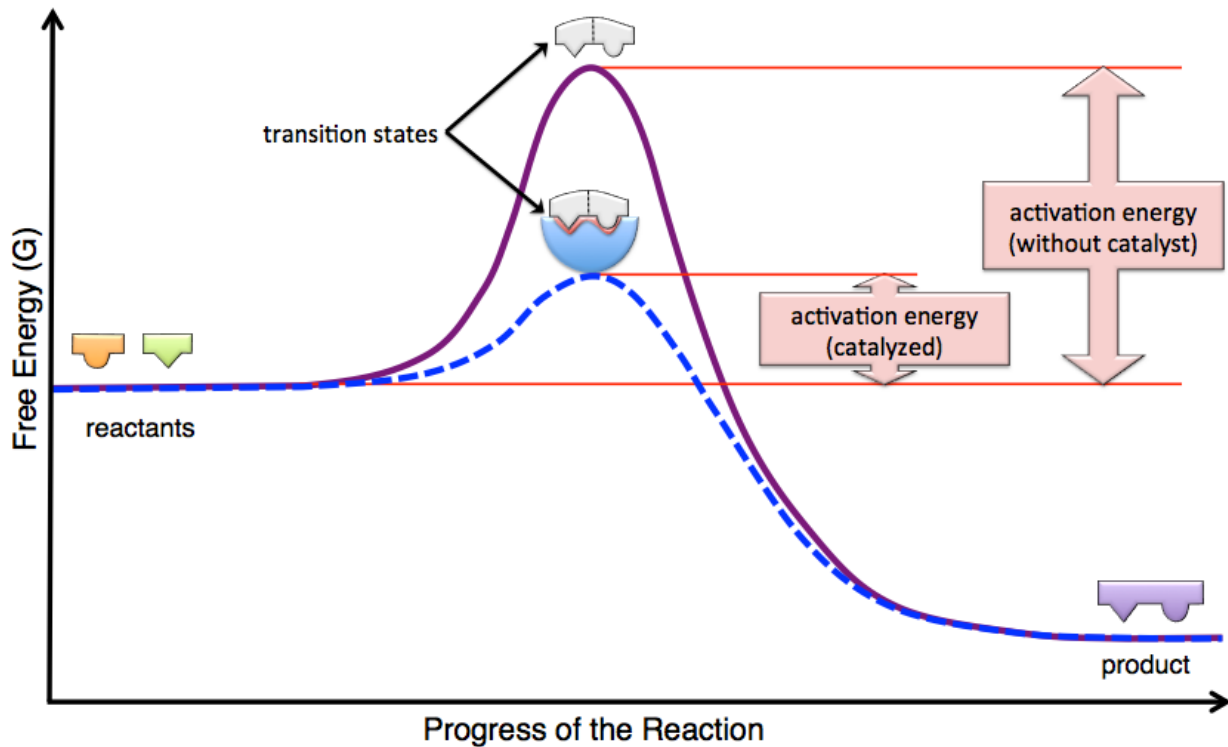
The *un-catalyzed* reaction is represented by the solid curve and the *enzymatically catalyzed* reaction is represented by the dashed curve. In catalyzed *and* un-catalyzed reactions, one or more of a reactant's covalent bonds and/or several noncovalent attractive interactions involving reactants are disrupted or completely broken. This process *requires* energy. At some point in the progress of the reaction, the energy reaches a *maximum value*. This state is a *temporary*, short-lived configuration of atoms called the ***transition state***. In chapter 6 you learned that amount of *energy* required to reach the *transition state* is called the ***activation energy***. As the reaction progresses, *new* covalent bonds and/or noncovalent attractive interactions form and generate the product; these processes *release* energy. The formation of the new covalent bonds and/or noncovalent attractive interactions is responsible for the *decrease in energy* that is seen in the diagram as the transition state changes to product.

How does an enzyme *increase the rate of a reaction*? When substrates bind to an enzyme's active site, ***interactions with the enzyme*** change the shape of the substrates (and enzyme) to a configuration that lowers the energy of the transition state (relative to an un-catalyzed reaction).

Understanding Check:

Determine whether each of the following statements are true or false.
   a. A catalyzed reaction has a lower activation energy than an un-catalyzed reaction.
   b. The greater the activation energy, the faster the reaction rate.
   c. At equilibrium, a catalyzed reaction will result in a greater amount of products than would an un-catalyzed reaction.

Example of Enzymatic Catalysis

As an example of enzymatic catalysis, let's consider an enzyme called *pyruvate kinase*. Kinases are a class of enzyme that catalyze reactions in which a phosphate group is transferred from one compound to another.

- Pyruvate kinase catalyzes the transfer of a phosphate group from *phosphoenolpyruvate* (**PEP**) to **ADP**, thereby forming *pyruvate* and **ATP**:
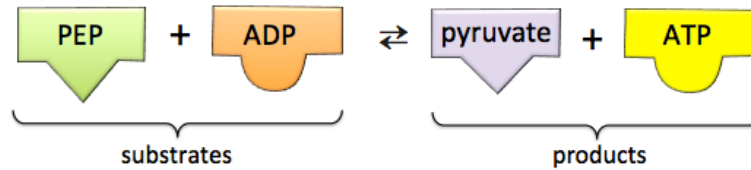
- This is the last reaction that occurs in a series of reactions called *glycolysis*.

A detailed knowledge of the bonding patterns involved in this reaction *is not important* at this time. One of the goals of the glycolysis process is to transfer potential energy stored within glucose (from our diet) to potential energy in the form of **ATP**. In chapter 15, I will discuss the details of how this is done, in part, by the reaction shown above.

The illustration below depicts the three steps of our enzymatic process model for the case of catalysis.
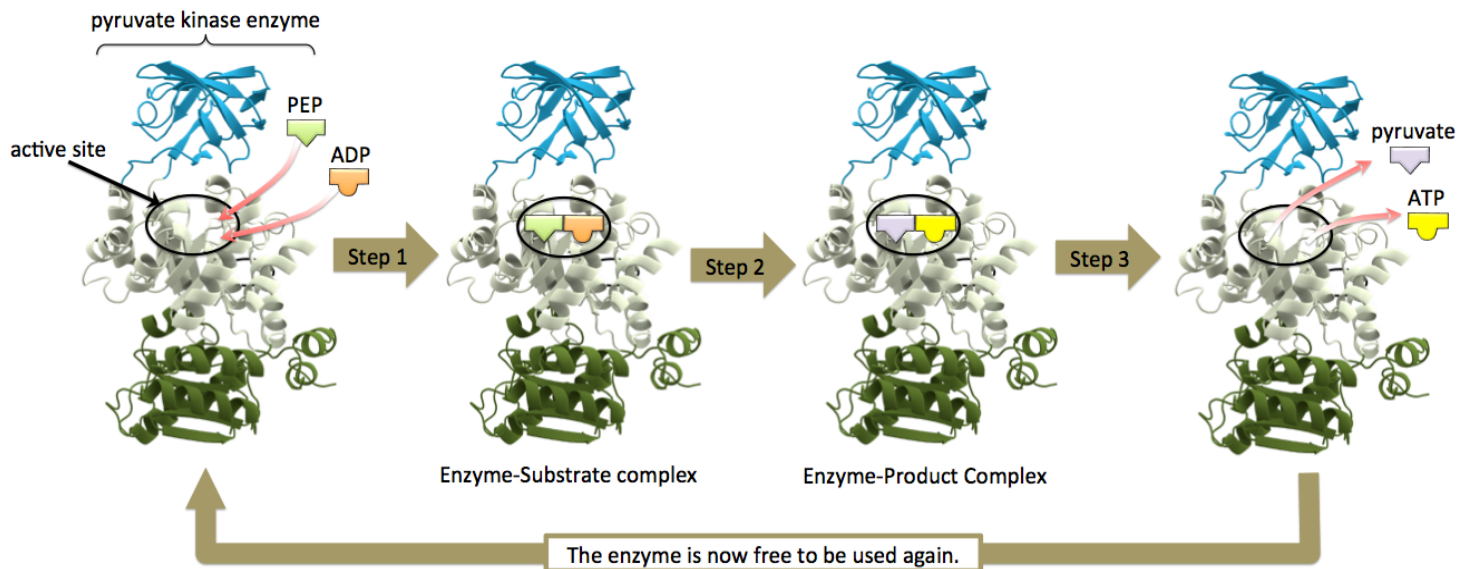
In **Step 1**, the substrates, PEP and ADP, bind to the *active site* of the *pyruvate kinase* enzyme.

In **Step 2**, the chemical reaction occurs.

- A phosphate group is transferred from PEP to ADP to form pyruvate and ATP.

In **Step 3**, the products, pyruvate and ATP, are released.

- The enzyme is free to accept new substrates so that the cycle can repeat.

Enzyme Specificity

Enzymes are _____ for particular substrates *or* groups of substrates.

- Their specificity is due to both the selective geometry of their active site and their ability to lower activation energy for particular substrates.

Some enzymes will only catalyze the reaction of a particular substrate; this is called _____ *specificity*.

- An example of an enzyme with *absolute specificity* is *urease*. *Urease* is used by some plants, fungi, and bacteria to catalyze a reaction in which *urea* (only) is converted to ammonium and bicarbonate.

Some enzymes are *less specific*, and will catalyzed reactions for a particular family of substrates; this is called _____ *specificity*.

- Examples of enzymes with r*elative specificity* include *proteases,* which catalyze the hydrolysis of various proteins.

Many enzymes will only catalyze the reaction of, or production of *one particular stereoisomer*; this is called _____.

- An example of an enzyme with stereospecificity is *stearoyl-CoA 9-desaturase, an enzyme that is involved in fatty acid metabolism and is present in every cell in the body.*

- *Stearoyl-CoA 9-desaturase* only catalyzes the production the *cis* stereoisomer, as shown below.

Catalyzed by **Stearoyl-CoA 9-desaturase**

The enzyme is **stereospecific**; it only produces the ***cis*** isomer
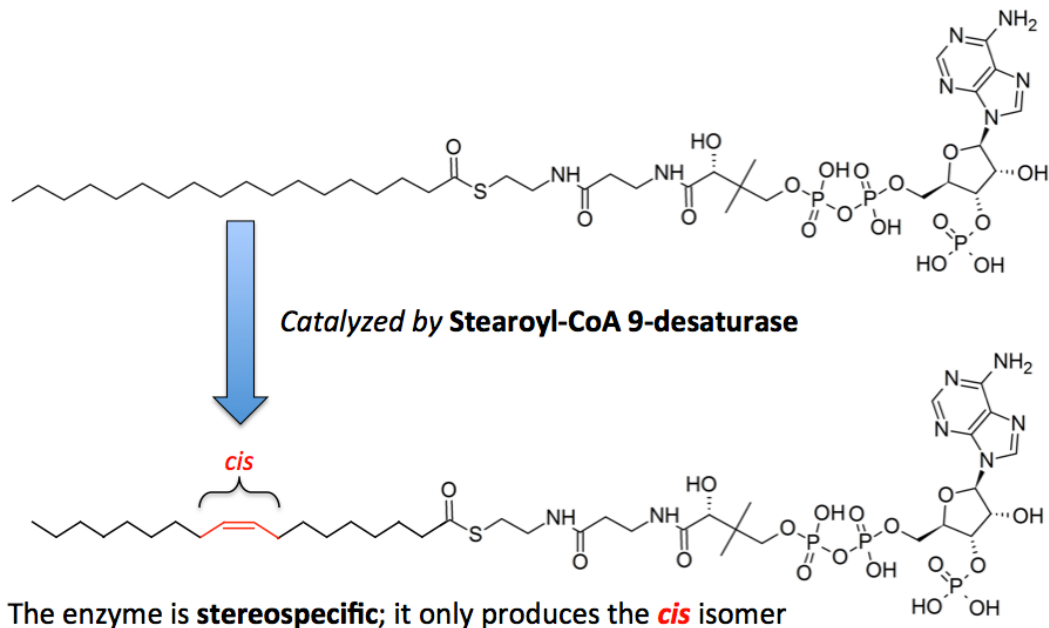
Almost all enzyme names use the "_____" suffix.

Enzymes are named and categorized based on their _____ *and/or* the _____ that they catalyze.

The table below lists some of the classes of enzymes, the reactions they catalyze, and some examples.

Enzyme Class	Reaction Involved	Examples
Isomerases	Catalyze rearrangement reactions: The reactant and the product contain the same atoms, only the bonding pattern changes.	Cis-trans isomerases - Convert *cis* to *trans* or vice versa.
Ligases	Use energy from ATP to form chemical bonds between substrates	DNA ligase - forms bonds between two DNA fragments.
Hydrolases	Catalyze hydrolysis reactions	• Lipases - hydrolyze ester bonds in lipids • Proteases - hydrolyze peptide bonds • Phosphatases - hydrolyze phosphoester bonds • Nucleases - hydrolyze bonds in DNA and RNA • Carbohydrases - hydrolyze glycosidic bonds
Oxidoreductases	Catalyze oxidation-reduction reactions	• Oxidases - oxidize a substrate • Reductases - reduce a substrate • Dehydrogenases - remove two hydrogens from neighboring carbons and form a double bond
Transferases	Catalyze the transfers of a group of atoms	• Kinases - transfer a phosphoryl group (PO_3^-) • Transaminases - transfer an amino group

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Understanding Check: Enzyme Specificity

Choose one of the enzyme classes (from the table above) that would catalyze each of the following reactions.

      a. The conversion of a *cis* double bond to a *trans* double bond.
      b. The digestion of fat.
      c. The conversion of starch to D-glucose.
      d. The conversion of a dipeptide into two amino acids.
      e. The hydrolysis of ATP to form ADP and P_i.

Cofactors

A _____ is defined as a non protein compound that must be permanently *or* temporarily bound to an enzyme in order for the enzyme to function.

- Example: A nickel ion (Ni^{2+}) must be bound to a *urease* enzyme in order for the enzyme to catalyze the conversion of urea to ammonium and bicarbonate.

Cofactors are either ***inorganic ions*** or ***organic compounds***.
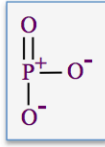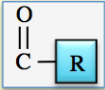
- When *cofactors* are *organic compounds*, they are often referred to as _____.

In most cases, coenzymes are actually one of the _____ in the catalyzed reaction.

- The reason that certain substrates are also referred to as *coenzymes* is that they are ***common substrates to many different enzymatic reactions*** in which they the ***donate atoms or groups of atoms*** to other substrates ***or*** accept ***atoms or groups of atoms*** from other substrates.

    - For example, ATP and ADP are classified as coenzymes because they are involved in the *transfer* of phosphoryl groups ($-PO_3^-$) ***in many different enzymatically catalyzed reactions***.

    - Many *coenzymes* are derived from dietary _____.

Some of the atom/group-transfer *substrates* that are also classified as *coenzymes,* and their dietary sources are listed below.

Coenzyme	Species that is Transferred	Dietary Source
ATP/ADP	phosphoryl group = $\overset{\displaystyle O}{\overset{\|\|}{P^+}}\!\!-O^-$ with O^- below	meat and sugars
NAD$^+$/NADH	hydride ion (H:$^-$) **or** electrons	niacin (vitamin B$_3$)
FAD/FADH$_2$	hydride ion (H:$^-$) **or** electrons	riboflavin (vitamin B$_2$)
coenzyme A	acyl group = $\overset{\displaystyle O}{\overset{\|\|}{C}}\!-R$	pantothenic acid (vitamin B$_5$)

Effect of Temperature on the Rates of Enzymatically Catalyzed Reactions

A typical graph of the rate of an enzymatically catalyzed reaction vs. temperature is shown below.

The temperature at which the rate of the reaction is greatest is called the enzyme's _____ *temperature*.

The reason that the reaction rate does not continue to increase after reaching the *optimum temperature* is that the enzyme begins to *denature* at the higher temperature.

An enzyme's optimum temperature is usually very close to the normal temperature of the organism in which it exists.

- For example, the optimum temperature of most human enzymes is at normal body temperature (~37 ^{o}C), as depicted in the graph.
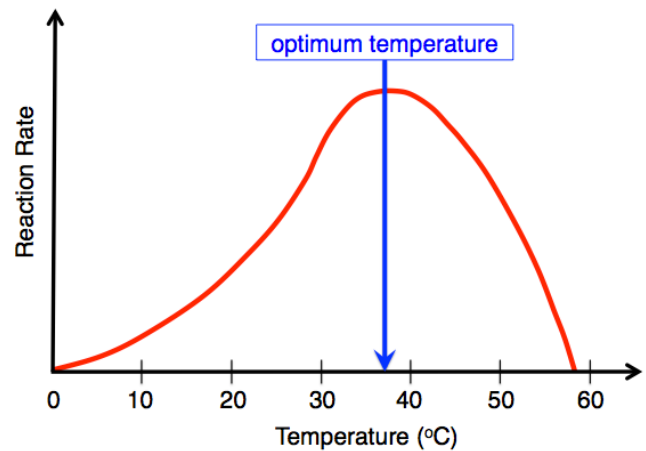
Effect of pH on the Rates of Enzymatically Catalyzed Reactions

A typical graph of the rate of an enzymatically catalyzed reaction vs. pH is shown below.

The pH at which the rate of an enzymatically catalyzed reaction is greatest is called the enzyme's

_____ **pH**.

An enzyme's *optimum* pH is usually very close to the normal pH of the region of an organism in which the enzyme exists.

- For example, the normal pH in most regions of the body is about 7.4 (physiological pH), so the *optimum* pH for enzymes found in these regions is also near 7.4 (as depicted in the graph).
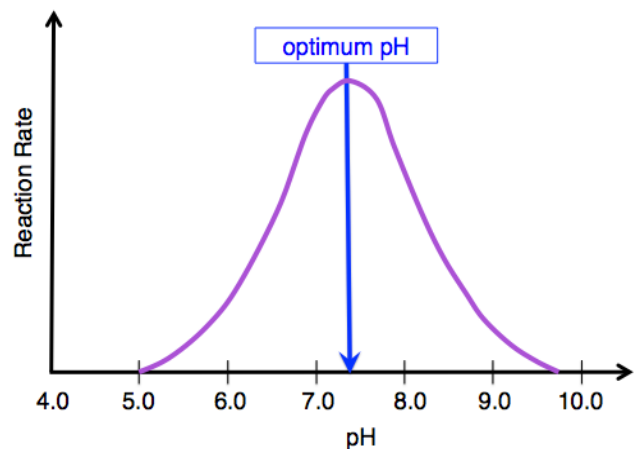
As the pH increases *or* decreases from its *optimum* pH value, the reaction rate decreases because of enzyme denaturation.

Not all parts of the body have a normal pH near 7.4. The stomach has a normal pH range of 1 to 3. It is not surprising that the digestive enzyme called *pepsin,* which functions in the stomach, has an optimum pH of 2.

Control of Enzymatic Reactions

All life forms employ reaction regulation mechanisms that involve *controlling* enzymatically-catalyzed reactions by processes called ***enzyme*** _____ and ***enzyme*** _____.

The body uses chemical feedback systems that can increase or decrease an enzyme's ability to catalyze a reaction.

The amount of substrate that an enzyme converts to product (per second) is referred to as the enzyme's "_____."

1) Enzyme Inhibition

When a particular molecule (or ion) forms a covalent or noncovalent bond with an enzyme, it can result in a decrease in the enzyme's *activity*.

A species that decreases a particular enzyme's activity is called an _____.

- Unlike temperature, pH, and denaturing agents, which affect all types of enzymes, inhibitors will only affect specific enzymes.

Enzyme inhibition can be classified as _____ **inhibition** or _____ **inhibition**.

i) Irreversible inhibition

Irreversible inhibition occurs when an *inhibitor reacts* with an enzyme, forming a ***new*** and _____ ***covalent bond*** to the enzyme.

- In almost all cases of irreversible inhibition, the new bond is made to the enzyme's *active site*, which results in *complete and permanent loss* of the enzyme's activity.
- In order to re-initiate catalysis, an organism must produce *new enzymes* (in the absence of the inhibitor).

An example of *irreversible inhibition* is ***aspirin's* mode of operation**. Aspirin *irreversibly inhibits* the *cyclooxygenase* (COX) enzyme, which catalyzes one of the reactions involved in prostaglandin production. *Prostaglandins* have a wide range of biological effects, including causing pain, inflammation, and fever. In order to *prevent* pain, inflammation, and fever, we use *aspirin* (or other **n**onsteroidal **a**nti **i**nflammatory **d**rugs (NSAIDs)).

Irreversible inhibition occurs when aspirin reacts with an amino acid side-chain in the COX enzyme's *active site,* as illustrated below.
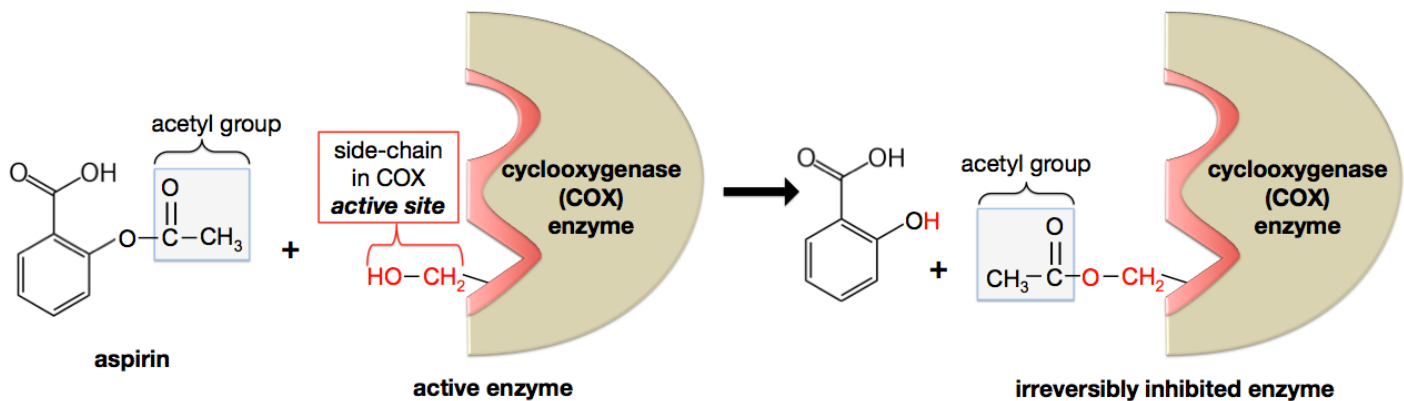
In this reaction, an *acetyl group* from **aspirin** is exchanged for a hydrogen atom (**H**) from a particular side-chain in the COX enzyme's active site. When an acetyl group is bonded to the enzyme's active site, it is no longer possible for *substrates* to bind to the enzyme, and therefore the enzyme is permanently inactivated.

Another example of *irreversible inhibition* can be seen in the mode of action of the antibiotic drug called **penicillin**. The structural formulas of the intravenously-administered *penicillin G* and the orally-administered *penicillin V* are shown below.

penicillin G
(given intravenously)

penicillin V
(given orally)
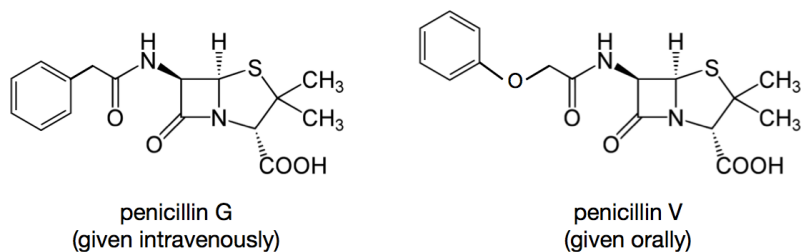
Penicillins are a class of antibiotics that work by *irreversibly inhibiting* a bacterial enzyme called DD-*transpetidase*. This enzyme is involved in constructing cell walls in some types of bacteria. If the cell wall cannot be correctly assembled, then the bacteria cannot divide (reproduce), and therefore do not persist. *Penicillin is **specific** for the DD-transpetidase* enzyme's active site because the shapes of the *penicillins* are quite similar to the shape of the substrate that is normally catalyzed by the enzyme. Once a penicillin is in the active site of this enzyme, a chemical reaction occurs in which *penicillin forms a* **covalent bond** to a particular side-chain in the active site. The reaction is *irreversible* and results in the complete loss of the enzyme's activity.

Some bacteria develop a resistance to *penicillin* G and V. In response, medical researchers have developed penicillin derivatives to which most bacteria have not yet developed a resistance. The structural formulas for a couple of these penicillin derivatives, *ampicillin* and *amoxicillin*, are shown below.

ampicillin

amoxicillin
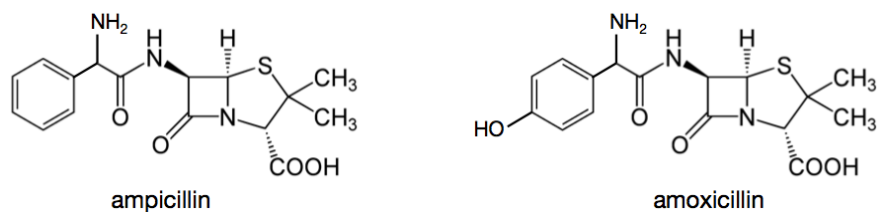
ii) **Reversible Inhibition**

_____ *inhibition* occurs when an inhibitor is weakly bound to an enzyme and decreases its activity.

- This type of inhibitor is called a **reversible inhibitor**.

Reversible inhibitors do not form covalent bonds to the enzyme, therefore they repeatedly attach to and detach from enzymes. When a reversible inhibitor detaches from an enzyme, the enzyme's activity is completely restored. The greater concentration of the inhibitor, the more frequently it will attach to enzymes, and the greater the reduction in enzyme activity. Reversible inhibitors decrease an enzyme's activity by attaching to either an enzyme's *active site* **or** to a region of an enzyme *other than the active site*.

An example of a *reversible inhibitor* is the antibacterial drug called *sulfanilamide*. Sulfanilamide, like most reversible inhibitors, reversibly binds to an enzyme's active site, forcing the enzyme's substrate to *compete* for access. Binding of reversible inhibitors to the active sites of enzymes can occur because the inhibitors' shapes often resemble the shapes of substrates, and are therefore complementary to the active sites. *Sulfanilamide* inhibits a bacterial enzyme that catalyzes the production of a compound that is essential for bacterial growth.

sulfanilamide
(antibacterial drug)
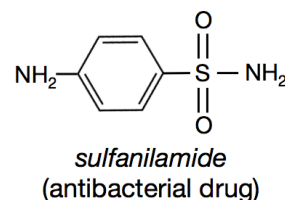
As shown below, *sulfanilamide* very closely resembles *p*-aminobenzoate ion, which is the bacterial enzyme's substrate.

sulfanilamide
(antibacterial drug)

p-aminobenzoate ion
(substrate)
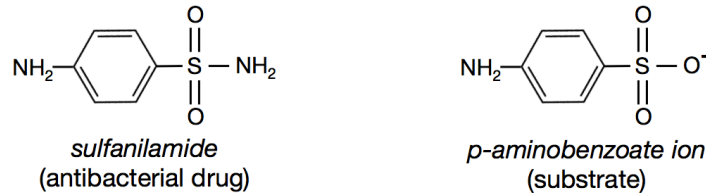
Sulfanilamide was first used extensively as an antibacterial agent in World War II. Since then, many other antibacterial agents have been synthesized by exchanging the amino group (that is bound to the sulfur) with other organic groups. These *sulfanilamide analogs* are called **antibacterial sulfa drugs**.

Organisms often use several reactions in series (one after another) in order to carry out the chemical changes they require to meet their physiological needs.

- These reaction series are referred to as _____ _____.

- Examples: *Photosynthesis*, *glycolysis,* and the *citric acid cycle.*

Many of the reactions in metabolic pathways require enzymes; therefore organisms can regulate (slow down) a metabolic process, according to their needs, by _____ one (or more) of the enzymes involved in the metabolic pathway.

The _____ of a reaction in a metabolic pathway often acts as a *reversible inhibitor* for one (or more) of the reactions in the pathway.

This biological strategy makes sense because when there is a relatively high concentration of a product in a metabolic pathway, it would be inefficient, and in some cases harmful, to continue its production. For example, consider the following hypothetical metabolic pathway that involves *four enzymatically-catalyzed reactions* and eventually converts compound "**A**" into compound "**E**."
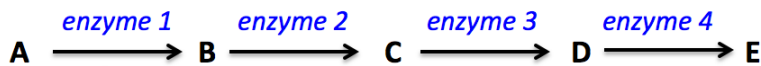
When the concentration of compound **E** is high enough to meet the organism's needs, it would be inefficient, and in some cases dangerous, for the metabolic pathway to proceed. For this reason, compound **E** acts as a r*eversible inhibitor* of **enzyme 1**:
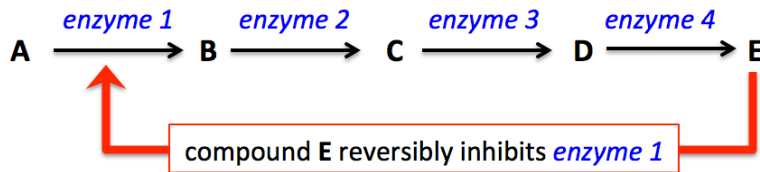
If compound **E** is not present, or is present in relatively low concentration, the reactions proceed, and therefore compound **E** is produced at a significant rate.

If compound **E** is produced at a greater rate than the organism uses it, then excess **E** is available to bind to and inhibit, **enzyme 1**.

- This decreases the production of **B**, **C**, **D**, and, ultimately, a decrease in the production of **E**.

Until the organism uses or breaks down a significant amount of compound **E**, compound **E** will continue to *inhibit its own production*.

The *regulation* of a metabolic pathway by *the inhibition of an enzyme* is called _____ **inhibition**.

An example of *feedback inhibition* is the regulation of *glycolysis*. Glycolysis is a metabolic pathway that involves a series of ten chemical reactions. It is used by organisms to convert glucose to ATP, NADH, and pyruvate. If the concentrations of these products are sufficient, it would be inefficient and potentially harmful to continue to produce them. Each of the ten reactions in the glycolysis pathway requires an enzyme. Three of the enzymes in the pathway are regulated by inhibitors in the *feedback inhibition* process.

2) Enzyme Activation

Enzyme activation can occur when an "**activator"** binds to an enzyme and _____ its activity.

Binding of the *activator* species to an enzyme induces changes in the active site that increases the enzyme's activity.

Just like the substrates and enzyme inhibitors, ***enzyme activators*** are specific for a particular enzyme or group of enzymes.

Enzyme activators can regulate metabolic pathways by activating one or more of the pathway's enzymes.

- Increasing the production of a metabolic pathway by an enzyme activator is called _____ **feedback**.

- An example of *positive feedback* is the activation of *pyruvate kinase*, an enzyme used in one of the *glycolysis* reactions. *Pyruvate kinase* is **activated** by PEP, which is also one of its own substrates (PEP).

One last note **on the** ***control of enzyme activity***: In this section, I discussed how enzyme activity could be decreased or increased by the binding of inhibitors or activators (respectively). Nature employs additional strategies in order to increase or decrease enzyme activity. In some cases, one enzyme catalyzes the breaking of chemical bonds, or the formation of new bonds, in a ***second enzyme*** in order to activate or deactivate the second enzyme. The details of these processes are beyond the scope of this course, however, you should know that this type of activation and deactivation is commonly employed by organisms to regulate metabolic pathways.

Examples of the Involvement of Enzymes in Disease

The underproduction or overproduction of enzymes, or the inability of an organism to control enzymes can lead to _____. When such diseases result from a defect (mutation) in a gene that is responsible for the production of a particular enzyme, they are categorized as **genetic diseases**. In the next chapter, you will learn details of how the information in DNA is used to produce proteins (including enzymes). There are thousands of different types of enzymes that are produced in the body, and the inability to correctly produce or control just one type of enzyme could result in death. You may recall that I discussed ***Tay-sach's*** and other ***sphingolipidosis*** genetic diseases that result from a deficiency of the enzymes responsible for the breakdown of sphingolipids. Although some forms of *sphingolipidosis* are treatable with **enzyme replacement therapy**, most sphingolipidosis cases result in death before five years of age. *Enzyme replacement therapy* is also used to treat other enzyme deficiencies, such as *lactose intolerance* (deficient lactase enzyme activity) and *exocrine pancreatic deficiency* (insufficient pancreatic production of digestive enzymes).

Another example of disease that is related to enzymes occurs when DNA is replicated. Before a cell divides, a duplicate copy of its DNA must be made. The new DNA is "proofread" for errors and then repaired. **DNA repair enzymes** catalyze the repair of mistakes made in the DNA replication process. If an individual's *DNA repair enzymes* are not functional, this results in an accumulation of new mutations, and leads to various types cancer.

Phenylketonuria (PKU) is an enzyme-related disease that can be controlled by a special diet. PKU is caused by deficient activity of the *phenylalanine hydroxylase* enzyme (PAH). This enzyme is responsible for breaking down excess phenylalanine (an amino acid). When the PAH enzyme is not fully functional, high levels of phenylalanine result, which affects brain development and causes intellectual disabilities, seizures, and other medical issues. If PKU is diagnosed and treated early, the damaging effects can be minimized and normal mental development can occur. For individuals with PKU, the consumption of foods rich in phenylalanine residues, such as meats and nuts, can be poisonous. Treatment of PKU is a strict life-time diet that *restricts* phenylalanine-containing foods, and *includes* dietary supplementation of the non phenylalanine amino acids, and other nutrients. Individuals with PKU must be careful not to consume the artificial sweetener called *aspartame* (NutraSweet) because phenylalanine is produced when aspartame is broken down in the body.

1) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 7.**

glycine	aspartic acid	lysine

2) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 1**

glycine	aspartic acid	lysine

3) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 14**

glycine	aspartic acid	lysine

4. Circle the peptide bonds and draw a star above the chiral carbons in the peptide below:

$$\overset{+}{N}H_3CH\overset{\overset{\displaystyle O}{\|}}{C}-NHCH_2\overset{\overset{\displaystyle O}{\|}}{C}-NHCH_2\overset{\overset{\displaystyle O}{\|}}{C}-NHCH\overset{\overset{\displaystyle O}{\|}}{C}-NHCH\overset{\overset{\displaystyle O}{\|}}{C}-O^-$$

5. Define the following:

a) peptide

b) peptide bond

c) peptide group

d) L-amino acid

e) D-amino acid

f) primary protein structure

g) secondary protein structure

h) tertiary protein structure

i) quaternary protein structure

j) enzyme

k) enzyme specificity (list the different types of enzyme specificities)

l) enzyme inhibition (compare and contrast reversible and irreversible inhibitors)

m) enzyme activation

n) active site

6. Draw the structures of peptide Val-Gly that would be predominant at pH = 1, 7, and 14.

pH = 1

pH = 7

pH = 14

7. List the ***attractive interactions*** involved in secondary, tertiary, and quaternary protein structure.

Protein Structure	Attractive Interaction
secondary	
tertiary	
quaternary	

KEY

1) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 7.**

glycine

aspartic acid

lysine

2) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 1**
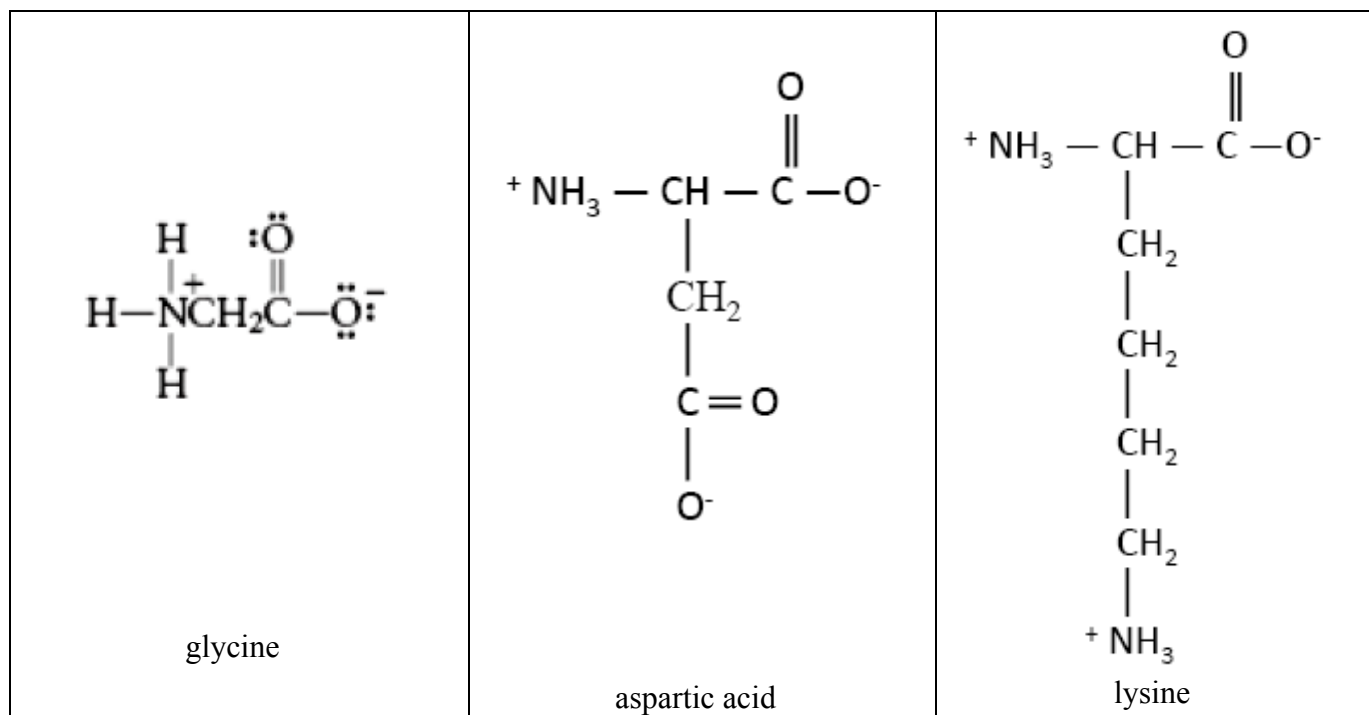
glycine

aspartic acid
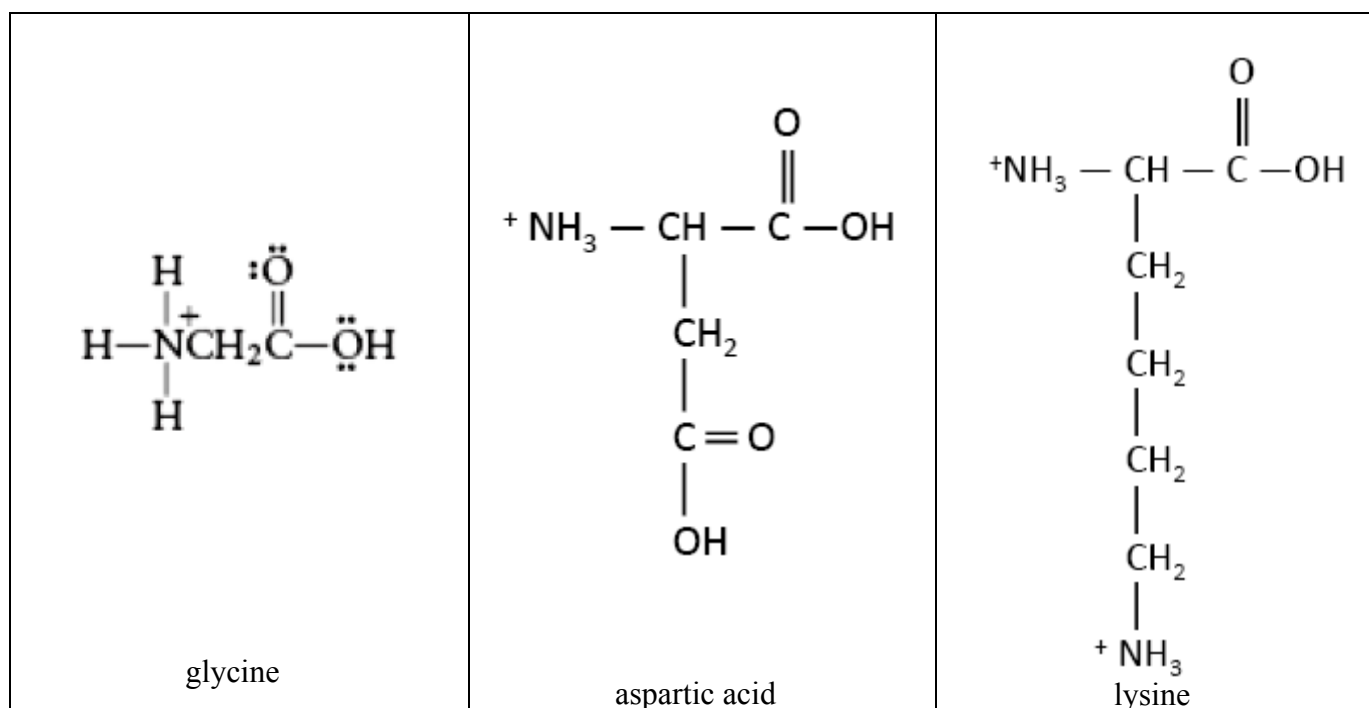
lysine

3) Draw the structures of glycine, aspartic acid, and lysine structures that would be predominant at **pH = 14**

glycine	aspartic acid	lysine
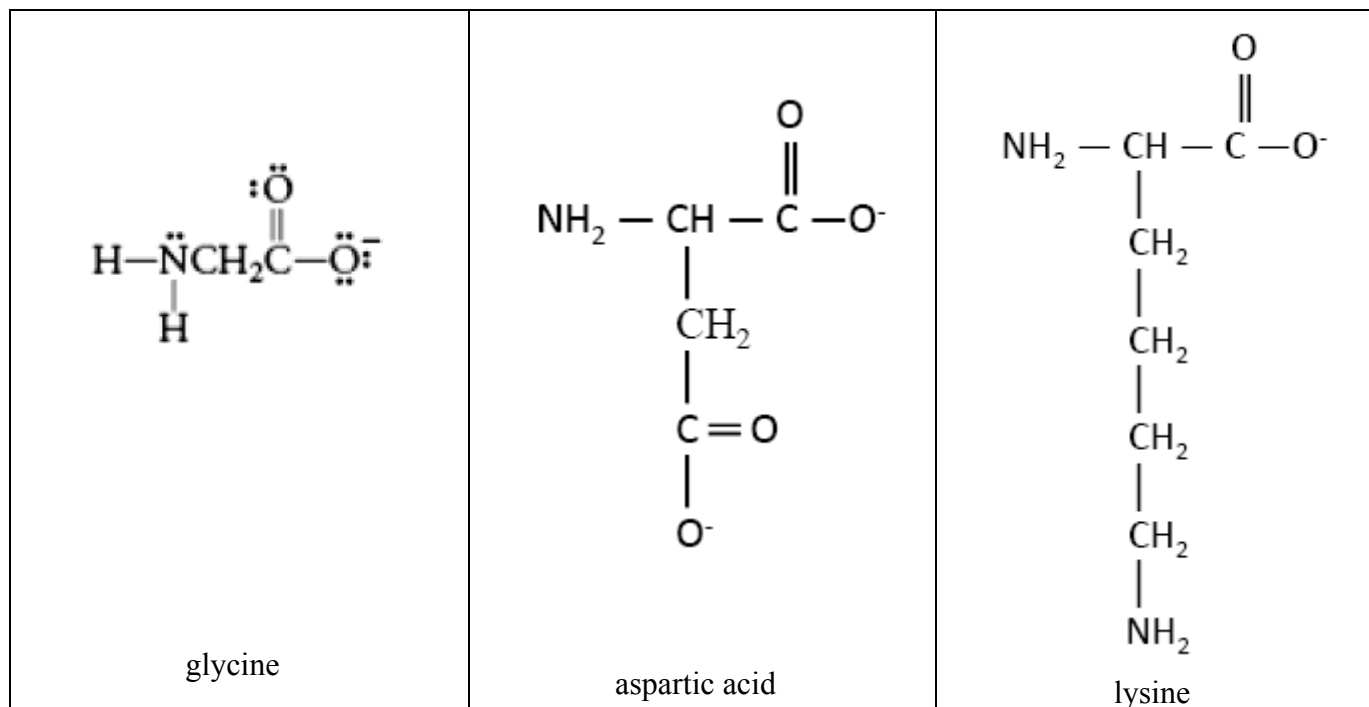
4. Circle the peptide bonds and draw a star above the chiral carbons in the peptide below:
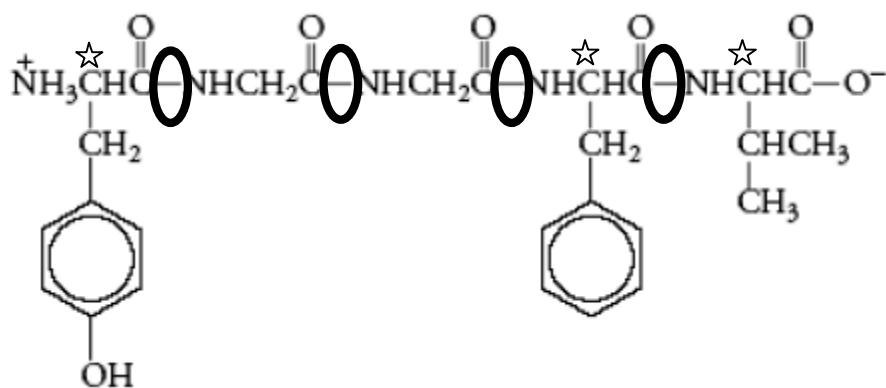
5. Define the following:

SEE YOUR LECTURE NOTES AND/OR TEXTBOOK TO CHECK THE DEFINITIONS

6. Draw the structure of peptide Val-Gly that would be predominant at pH = 1, 7, and 14.
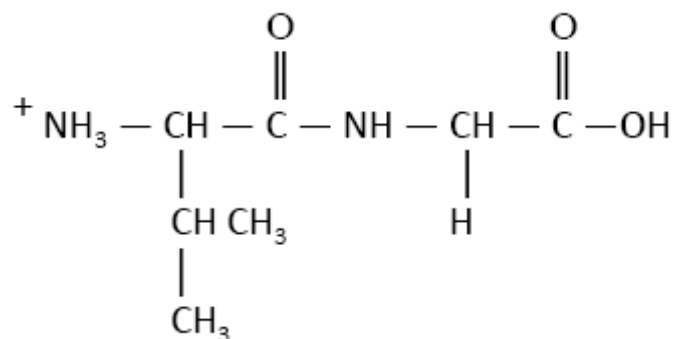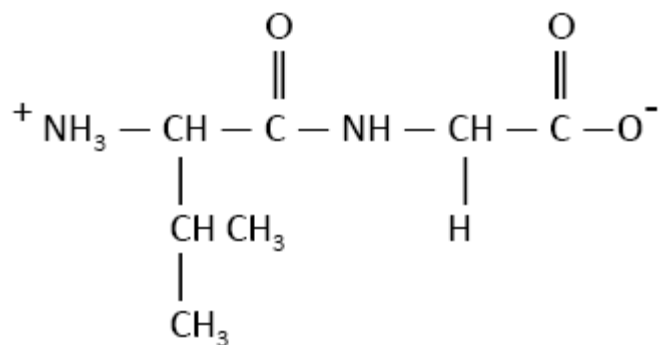
pH = 1

$$\overset{+}{N}H_3 - CH - \overset{\displaystyle O}{\overset{\|}{C}} - NH - CH - \overset{\displaystyle O}{\overset{\|}{C}} -OH$$

with CH side chains: CH CH₃ / CH₃ below the first CH, and H below the second CH

pH = 7

$$\overset{+}{N}H_3 - CH - \overset{\displaystyle O}{\overset{\|}{C}} - NH - CH - \overset{\displaystyle O}{\overset{\|}{C}} -O^-$$

with CH side chains: CH CH₃ / CH₃ below the first CH, and H below the second CH

pH = 14

$$NH_2 - CH - \overset{\displaystyle O}{\overset{\|}{C}} - NH - CH - \overset{\displaystyle O}{\overset{\|}{C}} -O^-$$

with CH side chains: CH CH₃ / CH₃ below the first CH, and H below the second CH

7. List the *attractive interactions* involved in secondary, tertiary, and quaternary protein structure.

Protein Structure	Attractive Interaction
secondary	hydrogen bonding
tertiary	hydrogen bonding, hydrophobic interactions, dipole-dipole, ion-dipole, disulfide bridges, and salt bridges
quaternary	same as tertiary: hydrogen bonding, hydrophobic interactions, dipole-dipole, ion-dipole, disulfide bridges, and salt bridges

Chapter 14 Lecture Notes: Nucleic Acids

Educational Goals

1. Know the *three* chemical components of a **nucleotide**: a *monosaccharide residue* (either ribose or deoxyribose), at least one *phosphate group*, and an "*organic base.*"

2. Identify **phosphoester** bonding patterns and *N*-**glycosidic bonds** within *nucleotides*.

3. Compare and contrast **ribonucleotides** and **deoxyribonucleotides**.

4. Understand the bonding patterns within **nucleotide diphosphates** and **nucleotide triphosphates**.

5. Predict the products for the hydrolysis of **ATP** and **ADP**.

6. Describe the bonding patterns within **cyclic nucleotides**.

7. Describe the chemical structure of **polynucleotides** (DNA and RNA) and identify the **phosphodiester bonding patterns** within *polynucleotides*.

8. Draw the structural formula of a **dinucleotide** that is formed by combining two specified nucleotides.

9. Compare and contrast the monosaccharide residues present in DNA vs. RNA.

10. Know the names of the **organic bases** that are present in DNA and RNA.

11. Given the structure of a DNA or RNA strand, identify the **sugar-phosphate backbone**, the **3' terminus**, and the **5' terminus**.

12. Describe the DNA **double helix structure**, and understand and define the term "**complementary base pairing**."

13. Understand how DNA folds back on itself and wraps around *histones* to form **chromatin**. Define, compare, and contrast **chromatin**, **genes**, and **chromosomes**.

14. Understand and explain how **DNA replication** takes place and how **DNA polymerase** is involved in the replication process.

15. Describe the **polymerase chain reaction**.

16. Know how **DNA fingerprinting** works and how it is used in forensic science.

17. Understand and explain **transcription** and how **RNA polymerase** is involved in the transcription process.

18. Understand and explain **translation** and define the term "**codon**."

19. Given the primary structure of DNA or mRNA, use the **genetic code** table to predict the sequence of amino acids in the polypeptide that would be produced in translation.

20. Describe the *three types of RNA* and understand the role of each in translation.

21. Define the term "**gene expression**."

22. Define the term "**operon**." Describe how the *lac* **operon** is *regulated* in order to control *gene expression* in *E. coli*.

23. Describe the structure of **viruses** and understand the way in which they can cause infections/diseases. Understand how the **reverse transcriptase** enzyme is used by HIV viruses.

24. Define and understand the terms "**mutation**," "**genome**," and "**gene therapy**." Explain how mutations can lead to **genetic diseases**. Give an example of a **monogenic disease**.

25. Define the terms: **recombinant DNA**, **genetically modified organism (GMO)**, **transfection**, and **bioethics**.

_____ _____ is a term used for the class of biological polymers consisting of **deoxyribonucleic acid (DNA)** *and* **ribonucleic acid (RNA)**.

- Nucleic acids are *polymers* that consist of _____ residues.

Nucleotides

A *nucleotide* is formed from *three* chemical components:

1) at least one _____ (hydrogen phosphate ion)

2) a _____ (either D-ribose *or* D-2-deoxyribose)

3) an _____ base

a phosphate (hydrogen phosphate ion)

D-ribose   D-2-**deoxy**ribose

nucleotides contain one of these monosaccharides

adenine   guanine   thymine   cytosine   uracil

nucleotides contain one organic base (the five most common organic bases are shown)
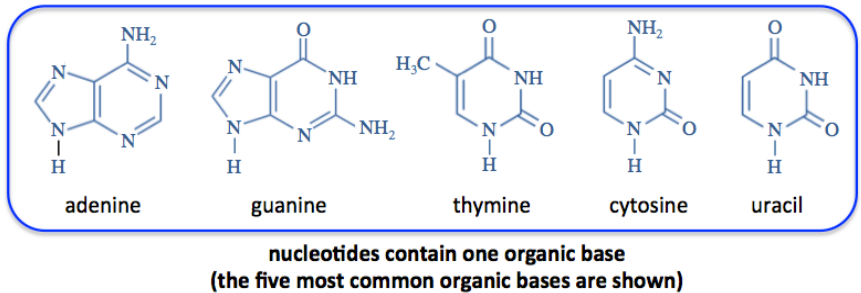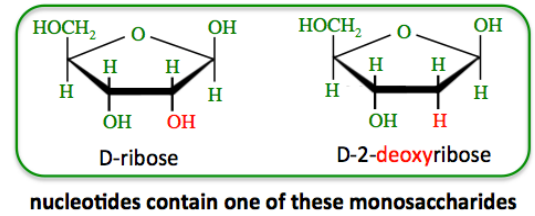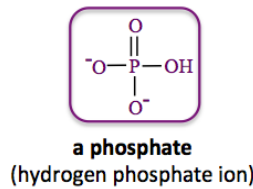
Example: a deoxyribonucleotide

phosphoester bonding pattern

an *N-glycosidic bond*

a nucleotide
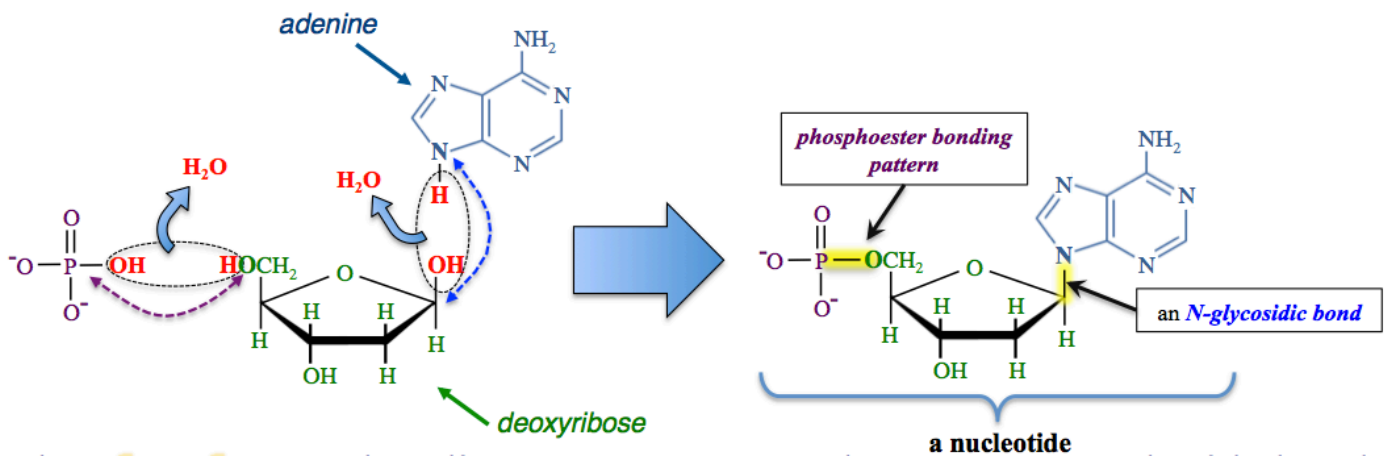
I used *adenine* as the *organic base* and *deoxyribose* as the *monosaccharide.*

The _____ bonding pattern occurs when a monosaccharide bonds with the phosphate group.

An _____ is made when the monosaccharide bonds to a nitrogen in the *organic base.*

In this example, the *phosphate residue* is bonded to the carbon in position number **5'** of the monosaccharide ring.

deoxyadenosine **5'-monophosphate**

Because this nucleotide is formed from one *phosphate* residue, a *deoxyribose* residue, and an *adenine* organic base, we write its name as "*deoxyadenosine* **5'-**monophosphate."

It is common to use abbreviations when naming nucleotides. In this case, we would abbreviate the name as "**5'-d**AMP," the lowercase "**d**" indicates "*deoxy.*"

Organisms synthesize DNA from **5'-**nucleotides.
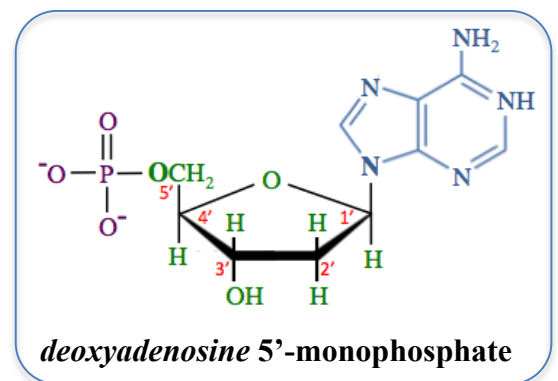
Deoxyribonucleotides

The nucleotides that make up **DNA** contain a _____ residue, a *phosphate* residue*,* and either *adenine*, *guanine*, *cytosine*, or *thymine* organic base residues.

The deoxyribonucleotide residues that comprise DNA

deoxyadenosine 5'-monophosphate
(5'-dAMP)

deoxyguanosine 5'-monophosphate
(5'-dGMP)

deoxycytidine 5'-monophosphate
(5'-dCMP)

deoxythymidine 5'-monophosphate
(5'-dTMP)
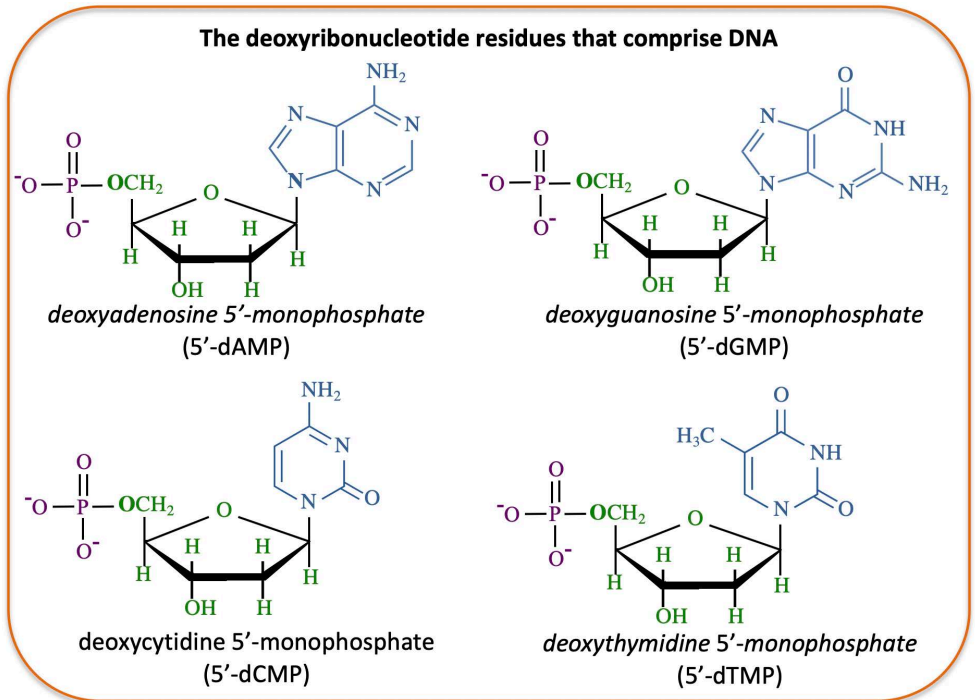
Ribonucleotides

The nucleotides that make up **RNA** contain a _____ residue, a *phosphate* residue*,* and either *adenine*, *guanine*, *cytosine*, or *uracil* organic base residues.

The ribonucleotide residues that comprise RNA

adenosine 5'-monophosphate
(5'-AMP)

guanosine 5'-monophosphate
(5'-GMP)

cytidine 5'-monophosphate
(5'-CMP)

uridine 5'-monophosphate
(5'-UMP)
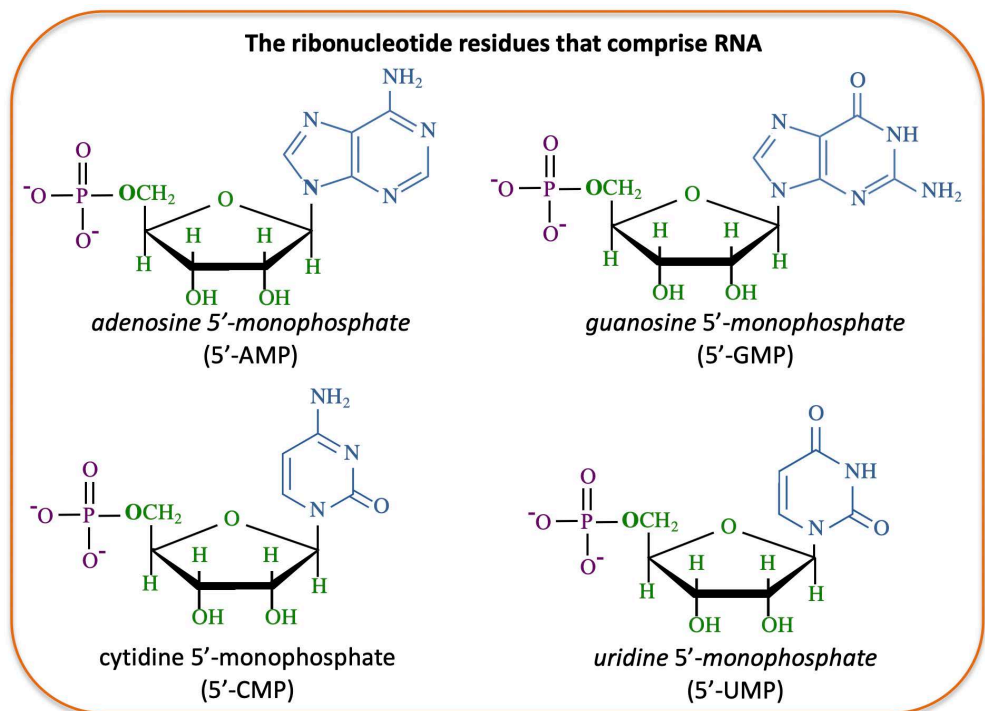
These **5'**-nucleotides are so frequently encountered in biology that the "**5**-" is usually omitted in the names and abbreviations. **3'**-nucleotides do exist, but they are rare.

Both DNA and RNA have *adenine, guanine*, and *cytosine* organic bases, **however** *thymine* is present only in DNA and *uracil* is present only in RNA.

3

Nucleotide Diphosphates and Triphosphates

Nucleotides have biological roles other than forming DNA and RNA.

One of these roles involves _____ _____.

The two most important energy-transfer nucleotides are *adenosine triphosphate* (ATP) and *adenosine diphosphate* (ADP).

adenosine diphosphate (ADP)

adenosine triphosphate (ATP)
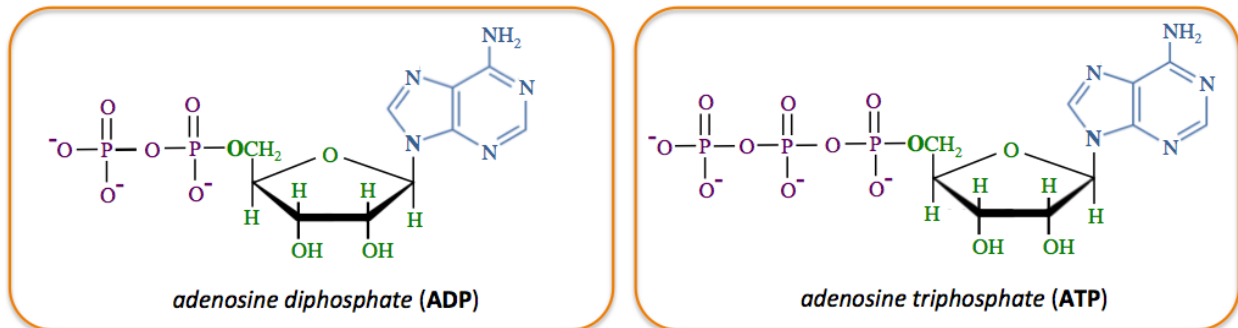
ATP contains ***more*** *chemical potential energy* than does ADP.

Organisms ***obtain energy*** from their environment (sunlight or chemical potential energy in food) when they use it to convert ADP to ATP.

Energy is ***released*** from ATP when it is converted to back to ADP.

- Organisms can do mechanical ***work,*** or drive chemical reactions that require energy by converting ATP to ADP. This is analogous to burning fuel in order to move a car, or discharging a battery while powering an electrical device. *One* way that energy can be released from ATP is by reacting it with H_2O to form ADP, hydrogen phosphate (abbreviated as P_i), and an H^+ ion. The chemical equation for this reaction is shown below.

$$H_2O \ (l) \ + \ ATP \ (aq) \ \rightleftharpoons \ P_i \ (aq) \ + \ H^+ \ + \ ADP \ (aq) \qquad \Delta G = -7300 \text{ Joules per mole of ATP}$$

adenosine triphosphate (ATP)

hydrogen phosphate (P_i)

adenosine diphosphate (ADP)
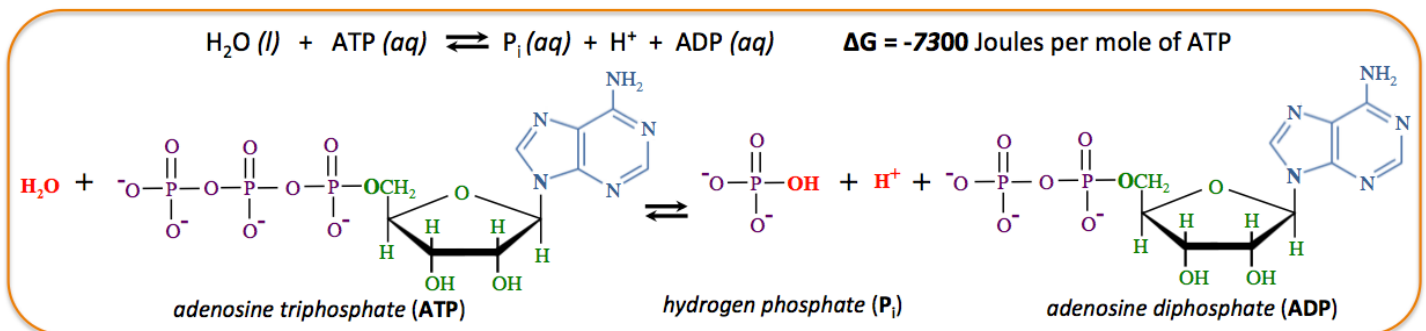
Cyclic Nucleotides

Another biological role of nucleotides is to act as _____ _____ compounds.

A type of nucleotide, called a _____ **nucleotide,** is often used for this purpose.

Cyclic nucleotides are nucleotides that contain a phosphate group *that bonds to the monosaccharide residue at two locations*, thereby forming a *phosphorus-containing* ring.

The lower-case "c" in the abbreviation (cAMP) indicates that it is a cyclic nucleotide.

cyclic adenosine monophosphate (cAMP)

4
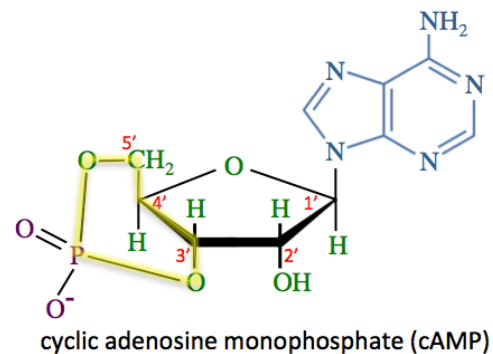
Understanding Check: Draw the structural formula of *cyclic* guanosine monophosphate (cGMP) by making the phosphoester bonds to the **3'** carbon and the **5'** carbon of the ribose monosaccharide residue. Also, label the N-glycosidic bond.

HINT: Look at the image of guanosine monophosphate (below) to see how *guanine* is connected to *ribose*.

guanosine 5'-monophosphate
(5'-GMP)
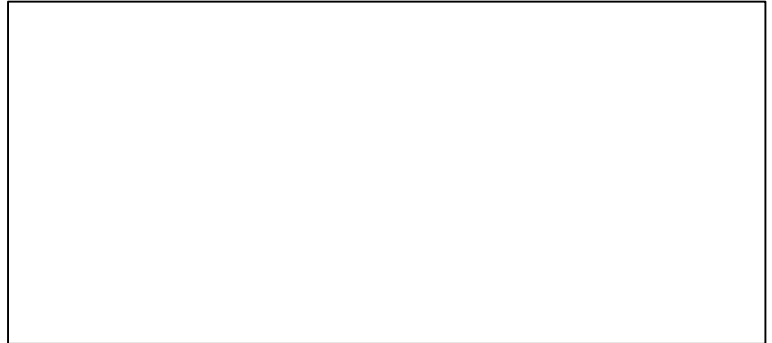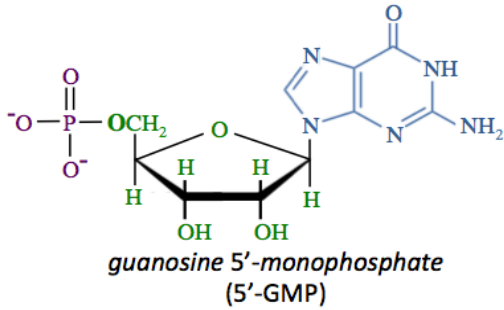
Polynucleotides: DNA and RNA

A _____ is a polymer made from ***nucleotide*** residues.
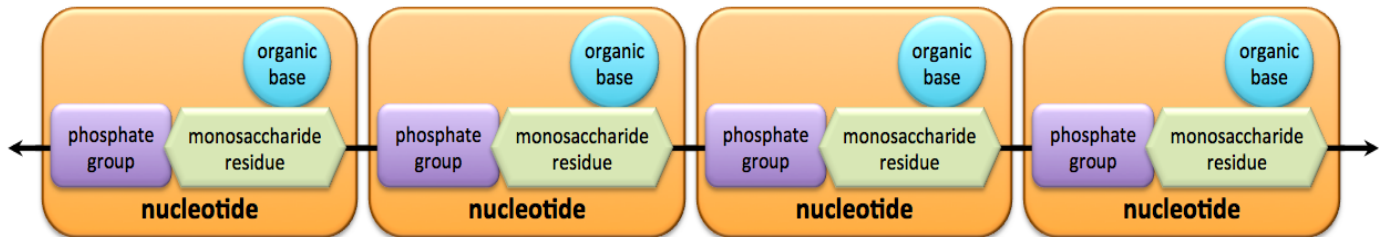
A chain of covalently bonded nucleotides is referred to as a "_____."

Example: A <u>Dinucleotide</u>

3'→5' phosphodiester bonding pattern
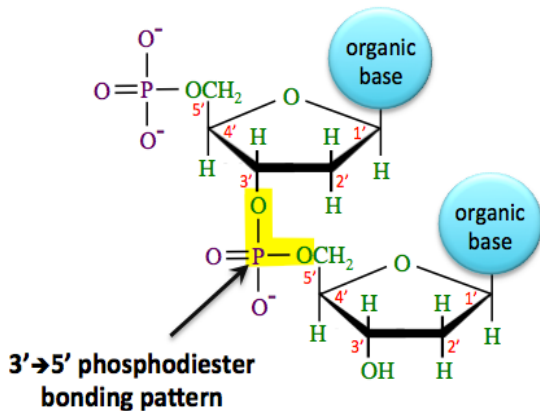
Nucleotides are covalently bonded to each other by a _____ bonding pattern between a   **3'** carbon on one monosaccharide and **5'** carbon on the other monosaccharide.

- We call this bonding pattern a 3'→ 5' *phosphodiester* because the phosphate group is between the 3' and 5' carbons.

Understanding Check: Starting with the dinucleotide, draw a *trinucleotide* by adding another nucleotide to the 3' carbon of the *bottom nucleotide residue*. Highlight the *phosphodiester* bonding patterns. You may use a circle to represent the organic base structures, as I did in the dinucleotide.

DNA Structure

DNA contains the "information" needed for life. This information enables cells to grow and divide. It is responsible for your physical characteristics, such as your height, skin tone, and eye color. Human DNA contains about three million deoxyribonucleotide residues. Eukaryotic cells, which are cells having membrane-bound nuclei, have most of their DNA in the nucleus, and small amounts in other organelles such as chloroplasts and mitochondria. The DNA of prokaryotic cells is contained in the cytoplasm.

Genetic information, the information used to make the various proteins and thereby enabling life, is contained in the _____ *of nucleotides* in DNA.

The sequence of nucleotides in DNA is referred to as **DNA's** _____ _____.

DNA is composed of a combination of *deoxyribonucleotides* that contain either adenine, guanine, thymine, or cytosine organic bases.
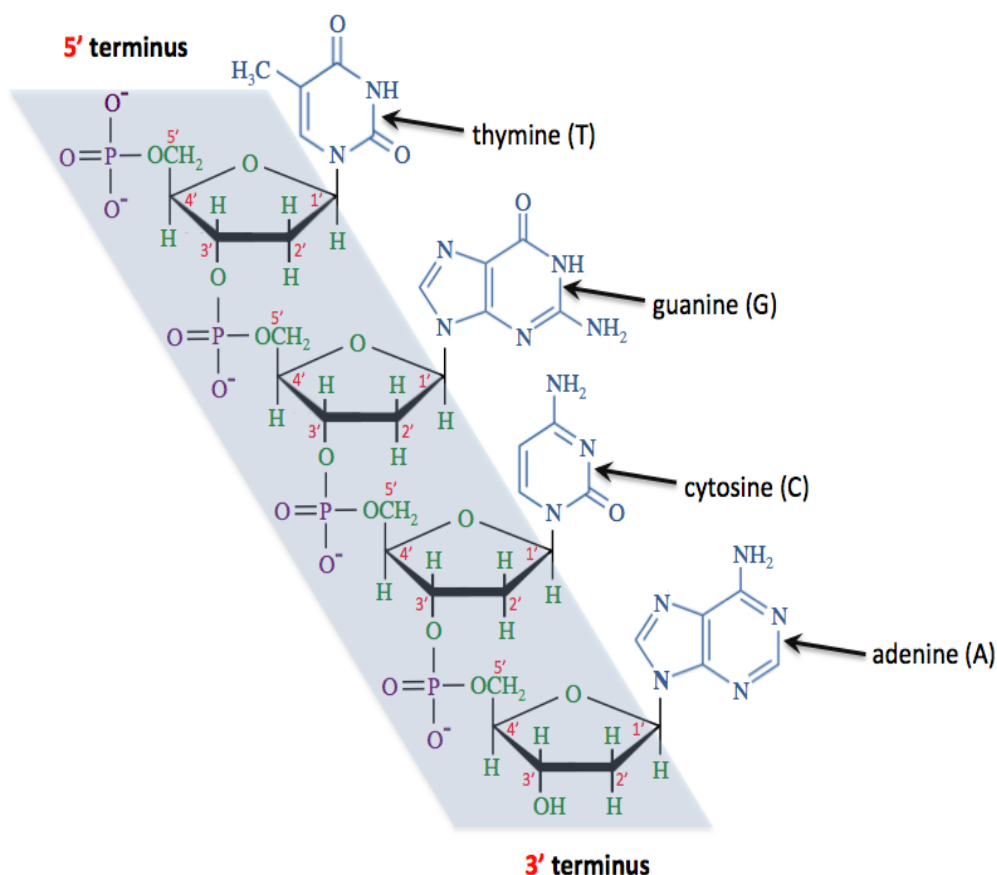
For example:

Nucleotides are given a one-letter abbreviation based on the **first letter in the name of their *organic base***, as shown in structure on the left.

In order to describe the primary structure of a DNA strand, it is customary to list the nucleotides' one-letter abbreviations in the order that the nucleotide residues appear in the strand.

For example, the primary structure of the DNA strand drawn on the left is written as:

5'-TGCA-3'

Another common method used to represent the primary structure of DNA and RNA is to draw the one-letter abbreviations of the organic bases branching from a line that represents the phosphate-sugar backbone. For example, the DNA strand shown above is represented as:

6
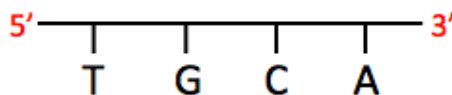
DNA exists as a _____ _____, which is made from **two** *polynucleotide strands*.

Guanine (**G**) bases hydrogen bond with *cytosine* (**C**) bases.

The reason for the strong hydrogen bonding between these organic base pairs is that they have _____ *shapes*.

The hydrogen bonding between these pairs of organic bases is referred to as _____ _____ *or* **complementary base pairing**.

- We say that the two polynucleotide strands in a double-stranded DNA particle are "**complementary**."

Example: Find the complement to this short DNA strand.
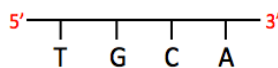
Solution:
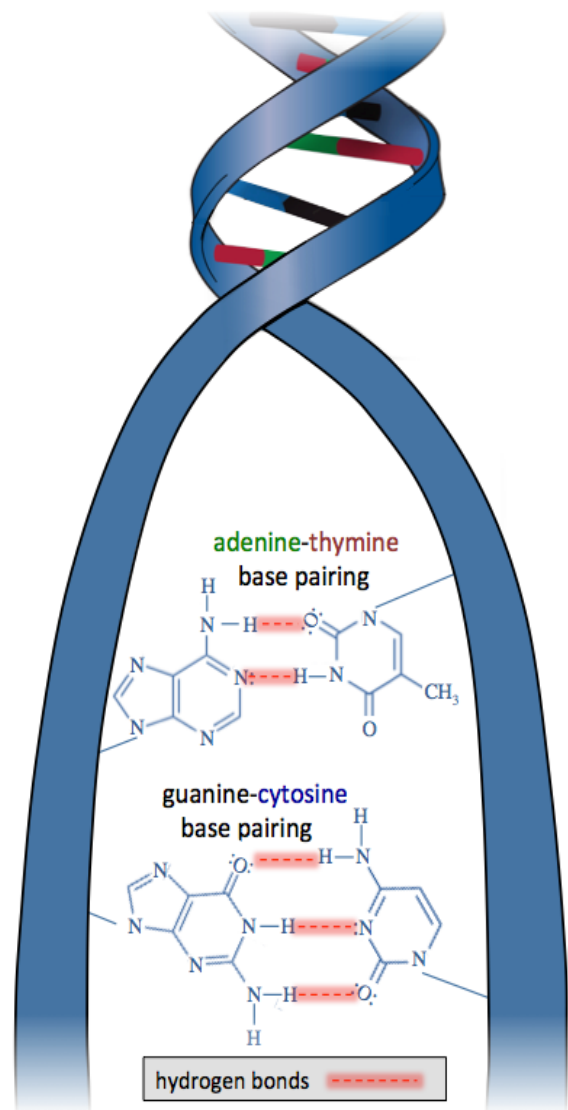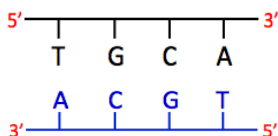
The sugar-phosphate backbones for each of the two DNA strands are illustrated as blue ribbons.

The two DNA strands of a DNA double helix have their **5'** terminuses and **3'** terminuses with opposite orientations. We call this opposing orientations of the DNA strands an "**antiparallel**" arrangement.

The two DNA strands are held together by especially strong _____ _____ between *specific* pairs of organic bases.

Adenine (**A**) bases hydrogen bond with *thymine* (**T**) bases.

5′ ──┬──────┬────┬────┬──────┬── 3′
     G   C   T   A   T

          C   G   G   A
3′ ──┴──────┴────┴────┴──────┴── 5′
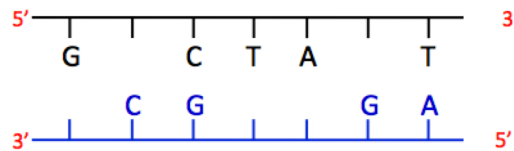
DNA Structure: Chromatin and Chromosomes

In eukaryotic organisms (plants, animals, and fungi), the DNA double helix coils into a more compact structure, as illustrated in the figure on the right.

In the coiling process, the double helix wraps around _____ proteins, as shown in figure on the right.

The DNA/histone further condenses into a fiber that is called _____.

Depending on the cell life cycle, *chromatin* can undergo further coiling. For example, before a cell divides chromatin is coiled into its tightest, *most compact shape*, which is called a

_____.

DNA double helix

The double helix wraps around **histone proteins**.

histone proteins

DNA/histones condense to form **chromatin**.

chromatin

a **chromosome**

Before a cell divides, *chromatin* condenses into a particle called a **chromosome**.

The amount of *chromosomes* that a cell contains depends on the organism. Humans have a total of 46 chromosomes per cell, 23 from each parent. Dogs have a total of 78 chromosomes, 39 from each parent. Fruit flies have a total of 8 chromosomes. The smallest human chromosome contains about 50 million base pairs, and the largest one contains about 250 million base pairs.

Bacterial DNA

DNA double helix
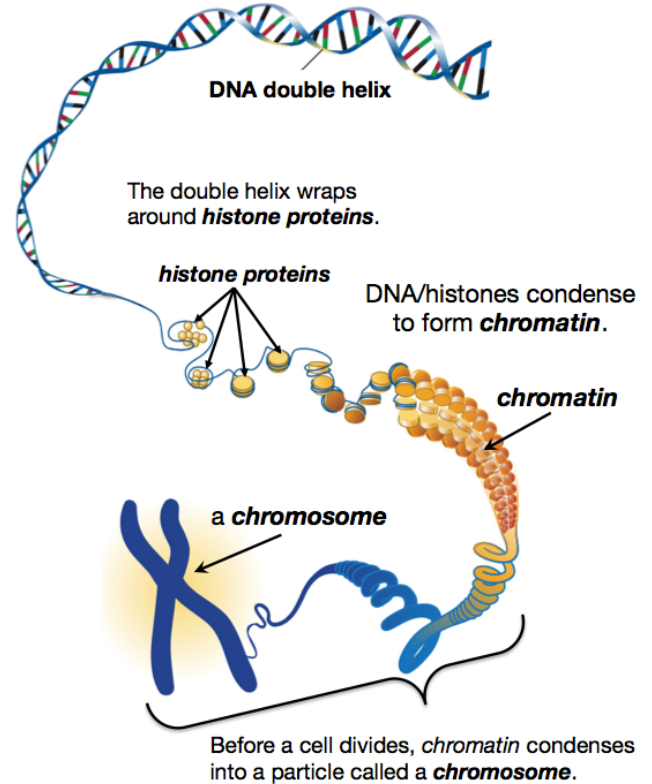
bacterial circular chromosome
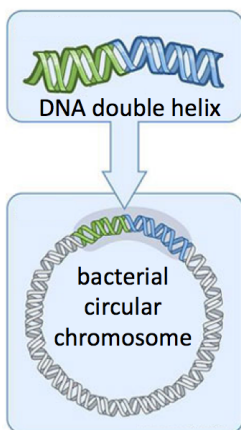
In *bacteria*, which do not have nuclei, chromosomes exist as circular units, called _____ *chromosomes*, (illustrated on the left).

- Circular chromosomes can twist/fold into more compact shapes.

In addition to *circular chromosomes*, bacteria contain smaller, *yet still circular*, double-stranded DNA units called _____.

Denaturation of the DNA Double Helix

Disruption of hydrogen bonding between complementary base pairs is called _____ _____.

- If enough disruption occurs, the DNA strands of a double helix will completely _____ from each other.

- DNA can be denatured by the same agents that are responsible for the denaturation of proteins.

Unlike protein denaturation, when *DNA* is denatured by heat and then allowed to cool to room temperature, the DNA strands will _____ into the original double helix shape.

- When complementary DNA strands re-form their double helix structure, it is referred to as _____.

- Annealing of DNA strands is possible because of complementary base pairing.

RNA Primary Structure

RNA is a polynucleotide that contains *ribose* residues, phosphate groups, and adenine, guanine, cytosine and uracil organic bases.

The sequence of nucleotides in RNA is referred to as **RNA's primary structure**.

The primary structure of a small section of RNA is shown below.
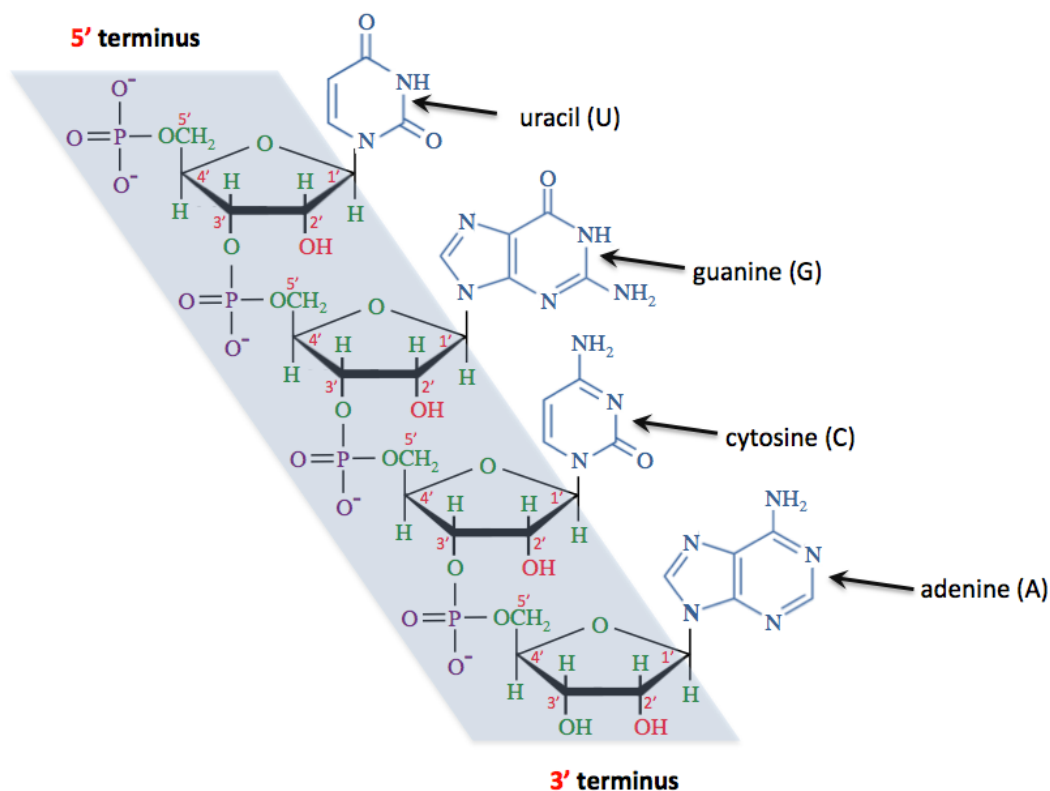
DNA contains *thymine* organic bases, however **RNA** does not; it contains _____ organic bases instead.

DNA has just one function - storing genetic information; **RNA** has _____ functions.

- The overall shape of an RNA particle depends on its _____.

- You will learn about the three types of RNA that are involved in protein synthesis in a later section of this chapter.

Differences Between the Two Classes of Polynucleotides: RNA vs. DNA

Polynucleotides

Contain *deoxyribose residues*:

DNA

Organic Bases:	*Function:*
adenine guanine cytosine thymine	storing genetic information

Contain *ribose residues*:

RNA

Organic Bases:	*Function:*
adenine guanine cytosine uracil	RNA has *multiple* functions. You will learn about these functions later in this chapter.
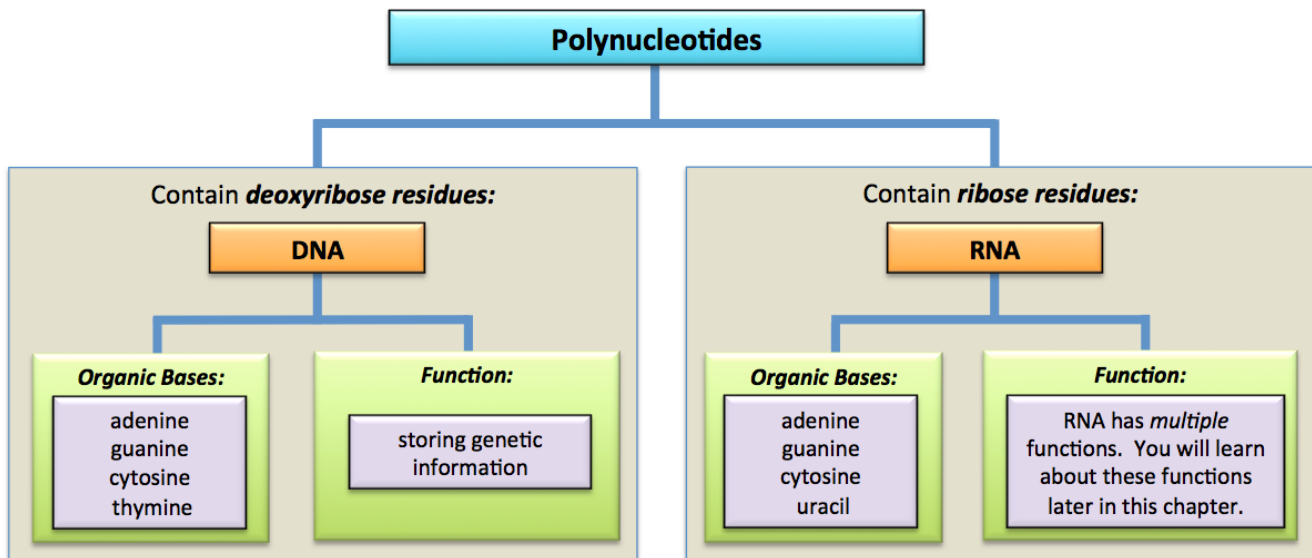
DNA Replication

When a cell divides, the original cell, called the *parent cell*, forms two new cells that are called the *daughter cells*.

Before a somatic cell (non germ/sex cell) physically splits into two daughter cells, an exact _____ of all of the parent cell's DNA must be made so that a copy can be placed in each daughter cell.

The process in which a duplicate copy of a DNA double helix is made is called _____ _____.

In DNA replication, each of the two original DNA strands (called the *parent strands*) is used as a "template" for the formation of a new "_____ _____."

- In eukaryotic cells, proteins called "helicases" unwind and then open sections of the double helices by disrupting the hydrogen bonds between base pairs.

parent (template) DNA strand · daughter strand · DNA polymerase · DNA polymerase · parent (template) DNA strand · daughter strand
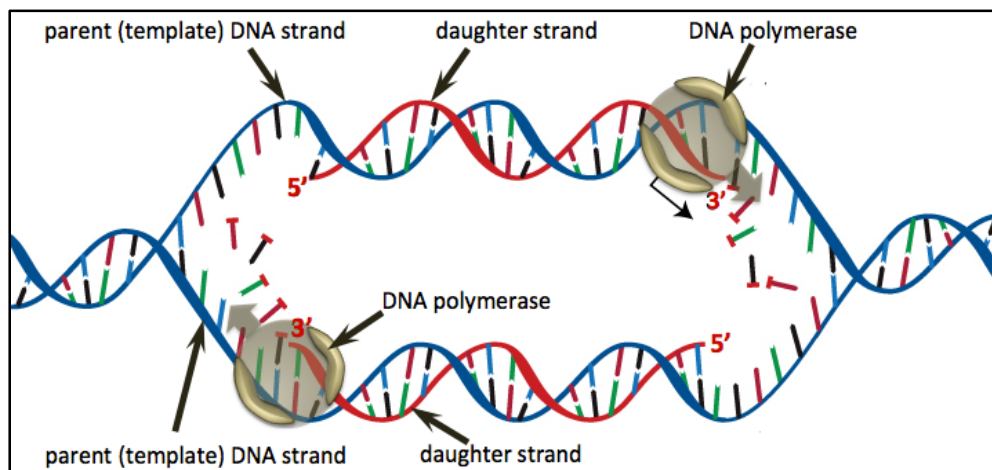
Once a double helix has opened, DNA polymerase enzymes catalyze the formation of complementary daughter strands *on _____of the parent strands*.

The daughter strands are formed by adding _____ deoxyribonucleotides, one-by-one to the growing daughter strands.

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Because each daughter strand is assembled, nucleotide by nucleotide, with organic bases that are *complementary* to one of the parent strands, then both of the double-stranded DNA particles that result from the replication process are **identical to the original DNA particle**.

DNA polymerase enzymes catalyze the addition of complimentary nucleotides to the _____ terminus of the growing **daughter strand**.

In order to do this, DNA polymerase moves along the **parent (template) strand** in the direction from **3'** terminus to **5'** terminus of the **parent** strand.

- In plants and animals, this process occurs simultaneously *at multiple places along each parent strand*. Although **not shown** in the image on the previous page, these multiple sections of a daughter strand are linked/bonded together with the help of *DNA ligase enzymes*.

Chemical Bonding in DNA Replication
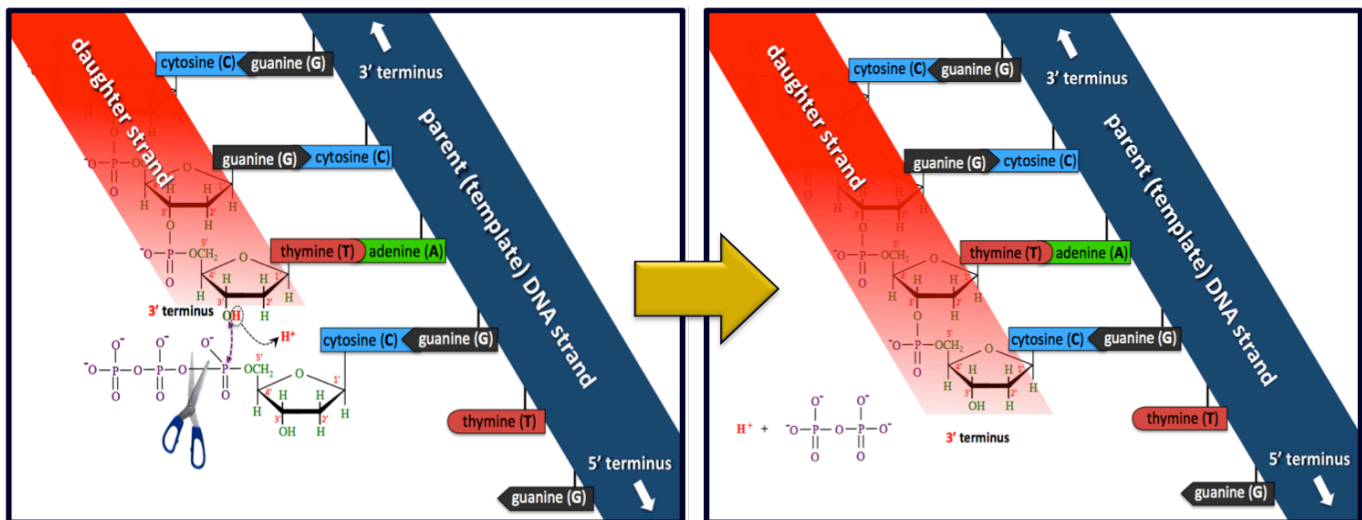
DNA polymerase enzymes catalyze the formation of _____ **bonds** between free nucleotide *tri*phosphates and the **3'** terminus of a growing daughter strand.

The daughter strands that are produced are _____ to their template parent strands because **DNA polymerase directs the addition of nucleotide triphosphates that are complementary to the adjacent parent strand bases**.

- In the image shown above, a triphosphate with the *cytosine* (C) base was added because of the adjacent complementary *guanine* (G) base in the template parent strand.

Proofreading and Repair

When adding new deoxyribonucleotides to a growing DNA strand, DNA polymerase inserts the wrong residue slightly less than once every 10,000 times.

The enzyme proofreads its work to see if the correct deoxyribonucleotide residue has been added; if a mistake has been made, DNA polymerase clips the residue and tries again.

If proofreading does not catch the error, then other DNA repair enzymes are likely to catch the problem. After proofreading and repair, the error rate during replication falls to *less than one in 1 billion bases*.

Understanding Check: Using the illustration on shown in the viewgraph, name the next *nucleotide triphosphate* that would be added to the growing daughter strand.

Protein Synthesis

The information contained in the sequence of DNA nucleotides is used to generate proteins. This process is central to the existence of all known life forms because proteins are critical in directing and controlling cell growth and function, and in regulating an organism's metabolism.

The process of making proteins from the information in DNA is called _____ _____ or _____ _____.

Protein synthesis can be divided into two sequential processes: **transcription** and **translation**.

Transcription: DNA to RNA

A _____ is generally defined as *a region of DNA that carries the information needed to produce a protein*.

  •   Human DNA contains about **_25,000_** genes.

The first step in *protein synthesis* is called _____.

In the transcription process, the information (sequence of nucleotides) in a gene is used to create a specific sequence of *ribo*nucleotides in a single-stranded _____ _____ (**mRNA**) particle.

The *transcription process* is similar to DNA replication, with three main differences:

  1) RNA is produced in transcription, whereas DNA is produced in DNA replication.

  2) In transcription, only *one* of the DNA double helix strands is used as a template to produce *one mRNA strand*, whereas in DNA replication, *each* of the two DNA strands in a double helix produce a daughter strand.

  3) Different enzymes are used.

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Transcription begins when an _____ _____ **enzyme** binds to a "**promoter site**" on the gene.

- *Promoter sites* are specific sequences of nucleotides at the beginning of a gene.   When RNA polymerase binds to the promoter site, the hydrogen bonding between base pairs within the DNA double helix is disrupted. This unwinds and opens a section of the gene's double helix.

Next, *RNA polymerase* moves along one strand of the gene while catalyzing the addition of *free ribonucleotides,* that are complementary to the DNA template, to the ____ end of a growing **mRNA** strand.
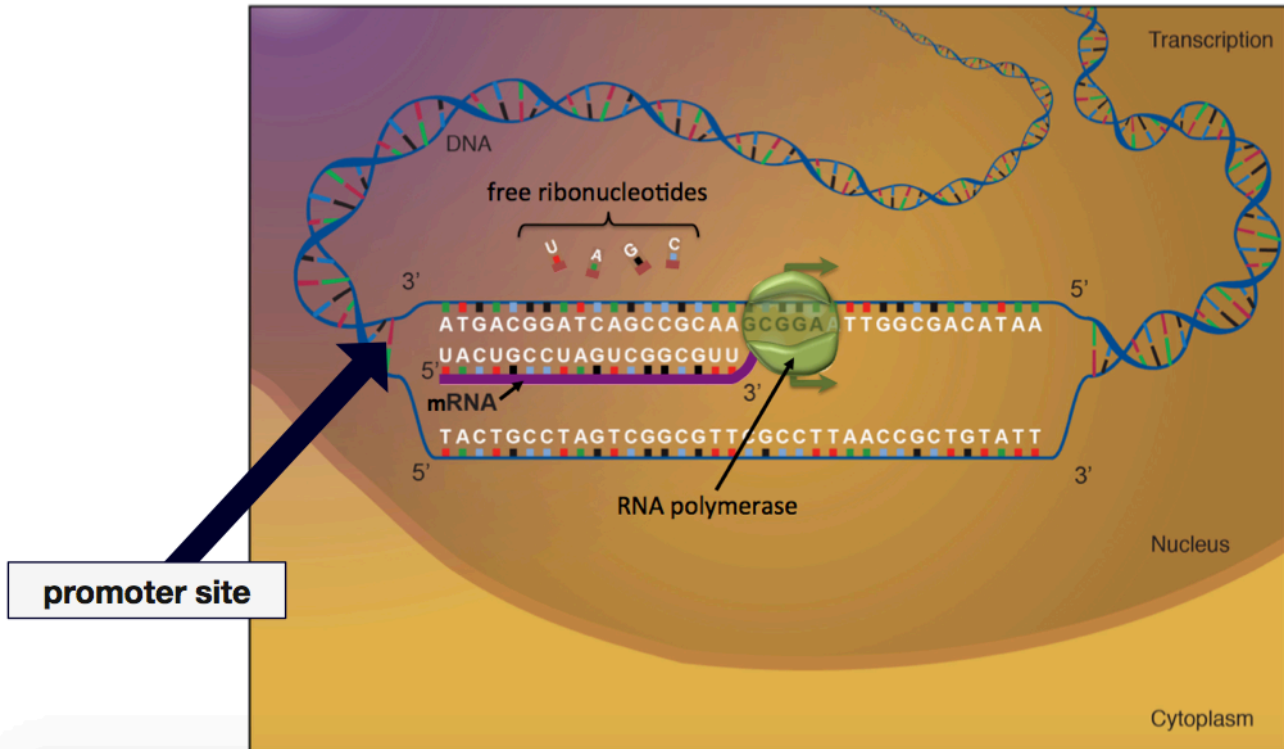
The DNA-to-RNA base pairing is a bit different from the DNA-to-DNA base pairing because RNA contains *uracil* (U) and does not contain *thymine* (T).
- *Adenine* (A) DNA organic bases base pair with *uracil* (U) RNA bases.
- DNA organic bases C,G, and T, base pair with RNA bases G, C, and A, respectively.
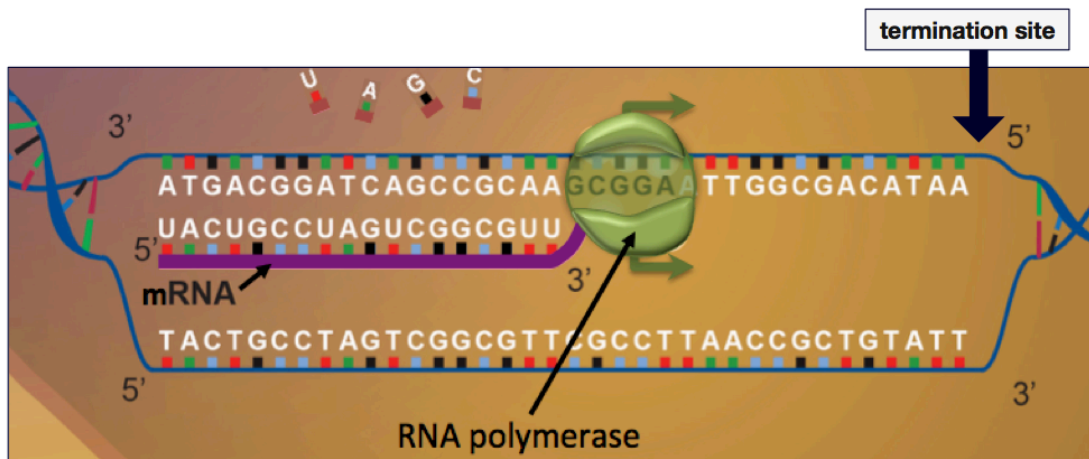
When the RNA polymerase reaches a nucleotide sequence in the gene, called the **termination site**, the mRNA strand is _____.

Transcription occurs in the _____ of eukaryotic cells and in the _____ of prokaryotic cells.

Although not shown in the illustration on the previous page, in eukaryotic cells, there are regions of RNA that undergo additions and deletions of nucleotides in a process called **co-transcriptional modifications**. A discussion of the details of co-transcriptional modifications is beyond the scope of this course.

Messenger RNA contains the _____ (message) from a gene that is required to produce a protein.

In eukaryotic cells, mRNA exits the nucleus through pores in the nuclear membrane and enters the cytoplasm where the *protein synthesis* process will be completed.

About 1.5% of human DNA is in the form of a gene; the remaining 98.5% is called **noncoding DNA**. Until recently, the noncoding DNA was called "junk DNA." It was thought that all noncoding DNA is extraneous DNA that has been passed down, through evolution, from ancestral species. More recently, research has shown that not all noncoding DNA is "junk." For example, noncoding DNA has been found to play a role in the regulation of transcription.

Translation: mRNA to Protein

The next step in *protein synthesis* is called _____.
- In this process, the information that was in a gene and is now contained in mRNA is used to construct the polypeptide chains that make up proteins.

In *translation*, the sequence of nucleotides in mRNA, is converted (translated) to a sequence of _____ _____residues in a *polypeptide*.

This is done using the _____ _____.

The *genetic code* is based on three-nucleotide sequences, called _____.

A *codon* directs the addition of a _____ amino acid residue to a polypeptide that is being formed.

The *genetic code* was completely known by the late 1950's and is shown in the table below.
- Example: the mRNA three-nucleotide sequence (codon) **GAU** codes for the addition of an *aspartic acid* (Asp) amino acid residue to a growing polypeptide chain.

Genetic Code Table: The mRNA Codons and the Amino Acids for which they Code

first mRNA codon base	second (middle) mRNA codon base				third mRNA codon base
	U	**C**	**A**	**G**	
U	UUU Phe	UCU Ser	UAU Tyr	UGU Cys	U
	UUC Phe	UCC Ser	UAC Tyr	UGC Cys	C
	UUA Leu	UCA Ser	UAA STOP	UGA = STOP	A
	UUG Leu	UCG Ser	UAG STOP	UGG = Trp	G
C	CUU Leu	CCU Pro	CAU His	CGU Arg	U
	CUC Leu	CCC Pro	CAC His	CGC Arg	C
	CUA Leu	CCA Pro	CAA Gln	CGA Arg	A
	CUG Leu	CCG Pro	CAG Gln	CGG Arg	G
A	AUU Ile	ACU Thr	AAU Asn	AGU Ser	U
	AUC Ile	ACC Thr	AAC Asn	AGC Ser	C
	AUA Ile	ACA Thr	AAA Lys	AGA Arg	A
	AUG = Met/START	ACG Thr	AAG Lys	AGG Arg	G
G	GUU Val	GCU Ala	GAU Asp	GGU Gly	U
	GUC Val	GCC Ala	GAC Asp	GGC Gly	C
	GUA Val	GCA Ala	GAA Glu	GGA Gly	A
	GUG Val	GCG Ala	GAG Glu	GGG Gly	G

The mRNA nucleotide sequences in the codons are listed in the direction of the mRNA **5'** terminus toward the **3'** terminus.

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Since there are *twenty-one* common amino acids, and only *four* types of RNA nucleotides (**C**, **G**, **A**, **U**), it was necessary for nature to use *three nucleotides per codon*. *If* there were only *one* nucleotide per codon, then only *four* amino acids could have been specified. *If* there were *only two nucleotides per codon*, then only *sixteen amino acids* could have been specified.

In nature, mRNA sequences contain hundreds to many thousands of nucleotide residues, however, for simplicity, I will use a very short mRNA sequence in the following example.

The "start" codon (**AUG**) determines the first amino acid residue to be used in the polypeptide.

Peptides are synthesized in the direction from their **N**-terminus to their **C**-terminus.
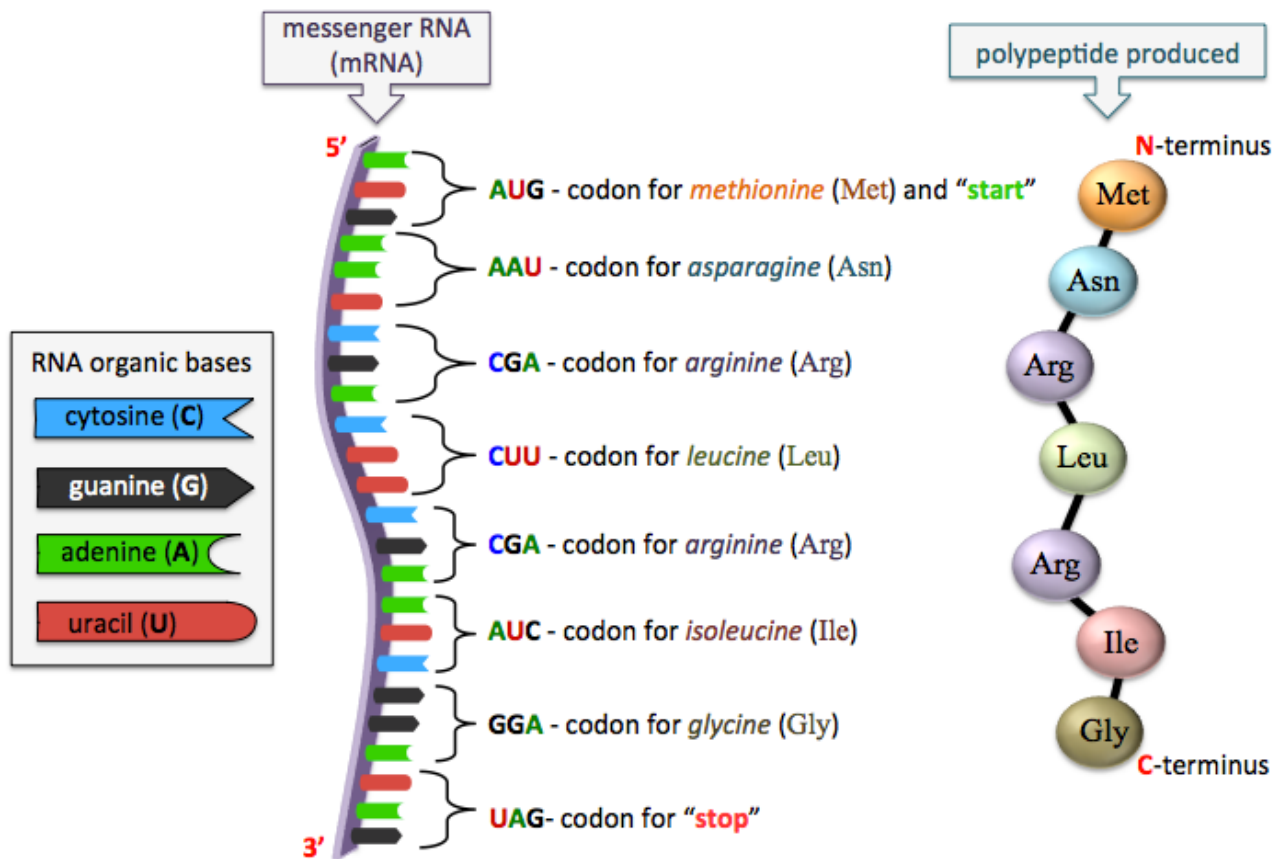
Nucleotides are added to the growing peptide chain until the stop codon is reached.

Understanding Check: Write the three-letter abbreviations for the amino acid residues, in order from **N**-terminus to **C**-terminus, of the polypeptide that would be produced in the translation of the mRNA shown below.

- Recall that in translation, polypeptides are formed in the direction from their **N**-terminus to the **C**-terminus.
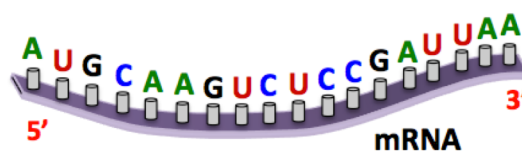
The Role of Transfer RNA (tRNA) in Translation

In order for you to understand how the codon information is used to direct the addition of specific amino acids to a growing peptide chain, we will consider another type of RNA, called **transfer RNA (tRNA)**.

The function of a tRNA particle is to _____ and then _____ the amino acid that is specified by an mRNA codon to a growing peptide chain.

A ribbon model and a simplified representation of a tRNA particle are shown below.

tRNA images adapted from: Wikimedia Commons, Author: Yikrazuul
CC-BY-SA, http://creativecommons.org/licenses/by-sa/3.0/legalcode
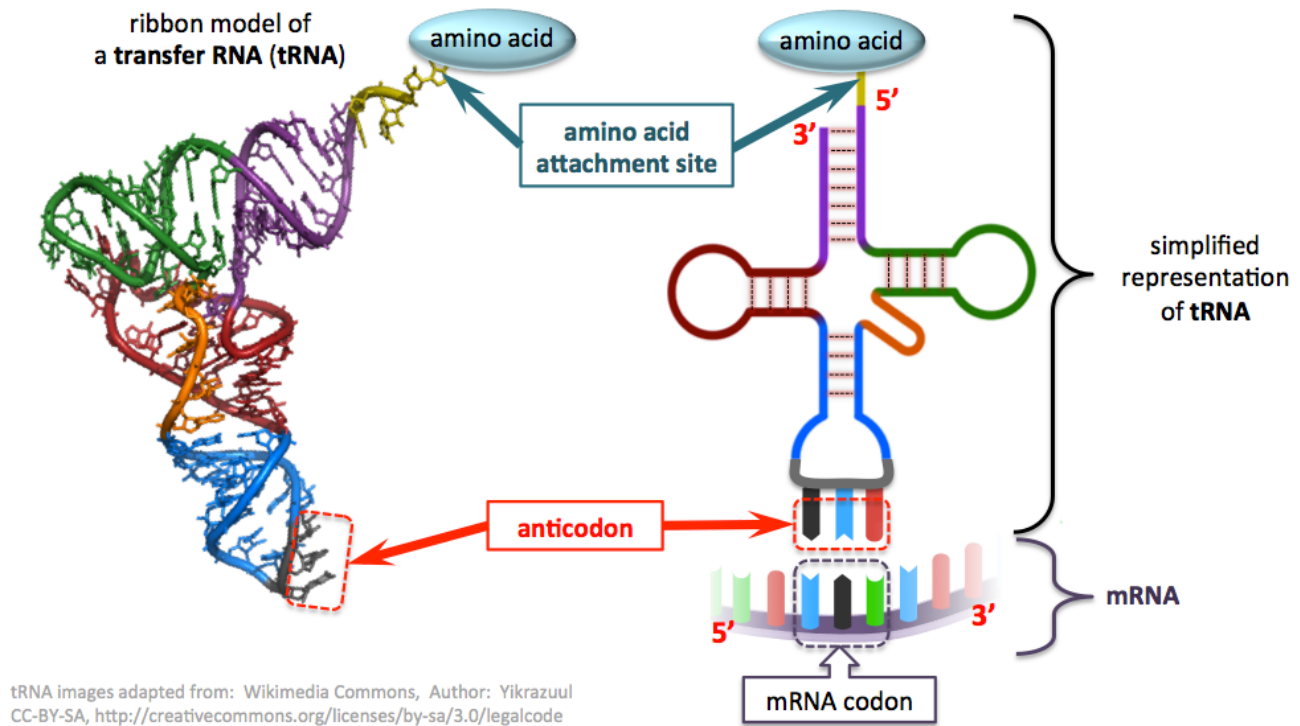
tRNA particles are single-stranded polynucleotides that contains 73 to 93 ribonucleotides. Base pairing causes the single tRNA strand to *fold back on itself*. Hydrogen bonding between tRNA base pairs is represented by the dotted lines that are highlighted in the simplified tRNA representation.

One region of tRNA has a site that attaches to an *amino acid residue,* and another region contains a three-nucleotide sequence called an _____.

The particular amino acid that a tRNA carries depends on the three-nucleotide sequence in its *anticodon*.

Anticodons are _____ to mRNA codons (as illustrated in the bottom-right of the image above).

In the illustration above, the mRNA codon (in the **5'** to **3'** direction) is **CGA**, therefore the tRNA anticodon (in the **3'** to **5'** direction) is **GCU**. Using the mRNA codon in this example (**CGA**), and the *genetic code table*, we find that this tRNA would carry an *arginine* (Arg) amino acid residue.

The Translation Mechanism

Translation occurs in ***three*** steps:

1) _____ 2) _____ 3) _____

1) Initiation

Once the *messenger RNA* leaves the nucleus and enters the cytoplasm, a _____ attaches to its "start" codon (**AUG**).

Ribosomes are relatively large particles that contain protein *and* very long RNA strands called **ribosomal RNA** (_____).

- The function of *ribosomes* is to provide a structure upon which polypeptides can be produced.

Next, a *transfer* RNA with a "_____" *anticodon* (**UAC**) binds to the mRNA start codon to form a ribosome/mRNA/tRNA complex. The formation of this complex, as illustrated below, is called the **initiation step**.
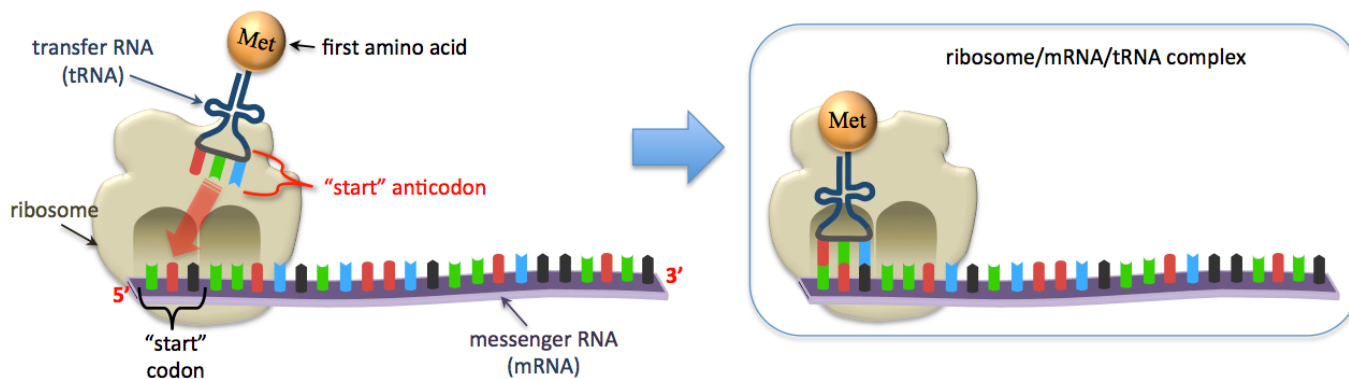
2) Elongation

Elongation begins when a second tRNA binds to the ribosome/mRNA/tRNA complex (as illustrated below).

- The second tRNA delivers the amino acid that corresponds to the codon that follows the start codon. In this example, the second tRNA delivers an asparagine (Asn) amino acid.

In elongation, a polypeptide chain is made by the formation of _____ *bonds* between the amino acid residues that are specified by the genetic code in mRNA.
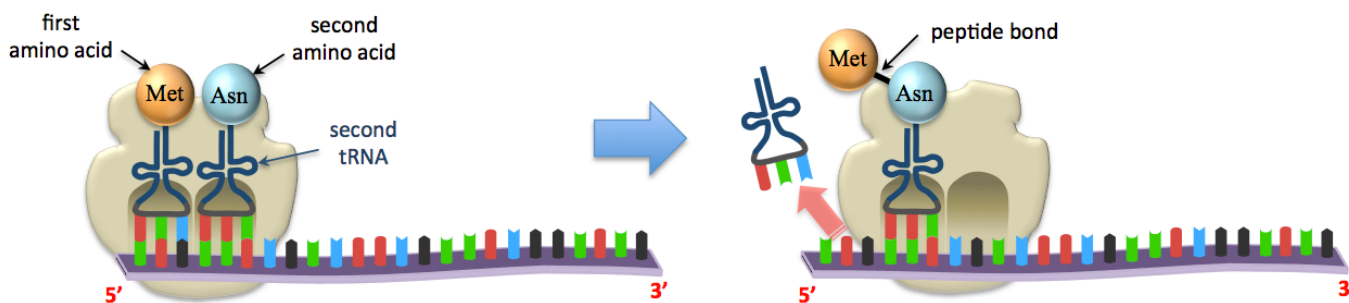
A part of the ribosome, called the *transferase center*, catalyzes the formation of *peptide bonds* between the amino acid residues.

Next, the ribosome moves a distance of three bases (a codon) along the mRNA strand in the **5'** to **3'** direction. The tRNA that was attached to the first amino acid detaches from the mRNA and diffuses throughout the cytoplasm where it will encounter an enzyme that catalyzes its reattachment *to an amino acid that matches its anticodon*.

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This entire process is repeated when a third amino acid binds to the next mRNA codon, as illustrated below.
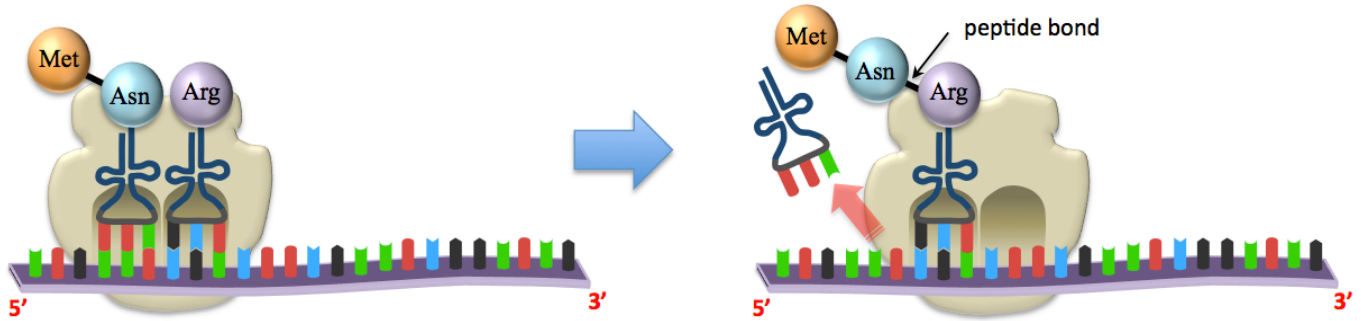
Peptides are synthesized in the direction from the **N**-terminus to the **C**-terminus because the new amino acid residues form peptide bonds with the **C**-terminus of a growing peptide chain.

After many cycles of amino acid addition, the ribosome will reach a "*stop*" codon as illustrated below.
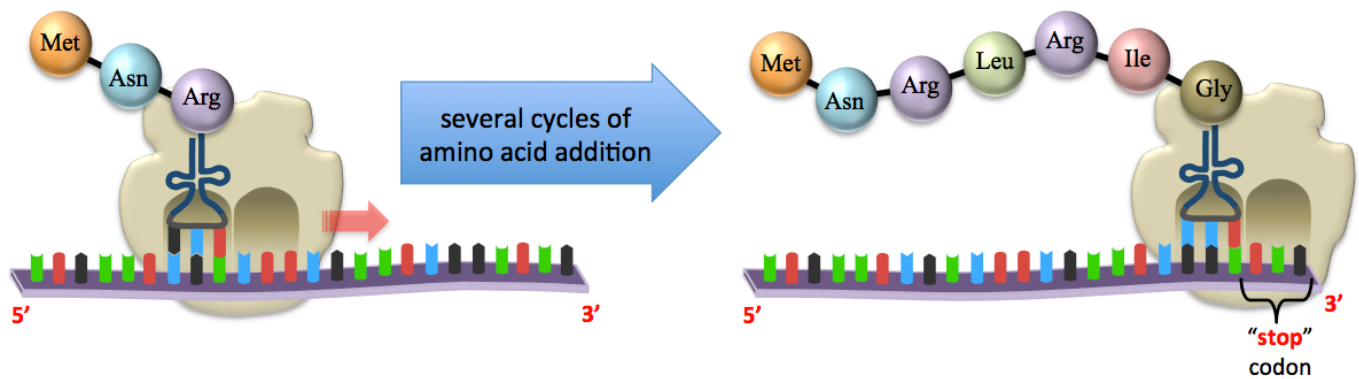
3) Termination

The ***termination*** step occurs when the ribosome reaches a _____ codon (**UAA**, **UGA**, or **UAG**).

When this happens, the polypeptide, mRNA, tRNA, and ribosome become separated, as illustrated below.
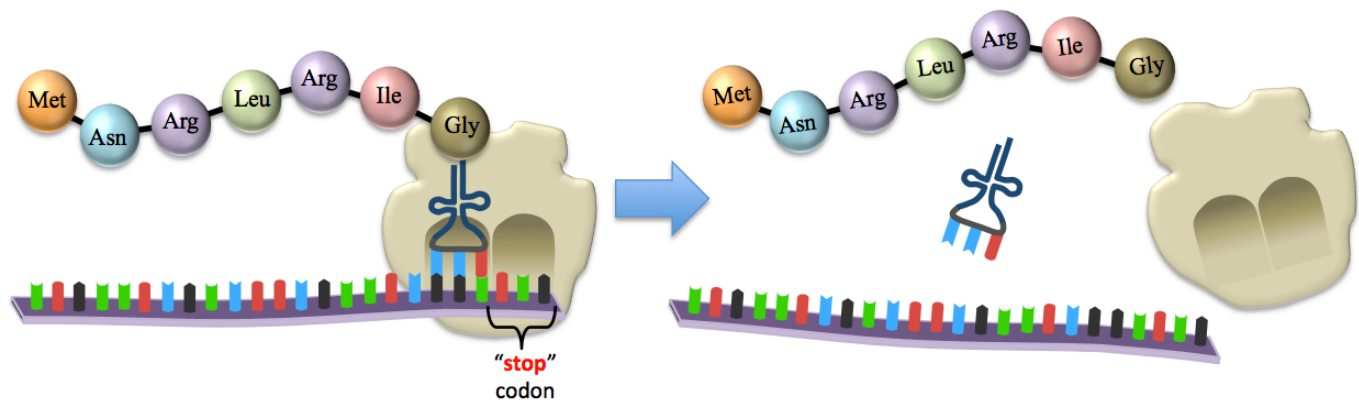
In some cases, the polypeptide that is produced in translation is a fully-functional protein. In other cases, the polypeptides undergo further folding to acquire the secondary and tertiary structures that they need in order to function. In many cases, multiple polypeptide subunits must assemble into a quaternary structure in order to form a fully-functional protein.

Some proteins require covalent bonding modifications, called **post-translational modifications**, after they are translated. An example of a *post-translational modification* is the addition of *heme groups* to heme-containing proteins, such as hemoglobin and myoglobin.

Although not discussed in this section, there are some differences in how prokaryotic and eukaryotic cells synthesize proteins. Many antibiotics take advantage of these differences in order to inhibit protein synthesis in prokaryotic pathogens while not harming the human (or animal) hosts. The table below lists some of these antibiotics and their effects on prokaryotic protein synthesis.

Antibiotic	Mode of Action
chloroamphenicol	inhibits peptide bond formation
erythromycin	prevents ribosome from moving along mRNA
streptomycin	inhibits initiation and cause misreading of mRNA
tetracycline	inhibits the binding of tRNA to mRNA/ribosome

Understanding Check: Write the three-letter abbreviations for the amino acid residues, in order from **N-terminus** to **C-terminus**, of the polypeptide that would be produced by the **transcription** *and* **translation** of **DNA** with a sequence of **3'-TACGGGGTACACACT-5'**.
- **CAUTION:** In this question, you were given the sequence of DNA, *not* mRNA.

Control of Gene Expression

_____ _____is another term used for *protein synthesis*
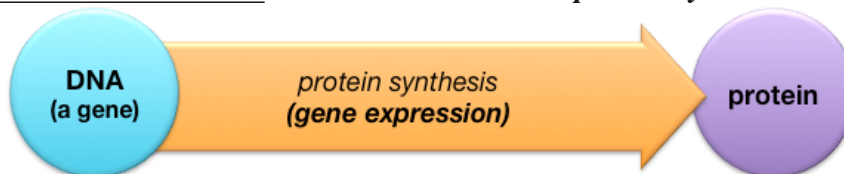
The DNA of each living thing contains *thousands* of **genes**.

These genes are not continually _____ (*read to make proteins*), because the production of unneeded proteins would be an inefficient use of resources.

In chapter 13, you learned how organisms often use several reactions in series, called **metabolic pathways**, in order to carry out the chemical changes they require to meet their physiological needs. You also learned that many of the reactions in metabolic pathways require enzymes and that organisms can regulate (slow down or speed up) a metabolic process, according to their needs, by *inhibiting* or *activating* one (or more) of the enzymes involved in the metabolic pathway.

Another way to control metabolic pathways, or other conditions that involve proteins, is to **regulate the** _____ ____ _____ **of a protein/enzyme**.

This is called _____ *gene expression*.

Increasing the rate of gene expression is called _____of the gene; decreasing the rate of gene expression is called _____of the gene.

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Example: Control of the *lac* operon.

Recall that *transcription*, the creation of mRNA from the information in a DNA, involves the *RNA polymerase enzyme*. In order for transcription to begin, *RNA polymerase* must bind to a "**promoter site**" on the DNA to be transcribed.

Sometimes, *several genes* are transcribed from the **same** *promoter site*.

A section of DNA made up from genes that are *transcribed from the same promoter site* is called an

_____.

Escherichia coli (*E. coli*) contain an operon comprised of three genes that code for proteins involved in the metabolism or transport of lactose.

This *operon* is called the ***lac* operon**.

The three genes of the *lac* operon are called *lac*Z, *lac*Y, and *lac*A. The *lac* operon is preceded by a *lac regulator* (*lacI*) *gene*, as illustrated below.
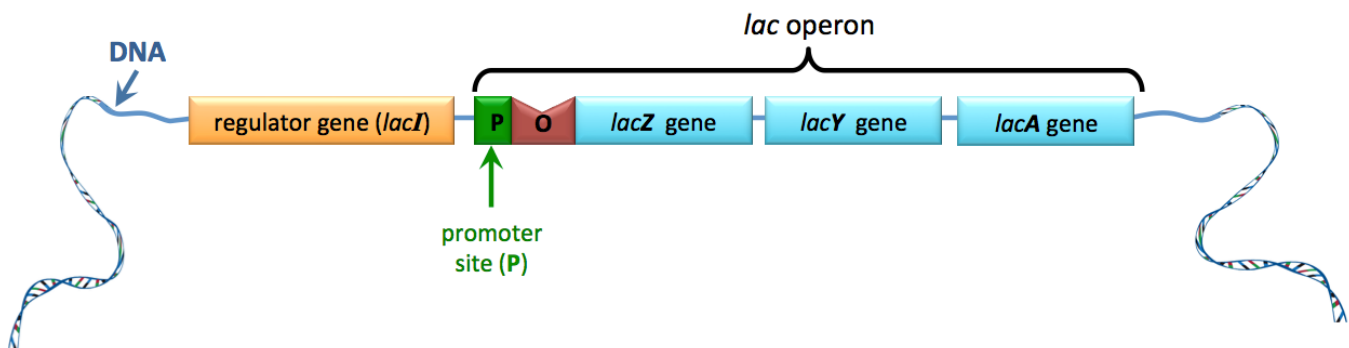
In the presence of glucose, lactose is not needed as an energy source and almost zero lactose is allowed into the bacterial cell, therefore it is not necessary for the genes of the *lac* operon to be expressed. It is for this reason that nature has provided a regulator gene (*lacI* gene).

The *lacI* gene produces an _____ *repressor protein*, which binds to a segment of DNA called an **operator site**, as illustrated below.
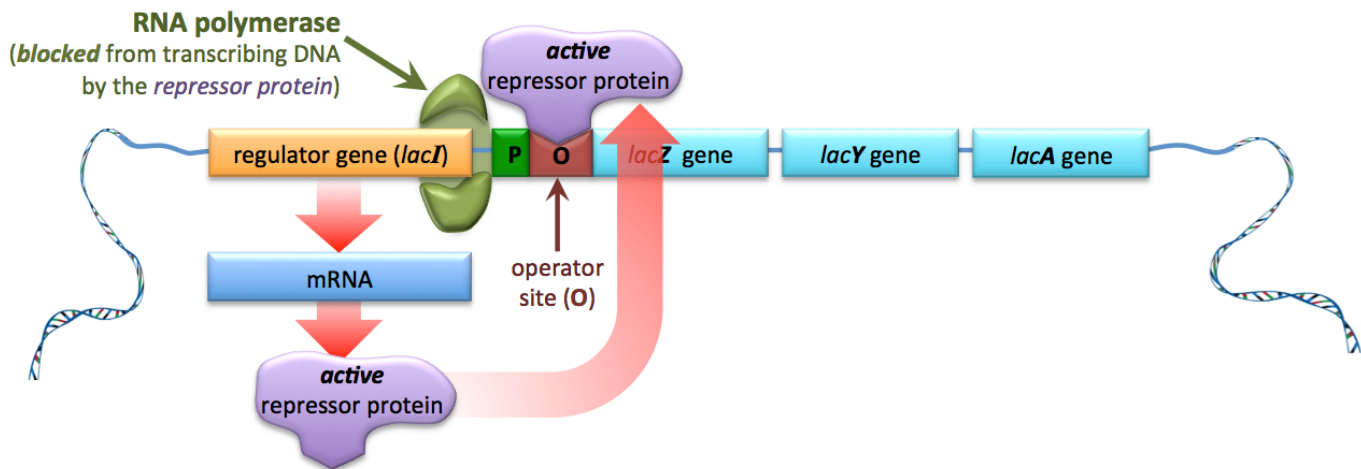
When the active repressor protein is bound to the operator site, ***RNA polymerase is _____ from moving along the lac operon* to transcribe the *lacZ, lacY*, and *lacA* genes**.

- Under normal conditions (glucose present), this is ideal for the *E. coli* because there is plenty of glucose present, and lactose is *not* being taken in, therefore the bacteria do not need the lactose metabolism or transport proteins that the genes of the *lac* operon express.

Let's consider the scenario in which *lactose* is present **in the absence of glucose**. In this case, lactose is allowed to enter the *E. coli*. Whenever lactose is present in the bacteria, some of it is converted to a compound called *allolactose*.

Allolactose will bind to, and thereby _____ *the repressor protein*.

The *inactive* repressor protein cannot _____ to the operator site, therefore RNA polymerase is no longer blocked and will move along the *lac* operon to transcribe the *lac* operon genes, as illustrated below.
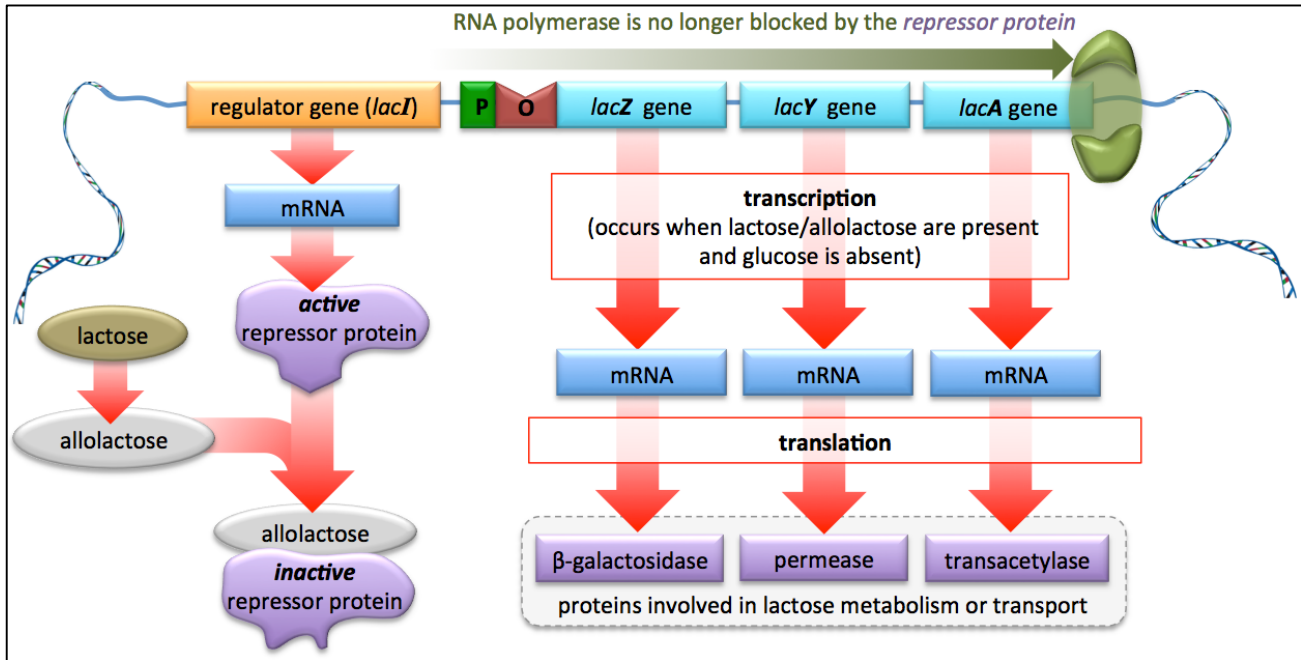
The mRNAs from the *lac* operon genes are *translated* to the three proteins: *β-galactosidase*, *permease*, and *transacetylase*.
- *β-galactosidase* is an enzyme involved in lactose metabolism.
- *Permease* is a transmembrane protein that transports lactose into cells.
- *Transacetylase* is an enzyme thought to be involved in the breakdown of some non lactose species that are transported into cells by *permease*.

The presence of lactose within *E. coli*, and the subsequent presence of allolactose, **upregulate** the genes of the *lac* operon. Allolactose and lactose are continuously being used up by the bacteria. Whenever lactose is no longer obtained from the surroundings, the concentration of allolactose within the cells will decrease, and then *active regulator proteins* become available again to **downregulate** the *lac* operon.

Understanding Check: Determine whether each of the following conditions would result in the genes of the *lac* operon being **upregulated** or **downregulated**.
- a. RNA polymerase is blocked from moving along the *lac* operon
- b. Allolactose binds to the repressor protein
- c. Lactose concentration within a cell is decreased
- d. Allolactose concentration within a cell is increased
- e. Active repressor proteins are present in the absence of allolactose
- f. Glucose is available.

Viruses

Viruses are small particles that are not able to _____ on their own.

- A typical virus is about 1/100 the size of a bacteria.

In order for a virus to reproduce, it must invade a cell of *another* organism.

A cell that is invaded by a virus is called a _____ **cell**.

Viruses have much less-complicated structures and contents than do cells; they do not have the components, such as nucleotides and certain enzymes, that are needed in order to self-replicate. Viruses come in a variety of shapes.

All viruses have a protein shell that encapsulates *either* _____ *or* _____, and some viruses contain a small set of enzymes.

- A virus that contains DNA is called a **DNA virus**. A virus that contains RNA is called an **RNA virus**. Some viruses have a lipid coating that surrounds their protein shell.

All forms of life can have their cells invaded by viruses.

When viruses take over plant or animal cells, we call this a _____ **infection**.

- Several human *infectious diseases*, some of which are *chronic diseases*, are caused by viral infection. Some of these diseases, the location of the infections, and the most common viral species involved are shown on the right.

Encephalitis/meningitis
- JC virus
- Measles
- LCM virus
- Arbovirus
- Rabies

Common cold
- Rhinoviruses
- Parainfluenza virus
- Respiratory syncytial virus

Pharyngitis
- Adenovirus
- Epstein-Barr virus
- Cytomegalovirus

Gingivostomatitis
- Herpes simplex type 1

Cardiovascular
- Coxsackie B virus

Hepatitis
- Hepatitis virus types A, B, C, D, E

Skin infections
- Varicella zoster virus
- Human herpesvirus 6
- Smallpox
- Molluscum contagiosum
- Human papillomavirus
- Parvovirus B19
- Rubella
- Measles
- Coxsackie A virus

Eye infections
- Herpes simplex virus
- Adenovirus
- Cytomegalovirus

Parotitis
- Mumps virus

Pneumonia
- Influenza virus, Types A and B
- Parainfluenza virus
- Respiratory syncytial virus
- Adenovirus
- SARS coronavirus

Myelitis
- Poliovirus
- HTLV-I

Gastroenteritis
- Adenovirus
- Rotavirus
- Norovirus
- Astrovirus
- Coronavirus

Sexually transmitted diseases
- Herpes simplex type 2
- Human papillomavirus
- HIV

Pancreatitis
- Coxsackie B virus

Viruses infect cells by introducing their DNA or RNA and, in some cases, a few types of enzymes, into the host cell. This is done in various ways depending on the particular virus. Once the viral DNA or RNA is introduced to the host cell, enzymes, nucleic acids, and amino acids *from the host cell* are employed to make more viral DNA or viral RNA, and viral proteins. The viral DNA or RNA and viral proteins are *reassembled into multiple, new virus particles* within the host cell. These new viral particles cause the host cell to burst or release the viral particles using the exocytosis process. The infection spreads as the new viruses infect other cells.

Viral DNA or RNA self-replicates and expresses viral proteins in several different ways, depending of the type of virus. A detailed description of each of these processes is beyond the scope of this course. Instead, I will give one example by describing how the *human immunodeficiency virus* (HIV) infects cells.

Viral infection example: the *human immunodeficiency virus* (HIV)

HIV is in a category of viruses called **retroviruses**. When taken into the host cell, the information in the *retroviral* RNA is converted to complementary DNA. This is called **reverse transcription** and is catalyzed by a viral enzyme called ***reverse transcriptase***. The name "*reverse transcriptase*" is applied because the chemical process is the *reverse* of transcription. The newly formed DNA is inserted into the host cell's DNA, and then *transcribed* into new *retroviral* RNA and viral proteins during the host cell's normal gene expression. The *retroviral* RNA and viral proteins are ***assembled into multiple retroviruses*** and then released from the cell. This process is illustrated below.
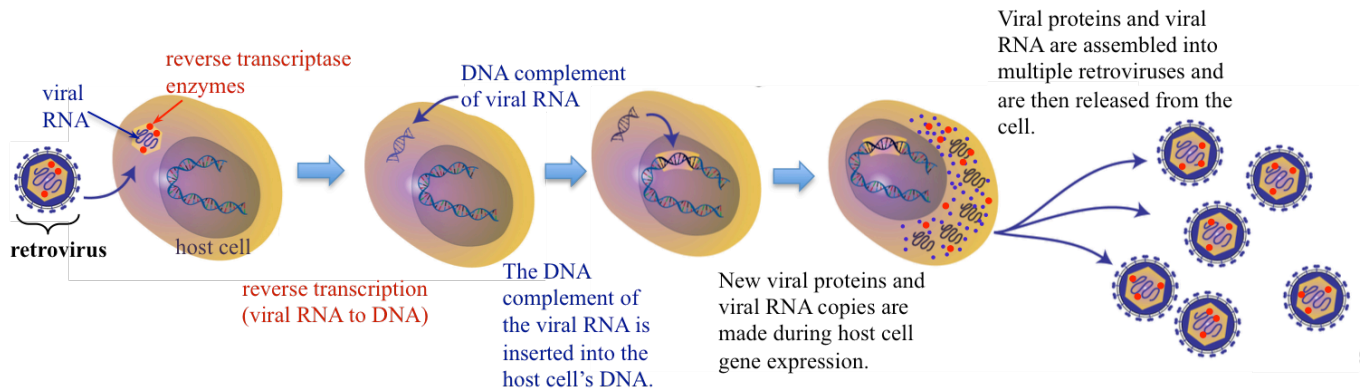
Animals are capable of producing immune responses that eliminate most viral infections. Vaccinations are effective as anti-viral agents because they allow vaccinated individuals to produce artificially acquired immune responses to many viral infections. Some viruses, such as HIV, herpes simplex virus (HSV), and hepatitis C virus (HCV), are capable of evading immune responses and therefore result in chronic (persistent or long-lasting) disease.

Understanding Check: Enzymes Involved in DNA and RNA Formation

Which enzyme (DNA polymerase, RNA polymerase, or reverse transcriptase) is involved in each of the processes below:

   a. Transcription
   b. Replication
   c. Using a DNA template to make RNA
   d. Using an RNA template to make DNA

Genetics

_____ is the study of genes, variation in genes, and heredity.

The information contained in the DNA of an organism is called its _____.

Individuals, other than identical twins, have different _____ _____ because the DNA of each person is not exactly the same as that of another person.

- Even identical twins have about *one hundred* incidents of differences in nucleotide sequences in their genome, although that is not enough to make differences in their appearances. Small differences in the appearances of identical twins are attributed to environmental, not genetic, differences.

- Examples of inherited traits in humans include eye, skin, and hair color.

- Sometimes, _____ result from an abnormal DNA sequence in a parent being passed to the next generation.

Mutations

Any permanent change in the primary structure of (sequence of nucleotide residues in) DNA is called a

_____.

- Mutations might involve the switching of one base pair for another or the addition or deletion of base pairs.

- Changes in the nucleic acid sequence of a gene (a mutation) can result in changes in the _____ _____ sequence of the protein that is expressed, and can thereby give rise to partially or completely *nonfunctional proteins*.

- A chemical or physical agent that induces mutations is called a _____.

- Errors in replication and exposure to mutagens (including x-rays, UV radiation, nuclear radiation, and chemicals) are the common causes of mutations.

- If the mutated gene results in a partially or completely nonfunctional protein that is important for an individual to function, the health of the individual may be diminished. *Some mutations result in premature death.*

Types of Mutations

Mutations that occur in multicellular organisms can be categorized as either _____ **mutations** or _____ _____ **mutations**.

Somatic mutations, also called *acquired mutations*, are mutations that occur within cell types that *are not involved in reproduction* (**somatic cells**).

- When a mutation arises in a *somatic cell*, then the mutation is limited to that cell or any of its cell-division descendants **within the organism**. Cancer is a disease that results from *somatic mutations* in genes that are responsible for cell growth or cell differentiation. Such mutations cause the formation of a mass of mutated cells (cancer cells) called a **tumor**. For example, a skin cell can acquire a mutation, very often from exposure to UV radiation, which causes it to begin to rapidly divide/replicate and form a tumor.

Germ line mutations are mutations that occur within germ line cells.

- Germ line cells are the cells that are involved in reproduction (e.g. sperm and ovarian cells).

- If a mutated germ line cell is passed to an offspring, then it results in a _____ **mutation**, which is a mutation occurring in the nuclei of *every cell of the offspring*.

- When a *constitutional mutation* causes a negative health condition, it is referred to as a _____ _____.

   - Note that mutations in germ line cells can be transmitted to offspring, whereas somatic cell mutations cannot.

Small-Scale Mutations vs. **Large-Scale Mutations**

Mutations can be classified as **small-scale** or **large-scale**, depending on the _____ *of nucleotides involved in the mutation.*

- *Small-scale mutations* involve a change in a small number of nucleotides (usually one to three nucleotides) within a single gene.

- *Large-scale mutations*, sometimes called ***chromosomal mutations***, involve changes in large sections of chromosomes.

Small-Scale Mutations:

1) **Point:** A single, incorrect nucleotide takes the place of the original nucleotide. This often happens during DNA replication.

2) **Insertions**: One or more extra nucleotides are inserted between two of the original nucleotides in a gene.

3) **Deletions**: A single nucleotide or a short sequence (usually 2 or 3 nucleotides) are removed from a gene.

Large-Scale Mutations:

Large-scale mutations involving a **single chromosome** (illustrated on the right):

1) **Deletions:** A large section of DNA within a single chromosome is removed/deleted.

2) **Duplication:** A large section of DNA within a single chromosome is duplicated and reinserted.

3) **Inversion:** A large section of DNA within a single chromosome is inverted (3' and 5' directions reversed).

large-scale mutations involving a *single* chromosome
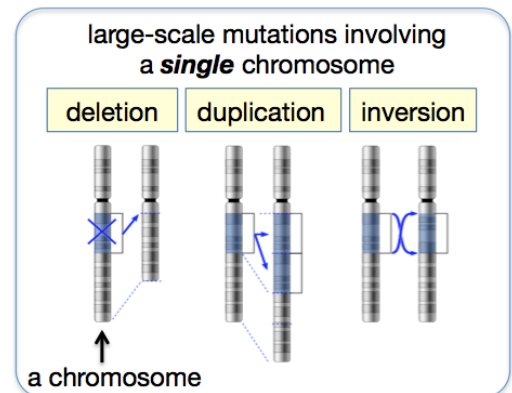
Large-scale mutations involving **two different chromosomes**:

1) **Insertion:** A large section of DNA within one chromosome is inserted into another chromosome (illustrated below, left).

2) **Translocation:** Large sections of DNA in two different chromosomes are exchanged (illustrated below, right).

large-scale mutations involving *two different* chromosomes
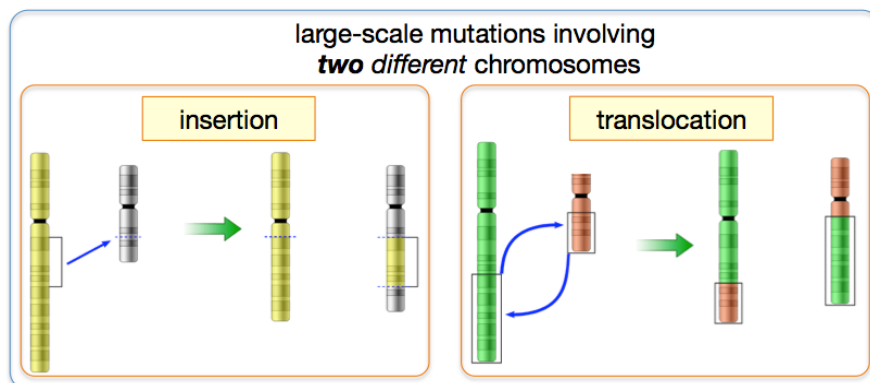
Human Genetic Diseases

The inheritance of one or more mutated genes can result in a **genetic disease**.

- Some genetic diseases involve a particular gene, others involve multiple genes.

Normally, individuals have **two copies** of each gene in the nucleus of every somatic cell in their bodies. One copy of the gene was inherited from mother, and one copy from father.

A _____ **disease** occurs when *one or both* copies *of a particular gene* contains a harmful mutation.

- **"Dominant diseases"** are monogenic diseases that occur when _____ *copies* of a gene are mutated.

- **"Recessive diseases"** are monogenic diseases that occur when _____ copy of the gene *is not* mutated *and* _____ copy *is* mutated.

   - The exceptions to these dominant/recessive disease definitions are *some genes* on the human X chromosome.

   - Example of a monogenic recessive disease: cystic fibrosis

Approximate Prevalence of Some Monogenic Diseases

monogenic disease	prevalence
familial hypercholesterolemia	1 in 500
polycystic kidney disease	1 in 1,250
Huntington's disease	1 in 15,000
sickle cell disease	1 in 625
cystic fibrosis	1 in 2,000
Tay-Sachs disease	1 in 3,000
Phenylketonuria (PKU)	1 in 12,000
glycogen storage diseases	1 in 50,000
Duchenne muscular dystrophy	1 in 7,000
hemophilia	1 in 10,000

The prevalences shown here are approximate values and can vary significantly between populations with different ancestral ethnicities as well as gender.

More than 7,000 different *monogenic diseases* have been identified. Despite this large number of diseases, monogenic diseases are quite rare. The table on the right lists some monogenic diseases and their prevalences.

A _____ **disease** occurs when *one or both* copies *of multiple, different genes* contain a harmful mutation.

- Examples: hypertension, coronary heart disease, and diabetes.

Treating Genetic Diseases: Gene Therapy

Some genetic diseases can be treated by _____ _____, which involves the delivery of functional (**un**mutated) genes to the cells of an individual who has a monogenic disease.

In some cases, the genes are introduced to the body by "infecting" the patient with inert DNA viruses that have had their genomes replaced with the gene that is to be delivered. A biological agent (a virus in this case) that is used to artificially deliver DNA to a cell is called a "**vector.**" An overview of this process is illustrated on the right.

viral vector

*un*mutated gene

*un*mutated gene

mutated gene

Nucleus

targeted cell
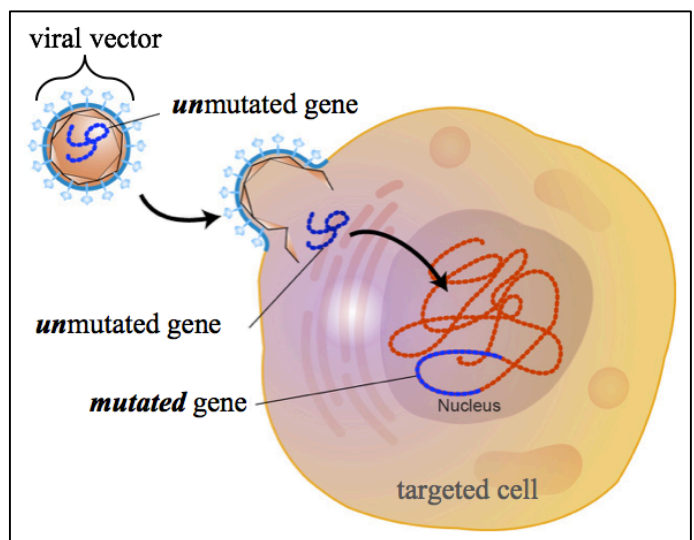
Recombinant DNA: Genetically Modified Organisms

It is possible to extract copies of a gene from one organism and then insert that gene into another organism's genome.

- This process forms "_____ **DNA**," which is *DNA made from two or more sources*.

- An organism that contains recombinant DNA is called a **genetically modified organism (_____)** or a _____.

GMO Examples:
1) Glyphosate Resistant Crops
2) Human Insulin from Bacteria
3) Measuring Gene Expression using Green Fluorescent Protein Mutants

Bioethics: Using What We Know

_____ is a term used to describe *the study of ethical issues that arise from biological technologies*.

Some of the bioethical concerns that involve human genetics include the following questions:

- What individuals or corporate entities can have access to personal genetic information?
- Is genetic information something that can be patented and owned?
- Who should be genetically tested and at what age should genetic testing be performed?
- Should we re-engineer the genes we pass on to our children?

These are complicated questions. The best solutions for complicated questions are usually not found by simple yes/no, or "one-size-fits-all" approaches. Furthermore, new research and emerging technologies make it necessary to frequently reconsider prior policies. Complicated questions often require complicated solutions. In order to reasonably address these bioethical questions, it is necessary to have an understanding of the fundaments of genetics and nucleic acid chemistry.   It was my intention to provide you with such an understanding in this chapter.

Chapter 15 Lecture Notes: Metabolism

Educational Goals

1. Define the terms **metabolism**, **metabolic pathway**, **catabolism**, and **anabolism**.

2. Understand how **ATP** is formed from **ADP** and inorganic phosphate (**P$_i$**), and vice versa.

3. Understand how **Coenzyme-A** is used to *transfer* **acyl groups**.

4. Understand the roles of the **NAD$^+$/NADH** and **FAD/FADH$_2$** coenzymes in the *transfer of electrons*. Identify the **oxidized** and **reduced form** of each of these pairs.

5. Understand the differences between **linear**, **circular**, and **spiral** *metabolic pathways* and give an example of each.

6. Name the products formed during the **digestion** of *polysaccharides*, *triglycerides*, and *proteins*, and know the part(s) of the digestive track where each occurs.

7. Identify the initial reactant and final products of **glycolysis**, and understand how this pathway is controlled.

8. Understand and compare **glycolysis** and **gluconeogenesis** pathways.

9. Know the *fate of pyruvate* under **aerobic** and **anaerobic** conditions.

10. Define the terms *hyperglycemic and hypoglycemic*.

11. Understand how the body controls **blood glucose concentration** by the release of **insulin** or **glucagon** into the bloodstream.

12. Understand and compare **glycogenesis** and **glycogenolysis**. Understand how these processes are involved in maintaining normal blood glucose concentration.

13. Understand and compare **type I**, **type II**, and **gestational diabetes**.

14. Identify the initial reactant and final products of the **citric acid cycle**; understand how this pathway is controlled.

15. Understand how the *oxidation of coenzymes* during **oxidative phosphorylation** is used to produce **ATP**.

16. Compare the **malate-aspartate shuttle** and the **glycerol 3-phosphate shuttle** and understand their significance in affecting the amount of **ATP** that can be produced from glucose.

17. Predict how many **ATP** are formed when **acetyl-CoA** undergoes *stages* **3** and **4** of catabolism.

18. Describe the catabolism of **triglycerides**, the **β-oxidation spiral**, and how *β-oxidation* differs from **fatty acid anabolism** (biosynthesis).

19. Given the structure of a **fatty acid**, predict how many **ATP** are formed when it undergoes the ***β-oxidation spiral***.

20. Understand and compare **lipolysis** and **fatty acid synthesis**.

21. Explain the biological origins of **ketosis** and **ketoacidosis**.

22. Understand how **transamination** and **oxidative deamination** are involved in the **catabolism of amino acids**.

23. Given the structure of an **amino acid** and **α-ketoglutarate**, predict the products of a **transamination reaction**.

24. Explain how *quaternary ammonium groups* (-NH$_3^+$) are removed from amino acids *and* eliminated from the body.

An Overview of Metabolism

_____ is defined as *the entire set of life-sustaining chemical reactions that occur in organisms.*

- These reactions number in the thousands and include reactions such as those responsible for getting energy from food, processing and removal of waste, building up muscles, growth, photosynthesis in plants, cell division, and reproduction.

The entire set of metabolic reactions is organized into smaller sets of sequential reactions called **metabolic** _____.

The species produced in the various reactions of a metabolic pathway are sometimes referred to as

_____.

Many of the reactions in metabolic pathways require enzymes; therefore organisms can control (accelerate or suppress) metabolic pathways, according to their current needs, by *upregulating*, *downregulating*, *inhibiting*, or *activating* one or more of the enzymes involved in the pathway.

Metabolic pathways can usually be classified as **catabolic** (catabolism) or **anabolic** (anabolism).

- ***Catabolic pathways*** involve the _____ of larger organic compounds into smaller compounds.

- ***Anabolic pathways*** involve _____ _____ of larger organic compounds from smaller ones.
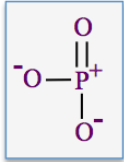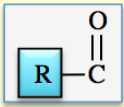
In this chapter, you will learn about the pathways that are involved in the metabolism of carbohydrates, proteins, and fats.

- An ultimate goal of these reactions is to convert the chemical potential energy contained in food into chemical potential energy in the form of _____.

The Coenzymes Involved in Metabolism

A *coenzyme* is a species that must bind to an enzyme in order for the enzyme to function.

- In most cases, a coenzyme is actually one of the *substrates* (reactants) in the catalyzed reaction.
- The reason that certain *substrates* are ***also*** referred to as *coenzymes* is that these *substrates* are ***common substrates in many different enzymatic reactions*** in which they ***donate electrons, atoms, or groups of atoms*** to other substrates, ***or accept electrons***, ***atoms or groups of atoms*** from other substrates.
- The five group-transfer coenzymes that are central to the metabolism of food, along with the species each transfers are listed in the table on the right.

Coenzyme	Species that is Transferred
ADP/ATP	phosphoryl group =
NAD+/NADH	hydride ion (H:$^-$) **or** electrons
FAD/FADH$_2$	hydride ion (H:$^-$) **or** electrons
coenzyme A	acyl group =
coenzyme Q	hydride ion (H:$^-$) **or** electrons

2

Phosphoryl Group-Transfer Coenzymes: ATP and ADP

ATP and **ADP** are classified as **coenzymes** because they are involved in the *transfer* of _____ groups (PO₃⁻) *in many different enzymatically catalyzed reactions*.

- When a compound gains/accepts a *phosphoryl group* in a reaction, we say that the compound became "**phosphorylated**."

- When a compound loses/donates a *phosphoryl group* in a reaction, we say that it was "**dephosphorylated**."

ATP and **ADP** are interconverted by the transfer of a *phosphoryl group*, as shown below.
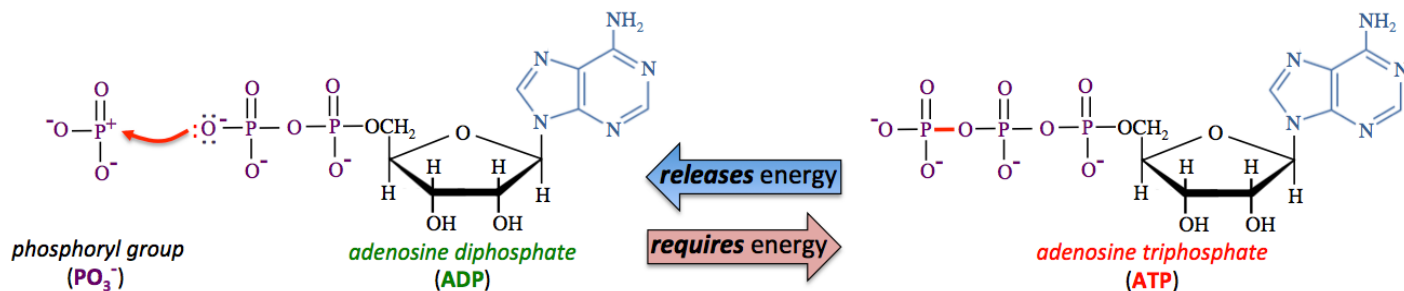
- Adding a *phosphoryl group* to **ADP** _____ energy.

- Removing a *phosphoryl group* from **ATP** _____ energy.

ATP is often formed by the reaction of **ADP** with *hydrogen phosphate* (HPO₄²⁻) and an **H⁺** ion, as shown below.
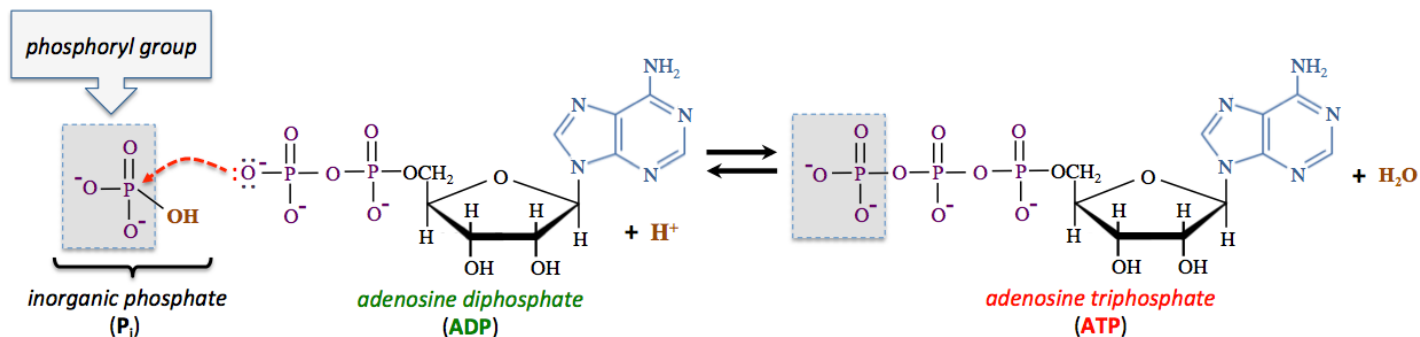
Biological literature refers to *hydrogen phosphate* as "_____ phosphate" (abbreviated as Pᵢ).

Another way that organisms convert **ADP** to **ATP** is by the reaction of **ADP** with an _____ molecule *that contains a phosphoryl group*. In this case, a *phosphoryl group* is transferred *from* the organic molecule *to* **ADP**, as shown in the chemical equation below.
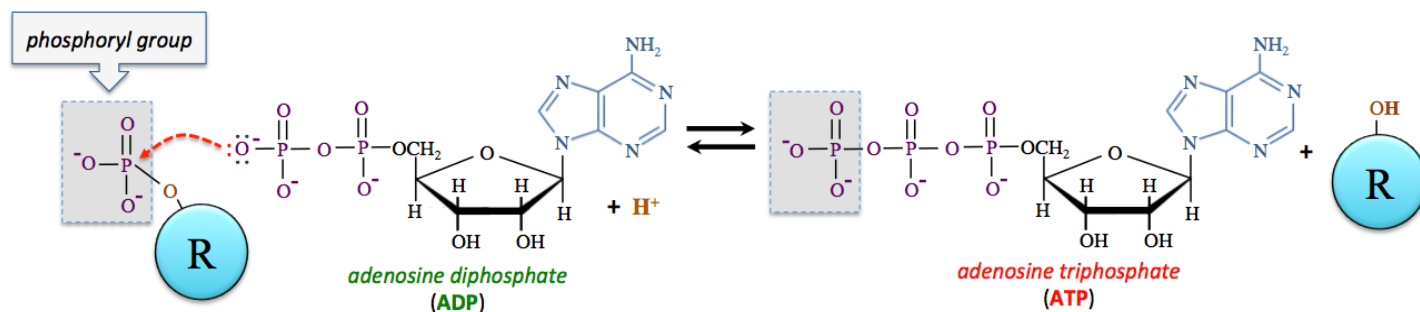
You will see hydrogen ions (**H⁺**) as reactants *in many of the reactions in this chapter*. Because these reactions occur in aqueous solutions, **H⁺** is *readily available* from **H₂O**, and can also come from **H₃O⁺** or the *acid forms* of other species that are present.

Energy is *released* from **ATP** when it is converted to **ADP**. This energy is used by organisms to drive energy-requiring reactions or physical processes that would otherwise not occur spontaneously. *One* way that energy can be released from **ATP** is by reacting it with H_2O to *form* ADP, *inorganic phosphate*, and an H^+ ion. Although this reaction is spontaneous (ΔG is negative), the reaction rate is quite slow, therefore organisms employ enzymes in order for the reaction to proceed at a useful rate. The chemical equation for this reaction is shown below.

ΔG = -7300 Joules per mole of **ATP**
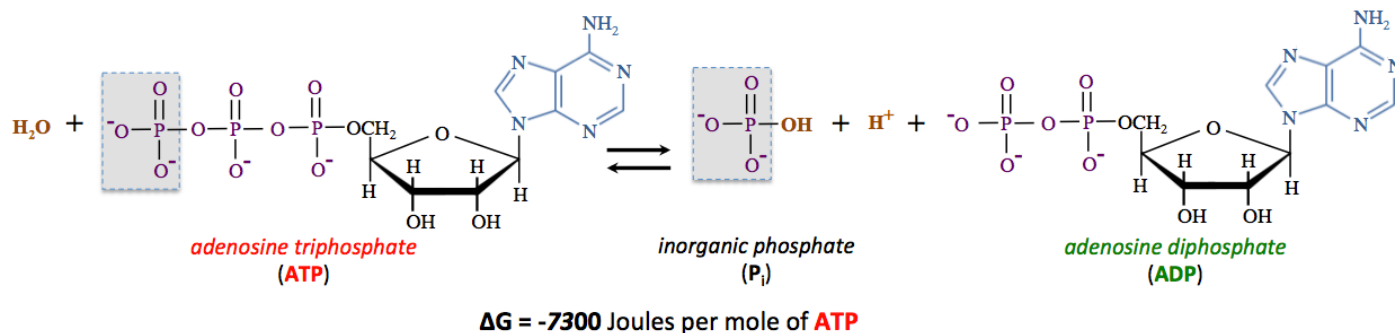
Note that H^+ is *produced* in this reaction. You will see H^+ ions as products *in many of the reactions in this chapter*. Keep in mind that the H^+ ions that are produced in aqueous solutions do not remain solvated as *isolated ions*; they quickly react with water to form H_3O^+. Alternatively, H^+ can react with OH^- or the *base form* of another species that is present.

Another way that organisms extract energy from **ATP** is to "energize" organic compounds by transferring a phosphoryl group *directly* to the compound. In this reaction, **ATP** is *dephosphorylated* and an organic compound is *phosphorylated*, as shown in the reaction below:

$$\textbf{ATP} + \text{organic compound} \rightleftarrows \textbf{ADP} + \text{phosphorylated organic compound} + \textbf{H}^+$$
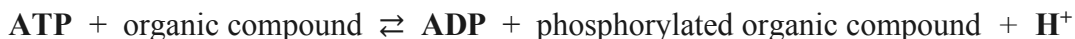
*Chemical potential energy **released** by the conversion of **ATP** to **ADP** is transferred to the phosphorylated organic product.*

- It is for this reason that we say "the organic compound is energized" in the reaction.

Example:
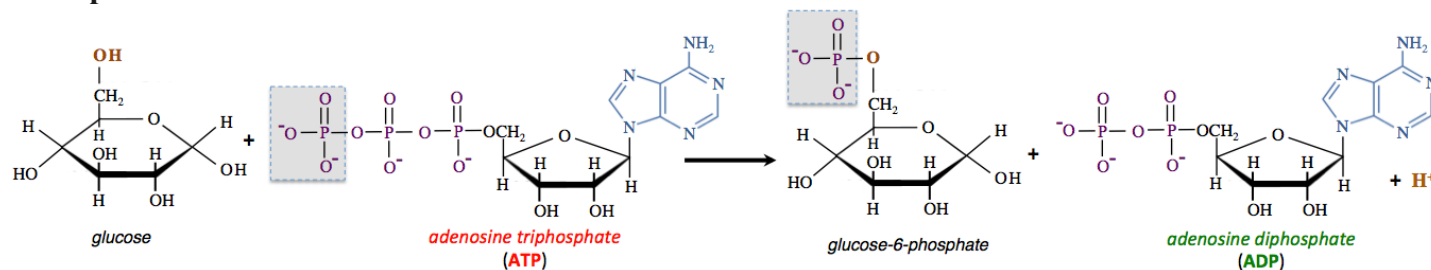
In this particular reaction, the reverse reaction occurs so slowly that it is negligible.

- In such cases, we refer to the reaction as an "_____ **reaction**."

When writing a chemical equation for an irreversible reaction, only a forward (left to right) arrow is used, as shown *above*.

Biochemical literature often uses an *alternative* chemical equation format. For example, the reaction shown above is often written as:

4
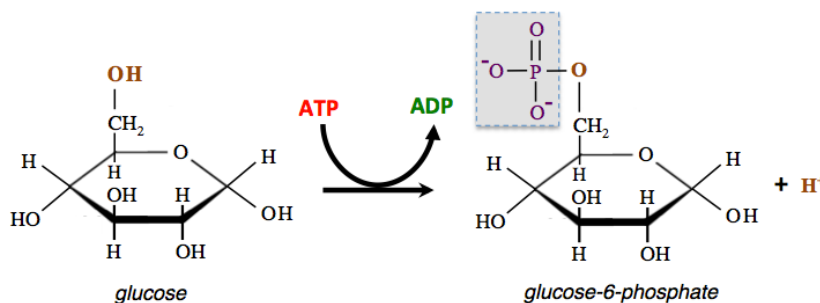
Electron-Transfer Coenzymes and Their Role as Oxidizing and Reducing Agents

Oxidation-reduction reactions, which involve the transfer of one or more electrons, are quite common in organisms.

Many of these reactions involve the transfer of an electron by way of the **hydride ion** ($H:^-$).

A **reduction** occurs when a _____ ion forms a bond with an organic compound.

- The transfer of a hydride ion is a reduction because of hydride's "extra" electron.

  - For example, aldehydes or ketones are **reduced** when a **hydride ion** forms a bond with them.
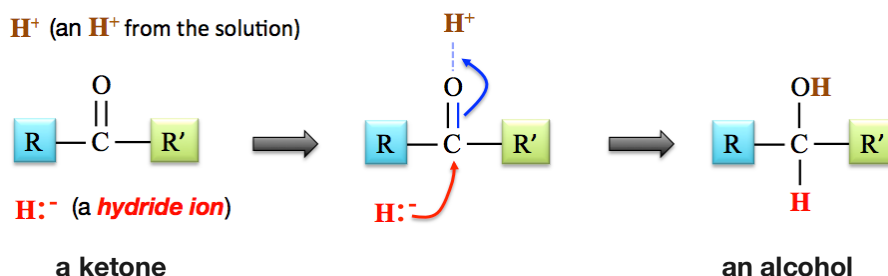
An _____ occurs when a *hydride ion* ($H:^-$) and an H^+ ion are *removed* from an organic compound.

- For example, 2° alcohols can be **oxidized** to ketones, as shown in the chemical equation below.
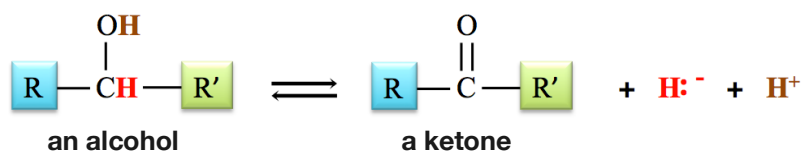
- This is considered an oxidation because the hydride ion carries away the "extra" electron.

Nicotinamide <u>a</u>denine <u>d</u>inucleotide (**NAD$^+$**) and <u>f</u>lavin <u>a</u>denine <u>d</u>inucleotide (**FAD**) are classified as **coenzymes** because they are common substrates, involved in the transfer of _____, *in many different enzymatically catalyzed reactions*.
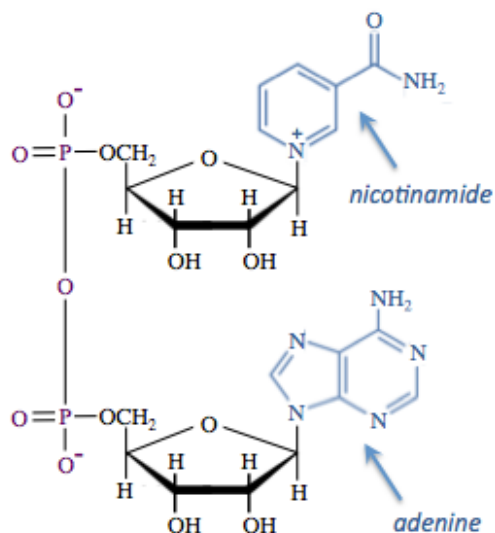
Nicotinamide Adenine Dinucleotide (NAD$^+$)

The structural formula of **NAD$^+$** is shown on the left. **NAD$^+$** contains *two* nucleotide residues. One of the nucleotides has an *adenine* base, and the other contains a *nicotinamide* base.

5

reduction
(requires energy)

oxidation
(releases energy)

oxidized form of the coenzyme
(**NAD⁺**)

reduced form of the coenzyme
(**NADH**)
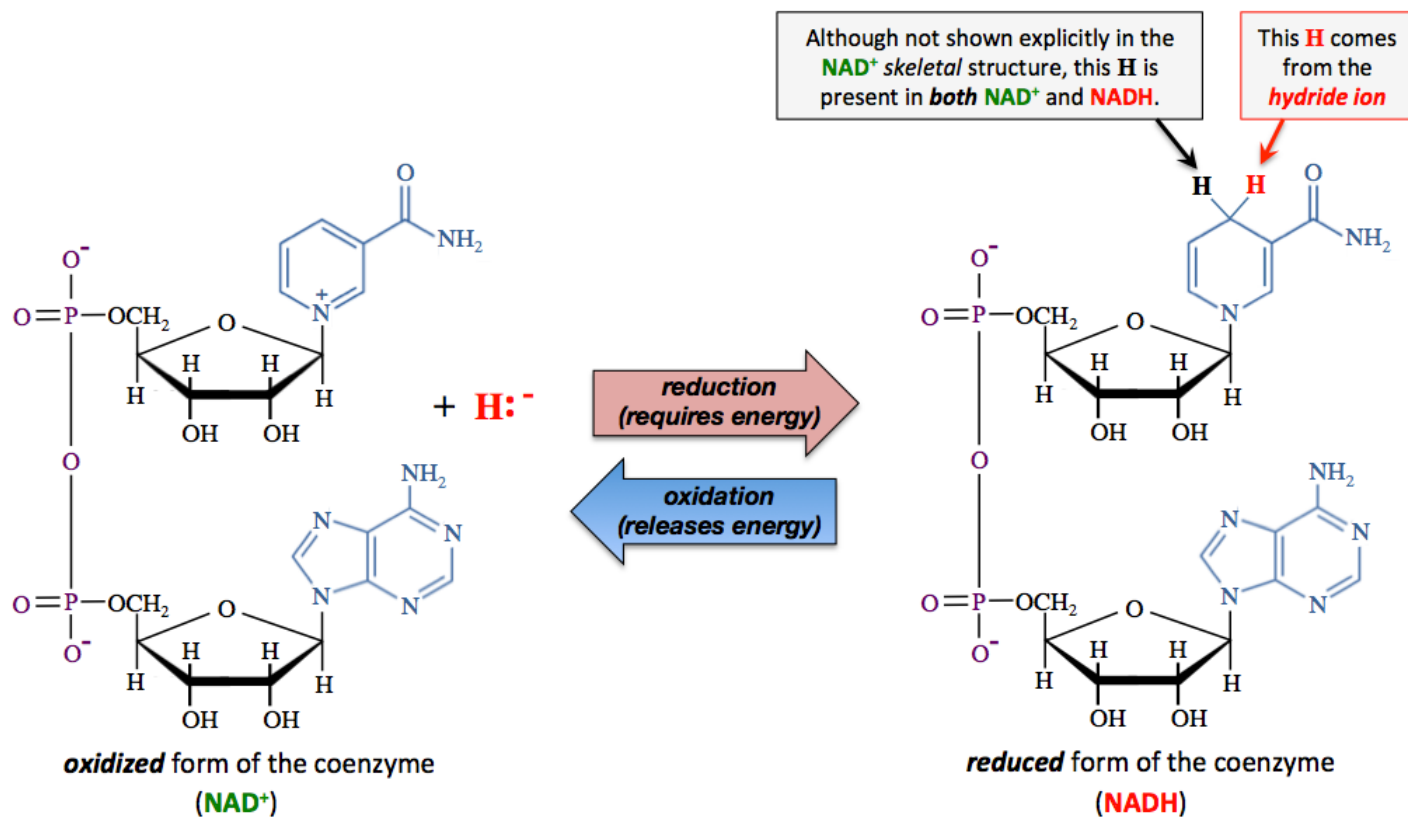
When **NAD⁺** *accepts* a hydride ion from another species, it is *reduced* to **NADH**.

- It is for this reason that **NADH** is referred to as a *reduced form of the coenzyme* or a "_____ _____."

- The reduction of **NAD⁺** *requires* energy.

When **NADH** *donates* a hydride ion (to another species) it is *oxidized* to **NAD⁺**.

- **NAD⁺** is referred to as the *oxidized form of the coenzyme* or an "_____ _____."

- Oxidation of **NADH** *releases* energy.

Example: The oxidation of an organic compound using **NAD⁺** as the *oxidizing agent:*
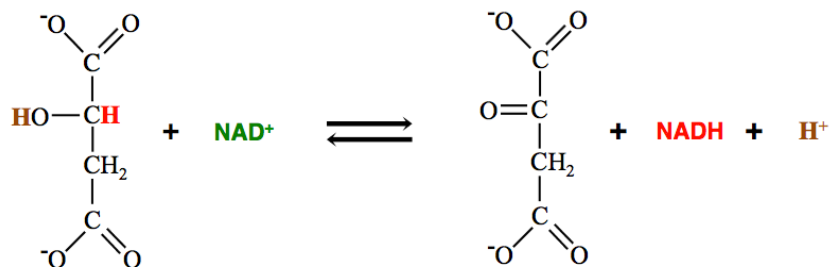
- In this reaction, *malate* is oxidized and **NAD⁺** is reduced.

Flavin Adenine Dinucleotide (FAD)

FAD
oxidized form of the coenzyme

FADH$_2$
reduced form of the coenzyme
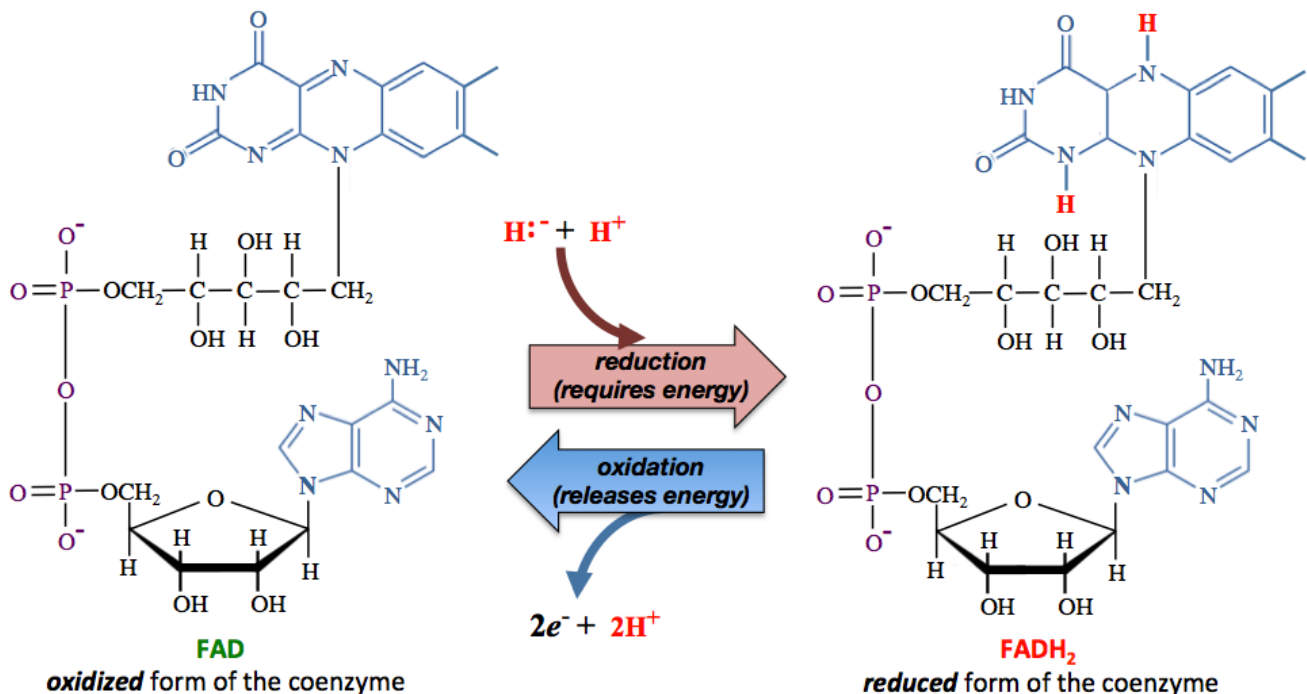
When **FAD** *accepts* a hydride ion from another species (and an **H$^+$** from solution), it is *reduced* to **FADH$_2$**.

- The reduction of **FAD** *requires* energy.

FADH$_2$ is **oxidized** to **FAD** by *donating two* electrons (and two **H$^+$** ions) to other species.

- The oxidation of **FADH$_2$** *releases* energy.

Much like **NAD$^+$/NADH** and **FAD/FADH$_2$**, **Coenzyme Q** (*not shown*), transfers electrons and hydrogen ions when it cycles between its oxidized and reduced forms.

Acyl Group-Transfer Coenzyme: Coenzyme A

Coenzyme A (H-CoA) is used in many metabolic reactions. Its structural formula is shown below.

coenzyme A (H-CoA)

(CoA)
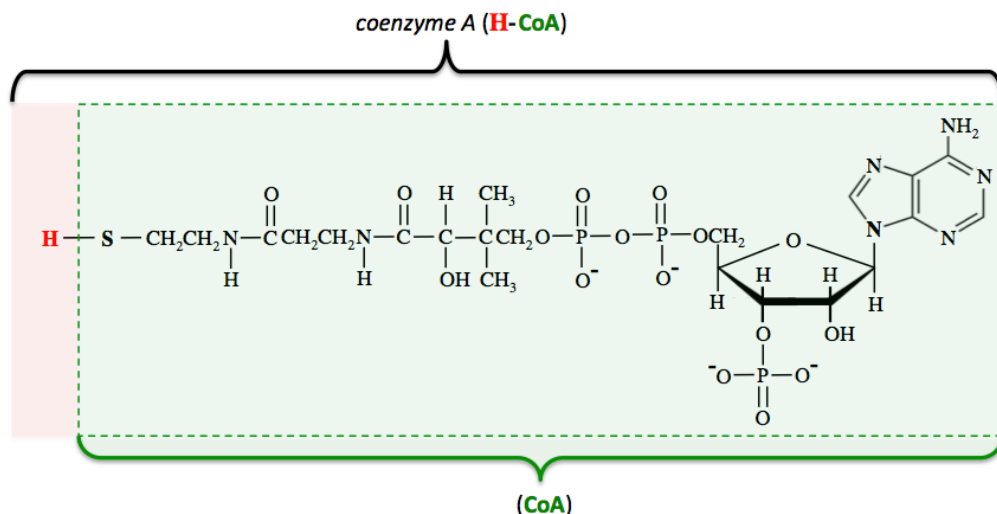
Coenzyme A is classified as a **coenzyme** because it is involved in the *transfer* of an _____ *group* in *many different enzymatically catalyzed reactions*.

- An *acyl group* consists of a carbonyl group bonded to an organic group (**R**), as shown *on the right*.

- When *coenzyme A* (**H-CoA**) accepts an **acyl group**, the *acyl group* replaces the *left-most* hydrogen in the *coenzyme A* structure.
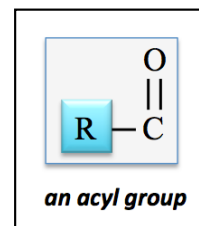
an acyl group

An **acyl group** that is central to the metabolism of food is the _____ **group**.

- *Acetyl groups* are donated and accepted by *coenzyme A*, as shown below:
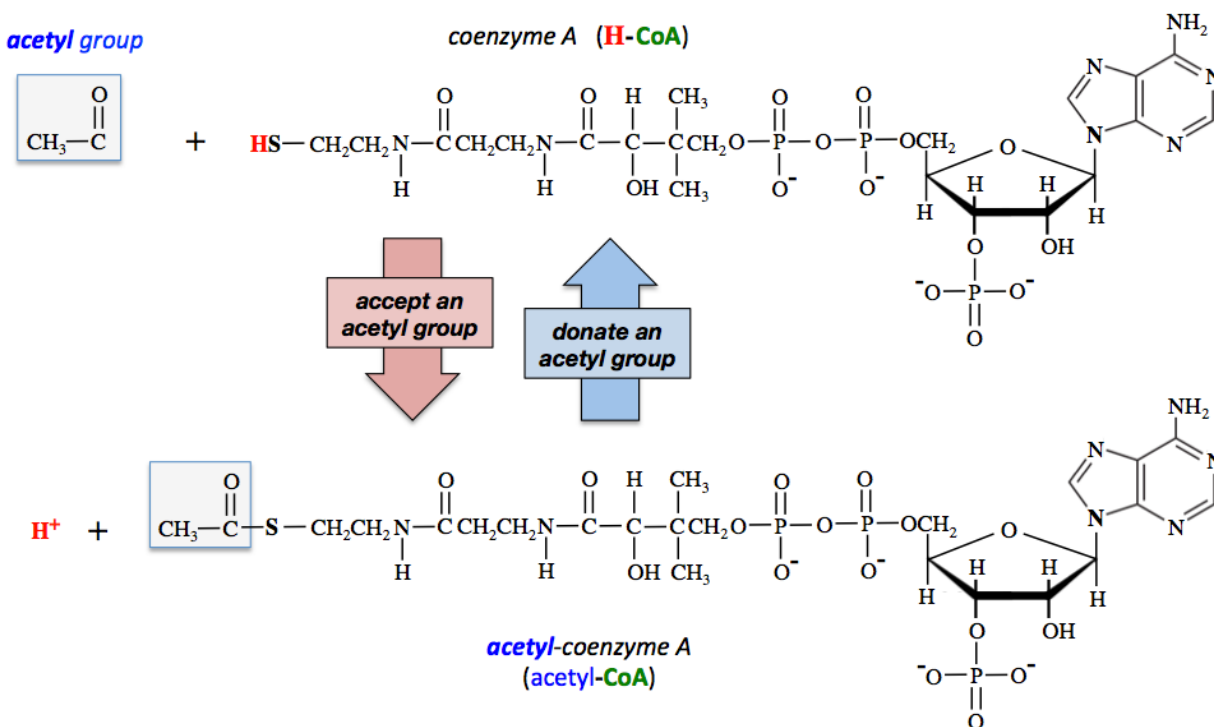
Carbohydrate Metabolism

The energy that is contained in food can be traced back to the _____.

- Energy from sunlight is captured by plants during *photosynthesis* as they convert CO_2 and H_2O into *glucose* and O_2.

- Without energy from sunlight, the reaction of CO_2 with H_2O to produce glucose and O_2 is not spontaneous.

- The input of energy from sunlight provides the energy that is required to convert CO_2 and H_2O to glucose and O_2.
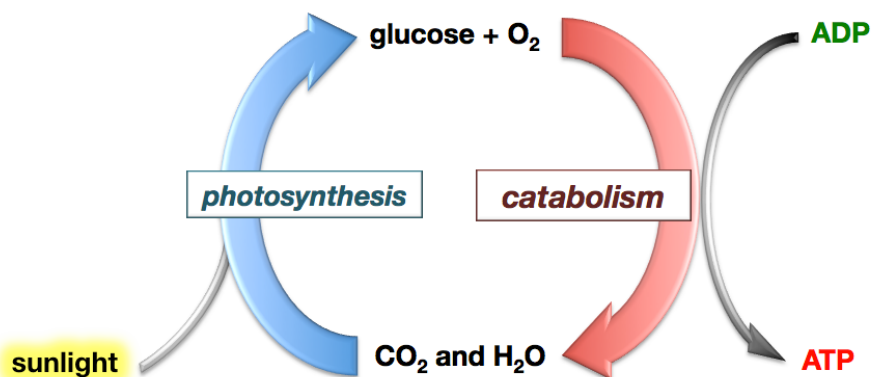
In photosynthesis, energy from the sun's light does not vanish; it is converted to
_____ _____ _____ within _____.

- Plants store excess *glucose* as **starch**.

Organisms, including humans, use a series of **catabolic** chemical reactions to *slowly* _____
carbohydrates and other food, eventually converting it back to CO_2 and H_2O.

Energy that is released in these oxidations is converted to chemical potential energy within _____.

All three classes of macronutrients in food, carbohydrates, triglycerides (fats), and proteins, are
catabolized in *four stages*:

Stage 1: _____

Stage 2: _____

Stage 3: _____

Stage 4: _____

Stage 1: Digestion of Carbohydrates

Digestion is the process in which the body breaks
down carbohydrate, protein, and triglyceride
polymers into their _____ residues.

- For example, carbohydrate polymers are
  converted to monosaccharides.

Digestion occurs in the **digestive system**.

The *digestive system*, sometimes referred to as
the **digestive track** or **gastrointestinal (GI)
track**, includes the organs that are responsible
for digesting food and eliminating the
*un*digestible components of food. The major
organs of the human digestive system are shown
on the right.

Major Organs of the Human Digestive System
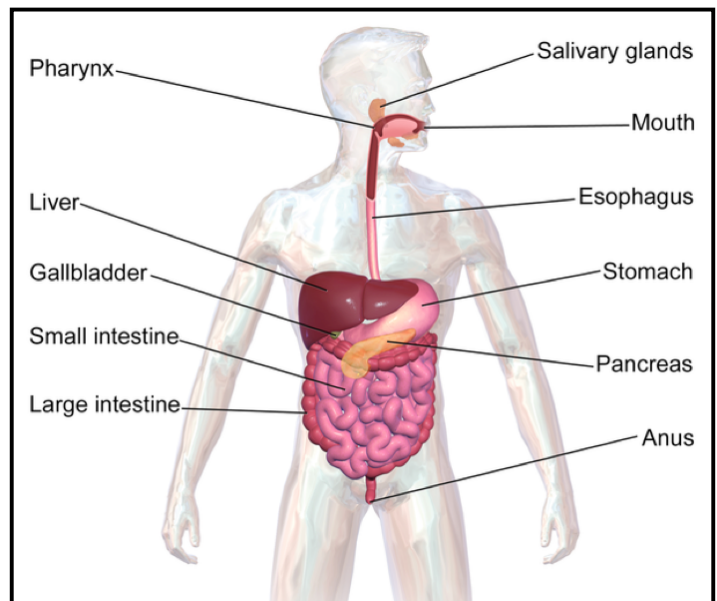
Image Source: Wikimedia Commons, Author: Blausen.com staff.
"Blausen gallery 2014". *Wikiversity Journal of Medicine*.
DOI:10.15347/wjm/2014.010. ISSN 20018762. CC-BY-SA,
https://creativecommons.org/licenses/by-sa/4.0/deed.en

During the digestion of carbohydrate polymers, most oligosaccharides (2-10 monosaccharide residues)
and polysaccharides (> 10 monosaccharide residues) can be broken down to _____.

- These reactions are catalyzed by _____ _____.

Approximately 50% of our dietary carbohydrates are in the form of **starch**.

- Starch has two components, amylose and amylopectin, both of which are composed entirely of
  _____ residues.

Digestion of amylose and amylopectin (starch) begins in the _____.

Saliva contains _____ _____ *enzymes*, which catalyze the hydrolysis of some of the **α-(1→4)** glycosidic bonds in amylose and amylopectin.

In the hydrolysis of carbohydrates, water molecules are used to lyse (break) _____ *bonds*.
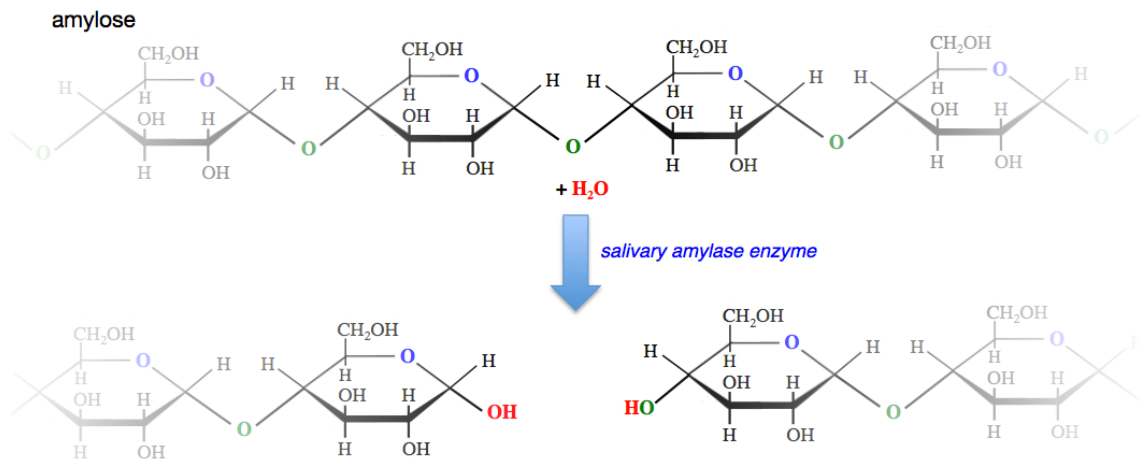
amylose

An Illustrative Overview of the Digestion of Carbohydrates
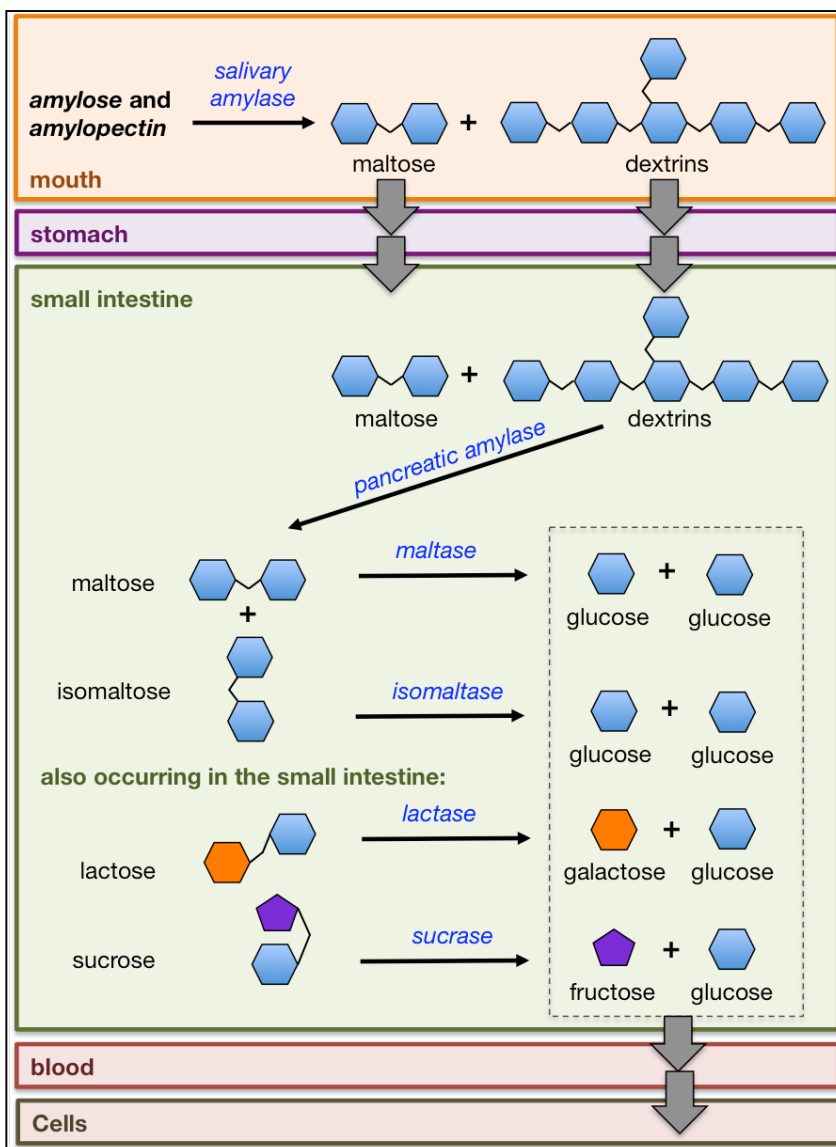
Salivary amylase catalyzes the hydrolysis of amylose and amylopectin to form *maltose* (an **α-(1→4)** glucose-glucose disaccharide) and small oligosaccharides called **dextrins**.

Dextrins are oligosaccharides that generally contain between *three* and *eight* glucose residues.

The maltose, dextrins, and other non-starch dietary carbohydrates then pass through the stomach, where carbohydrate digestion temporarily stops because the *salivary amylase* is denatured by the stomach's low pH (very acidic) environment.

Digestion continues in the small intestine with the help of more digestive enzymes.

Pancreatic amylase catalyzes the hydrolysis of *dextrins* to form *maltose* and *isomaltose*. *Isomaltose* is an **α-(1→6)** glucose-glucose disaccharide that comes from the branching points in amylopectin.

Maltase and *isomaltase* enzymes catalyze the hydrolysis of maltose and isomaltose (respectively) into glucose.

10

The **non starch** dietary carbohydrates, *lactose* and *sucrose,* are converted to monosaccharides with the help of *lactase* and *sucrase* enzymes, respectively.

- Lactose is hydrolyzed to galactose and glucose.
- Sucrose is hydrolyzed to fructose and glucose.

It is critical that oligosaccharides and polysaccharides be converted to monosaccharides in order for the sugars to pass through the intestine wall and into the bloodstream so that they are available to cells throughout the body.

Monosaccharides are transported into the cells by passive diffusion through transmembrane proteins.

Not all dietary carbohydrates can be digested.

- For example, cellulose cannot be digested because humans do not have a dietary enzyme capable of hydrolyzing **β-(1→4)** glucose-glucose glycosidic bonds. Cellulose cannot pass through the small intestine and therefore passes through the digestive track until it is excreted in feces.

Stage 2: Acetyl-Coenzyme A Production

When glucose enters a cell, it can then undergo **stages 2**, **3**, and **4** of catabolism.

In **stage 2** of carbohydrate catabolism, ***glucose*** is converted into **acetyl-coenzyme A**, CO_2, and H_2O.

This process begins with a *catabolic pathway* called _____.

Glycolysis is a series of _____ sequential reactions that ultimately converts one glucose molecule to two pyruvate ions and two H_2O molecules.

NOTE: I want to minimize any possible student anxiety by informing you that is not my intention for you to memorize these reactions, the names of the intermediates, or the names of the enzymes that are involved.

The **reactions of glycolysis**:

11

fructose 6-phosphate

Reaction 3 — *phosphofructokinase*

ATP → ADP

fructose 1,6-biphosphate + H⁺

Reaction 4 — *aldolase*

dihydroxyacetone phosphate + glyceraldehyde 3-phosphate

Reaction 5 — *triose phosphate isomerase*

glyceraldehyde 3-phosphate

Note that after **reaction 5**, glucose has been converted into *two* **glyceraldehyde 3-phosphate** ions.
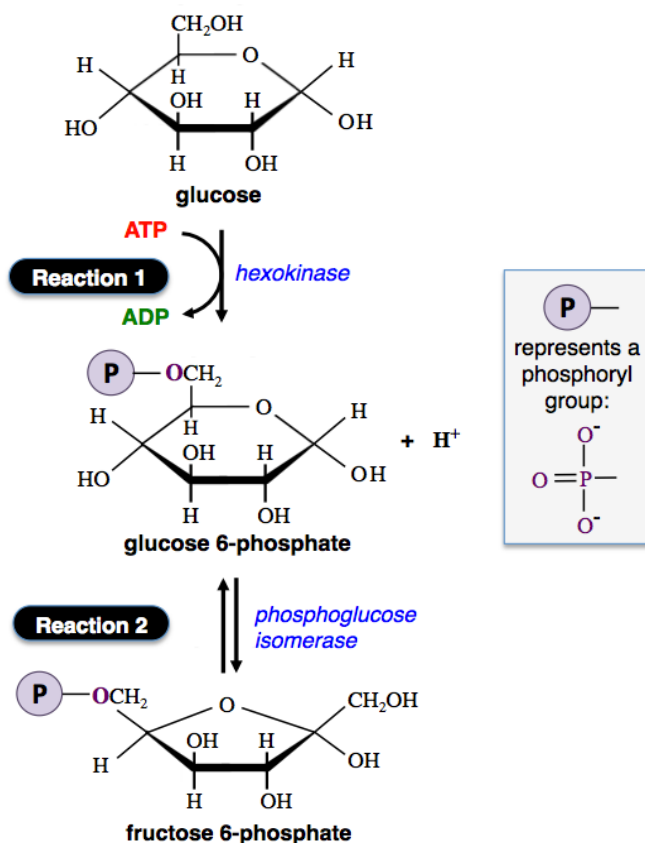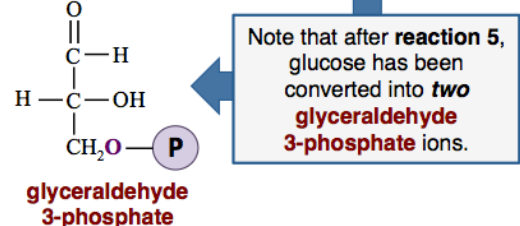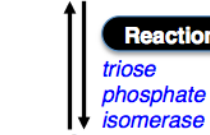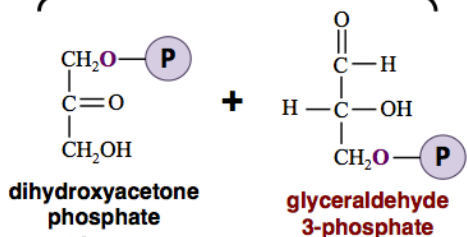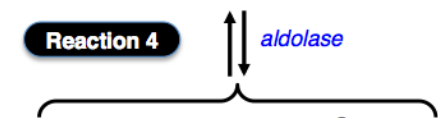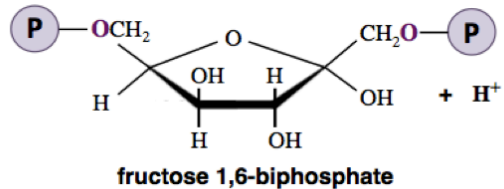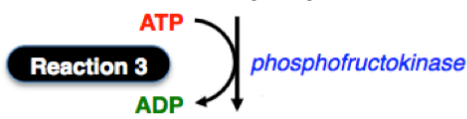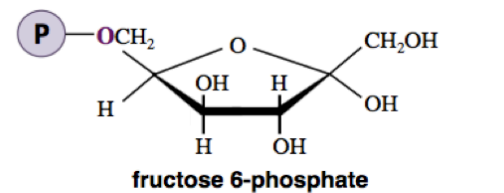
Notice that *one glyceraldehyde 3-phosphate* is produced in **reaction 4** and a second *glyceraldehyde 3-phosphate* is produced in **reaction 5**. Therefore, each of the *subsequent* reactions in the pathway **will occur twice for each molecule of glucose that undergoes glycolysis**.

It is for this reason the reactants and products in the chemical equations that follow have a stoichiometric coefficient of "**2**."

2 glyceraldehyde 3-phosphate

2 NAD⁺ + 2 Pᵢ

Reaction 6 — *glyceraldehyde 3-phosphate dehydrogenase*

2 NADH

2 [1,3-biphosphoglycerate] + 2 H⁺

1,3-biphosphoglycerate
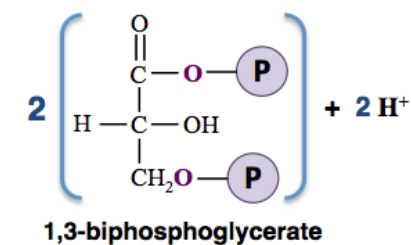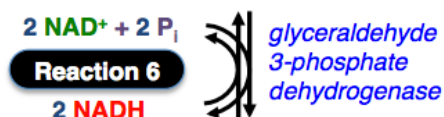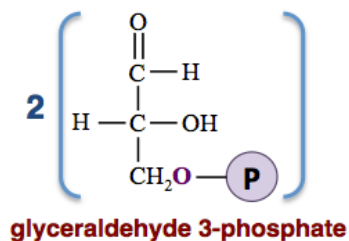
Reaction 6) In this reaction, *glyceraldehyde 3-phosphate* is *oxidized*. *An oxidation cannot occur without a reduction.* In this case, **NAD⁺** is *reduced* to **NADH**. This occurs when a hydride ion (**H:⁻**) is transferred from glyceraldehyde 3-phosphate's carbonyl carbon to **NAD⁺**. The reduction of **NAD⁺** to **NADH** requires energy, that energy comes from glyceraldehyde 3-phosphate.

The energy that is acquired by **NADH** can later be used to convert **ADP** to **ATP**.

- You will learn how that happens when I discuss **stage 4** of metabolism.
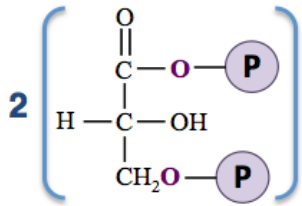
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1,3-biphosphoglycerate

$$2\begin{bmatrix} O \\ \| \\ C-O-\text{P} \\ | \\ H-C-OH \\ | \\ CH_2O-\text{P} \end{bmatrix}$$

1,3-biphosphoglycerate

Reaction 7
2 ADP
2 ATP
phosphoglycerate kinase

$$2\begin{bmatrix} O \\ \| \\ C-O^- \\ | \\ H-C-OH \\ | \\ CH_2O-\text{P} \end{bmatrix}$$

3-phosphoglycerate

Reaction 8
phosphoglycerate mutase

$$2\begin{bmatrix} O \\ \| \\ C-O^- \\ | \\ H-C-O-\text{P} \\ | \\ CH_2OH \end{bmatrix}$$

2-phosphoglycerate

Reaction 9
enolase
2 H_2O

$$2\begin{bmatrix} O \\ \| \\ C-O^- \\ | \\ C-O-\text{P} \\ \| \\ CH_2 \end{bmatrix}$$

phosphoenolpyruvate

Reaction 10
2 ADP + 2 H^+
2 ATP
pyruvate kinase

$$2\begin{bmatrix} O \\ \| \\ C-O^- \\ | \\ C=O \\ | \\ CH_3 \end{bmatrix}$$
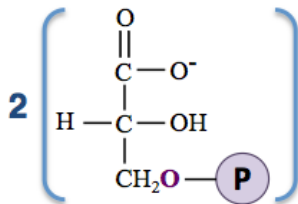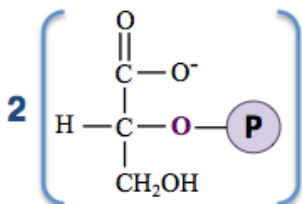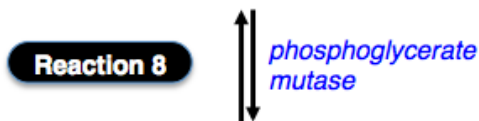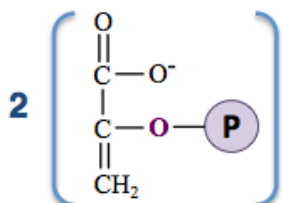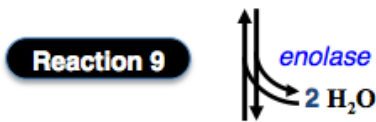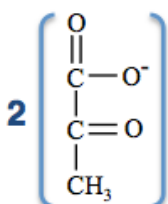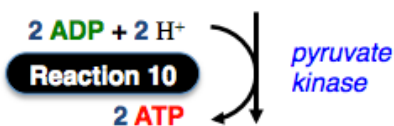
pyruvate

The reactions of glycolysis result in a net gain of *two* **ATP** and *two* **NADH**.

When there is a sufficiently high concentration of **ATP**, pyruvate, or other pathway products, then the rate of glycolysis can be slowed down. If the **ATP** concentration becomes low, then glycolysis can be accelerated. The rate of the glycolysis pathway is controlled by enzyme inhibitors and enzyme activators of the enzymes involved in the **irreversible reactions** (**1**, **3**, and **10**).

- For example, **ATP** and phosphoenol pyruvate (the product of **reaction 9**) act as inhibitors of the *phosphofructokinase* enzyme that catalyzes **reaction 3**.

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Summary of Glycolysis

The chemical equation for the *overall* glycolysis pathway is:

$$\textbf{glucose} + 2\ \textbf{ADP} + 2\ \textbf{P}_i + 2\ \textbf{NAD}^+ \rightleftharpoons 2\ \textbf{pyruvate ions} + 2\ \textbf{ATP} + 2\ \textbf{NADH} + 2\ \textbf{H}_2\textbf{O} + 2\ \textbf{H}^+$$

The **ten reactions** of glycolysis result in a net gain of _____ **ATP** and _____ **NADH**.

Not *all* of the energy from **glucose** is transferred to the **ATP** and **NADH** formed in glycolysis.

- Some energy was lost as *heat* during the reactions, however, **most** of glucose's chemical potential energy remains in the two *pyruvate ions*.

Glycolysis is characterized as a _____ *metabolic pathway*.

- A *linear metabolic pathway* is a series of reactions that are not repeated.

> Understanding Check:
> a. How many **ATP** are produced when *six* glucose molecules undergo glycolysis?
> b. How many **NADH** are produced when *six* glucose molecules undergo glycolysis?

Before we take a look at the *fate of the pyruvate* that is produced in glycolysis, let's consider how *non glucose monosaccharides* are metabolized.

The Entry of Non Glucose Monosaccharides into Glycolysis

Although *glucose* is the major product of *carbohydrate digestion*, *it is not the only monosaccharide that is produced*.

Other monosaccharides can be catabolized when they are *converted to* _____ *in the glycolysis pathway*.

- For example, fructose, galactose, and mannose monosaccharides are produced in carbohydrate digestion and can be converted to the glycolysis intermediates as shown on the right.

glucose
Reaction 1
glucose 6-phosphate ← galactose
Reaction 2
fructose 6-phosphate ← mannose
fructose →
Reaction 3
fructose 1,6-biphosphate
Reaction 4
dihydroxyacetone phosphate + glyceraldehyde 3-phosphate
Reaction 5
glyceraldehyde 3-phosphate
Reaction 6
1,3-biphosphoglycerate
Reaction 7
3-phosphoglycerate
Reaction 8
2-phosphoglycerate
Reaction 9
phosphoenolpyruvate
Reaction 10
pyruvate

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The Fate of Pyruvate

The fate of the pyruvate that is produced by *aerobic organisms* (organisms that require O_2 to grow), such as humans and most other organisms, *depends on the availability of _____ in cells*.

During strenuous physical activity, the oxygen in muscle cells becomes depleted (**anaerobic condition**).

- When this occurs, the *pyruvate* that is made in glycolysis remains in the cytoplasm and is converted (***reduced***) to _____, as shown in the reaction below.
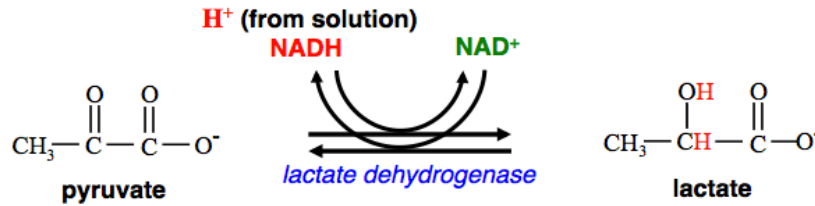
The presence of lactate in a muscle causes the muscle to tire and feel sore.

Lactate is released by muscle cells into the circulatory system and then taken up by _____ cells. **In the liver, lactate can be cycled *back to pyruvate*.**

After lactate is transformed back to pyruvate, it can be converted to glucose and stored for future use.
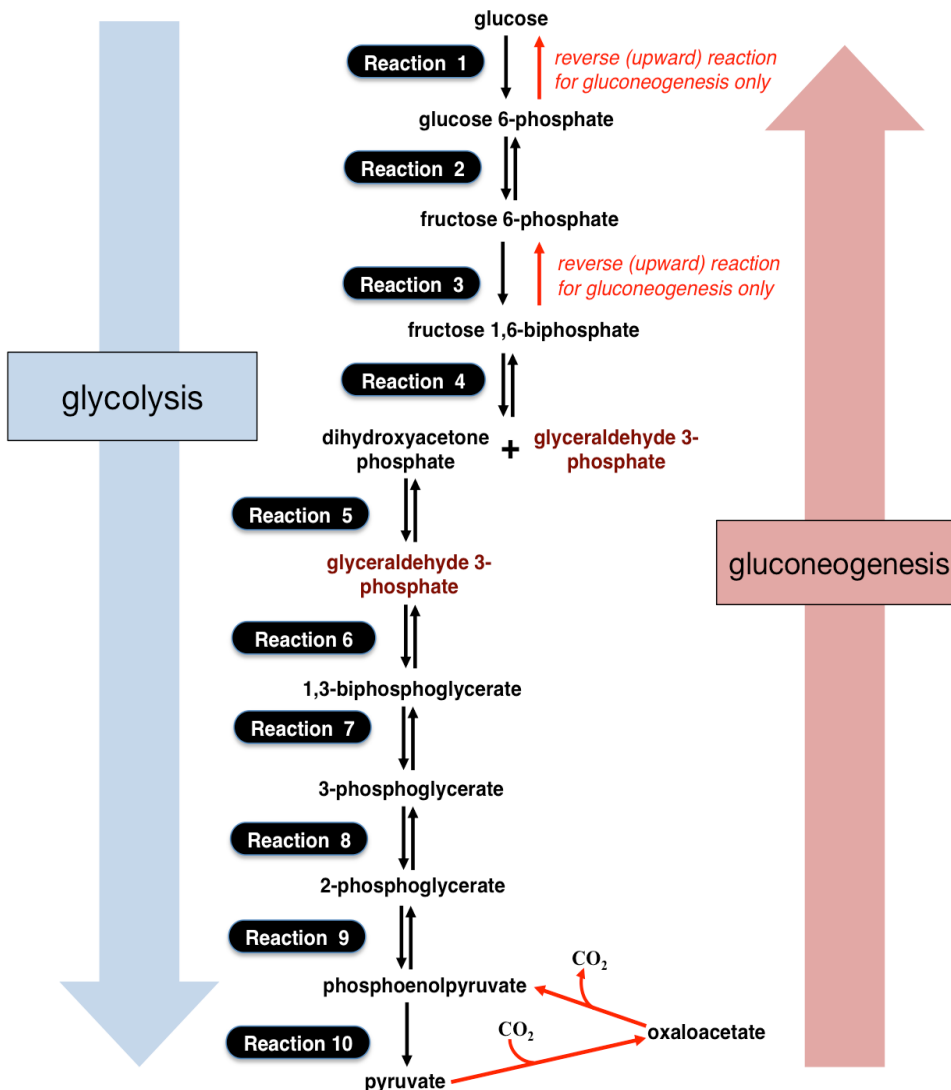
The conversion of ***non carbohydrate species to glucose*** is called

_____.

- The conversion of lactate and pyruvate to glucose is an example of *gluconeogenesis*.

The *gluconeogenesis* and *glycolysis* pathways share many reactions. The differences occur at the three *irreversible* glycolysis reactions (reactions 1, 3, and 10), as shown in the figure on the left.

Gluconeogenesis does not use reaction 10 of glycolysis, and it uses different enzymes in order to enable the reverse of reactions 1 and 3 of glycolysis.

Gluconeogenesis takes place primarily ***in the liver***.

In the figure above, *glycolysis* proceeds in the ***downward*** direction, and *gluconeogenesis* proceeds in the ***upward*** direction.

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When oxygen is present (_____ **conditions**), much more energy can be derived from pyruvate.

Under aerobic conditions, pyruvate passes from the *cytoplasm* into the _____ and is then converted to **acetyl-coenzyme A** and CO_2 (as shown in the equation below).
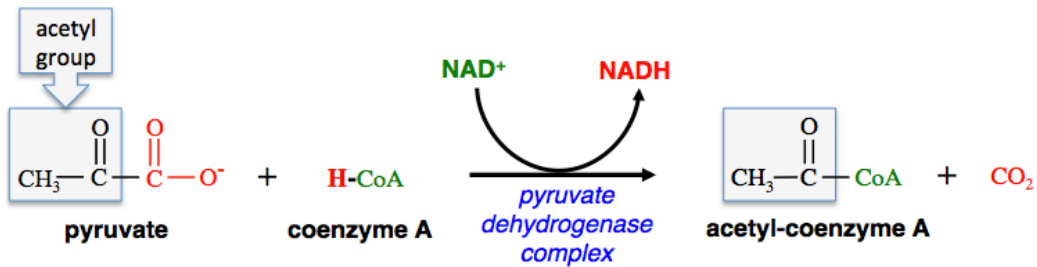
In this reaction, pyruvate is **oxidized** and **decarboxylated**.
- The decarboxylation produces CO_2.
- In the oxidation process, electrons from pyruvate are passed through intermediate compounds (not shown), until they are eventually transferred, along with a hydrogen, to **NAD⁺**.
- Energy *released* by the oxidation of pyruvate is transferred to **NADH**.
- _____ is produced.

The acetyl groups are relatively high-energy because they still contain much of the energy that was originally in glucose.

In the next stage of catabolism (the citric acid cycle), the energy contained in the acetyl groups is used to produce more **NADH** and more **ATP**.

Summary of Stage 2 of Carbohydrate Catabolism and the Fate of Pyruvate
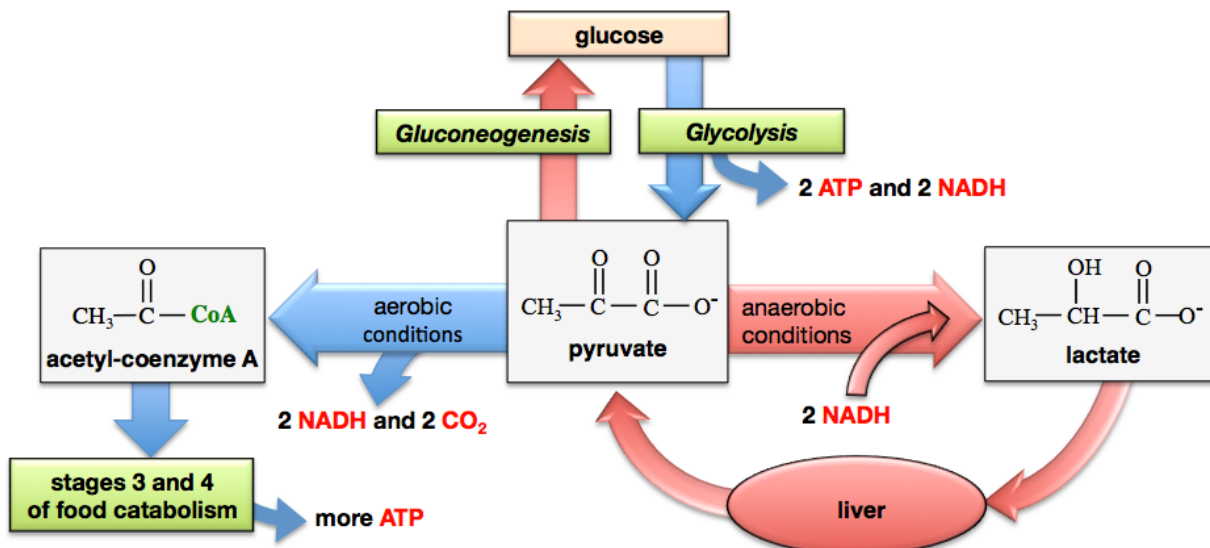
In Stage 2 of carbohydrate catabolism, **under aerobic conditions**, *one* glucose molecule has produced two **acetyl-coenzyme A ions**, and provided the energy for the formation of *four* **NADH** and *two* **ATP**.

Stage 3: The Citric Acid Cycle

The **citric acid cycle** is also referred to as the **Krebs Cycle** because it was H. A. Krebs who, in 1937, discovered these reactions and recognized their significance in energy-transfer reactions.

NOTE: you *do not* need to memorize these reactions, the names of the intermediates, or the names of the enzymes that are involved.

Reactions of the **Citric Acid Cycle**
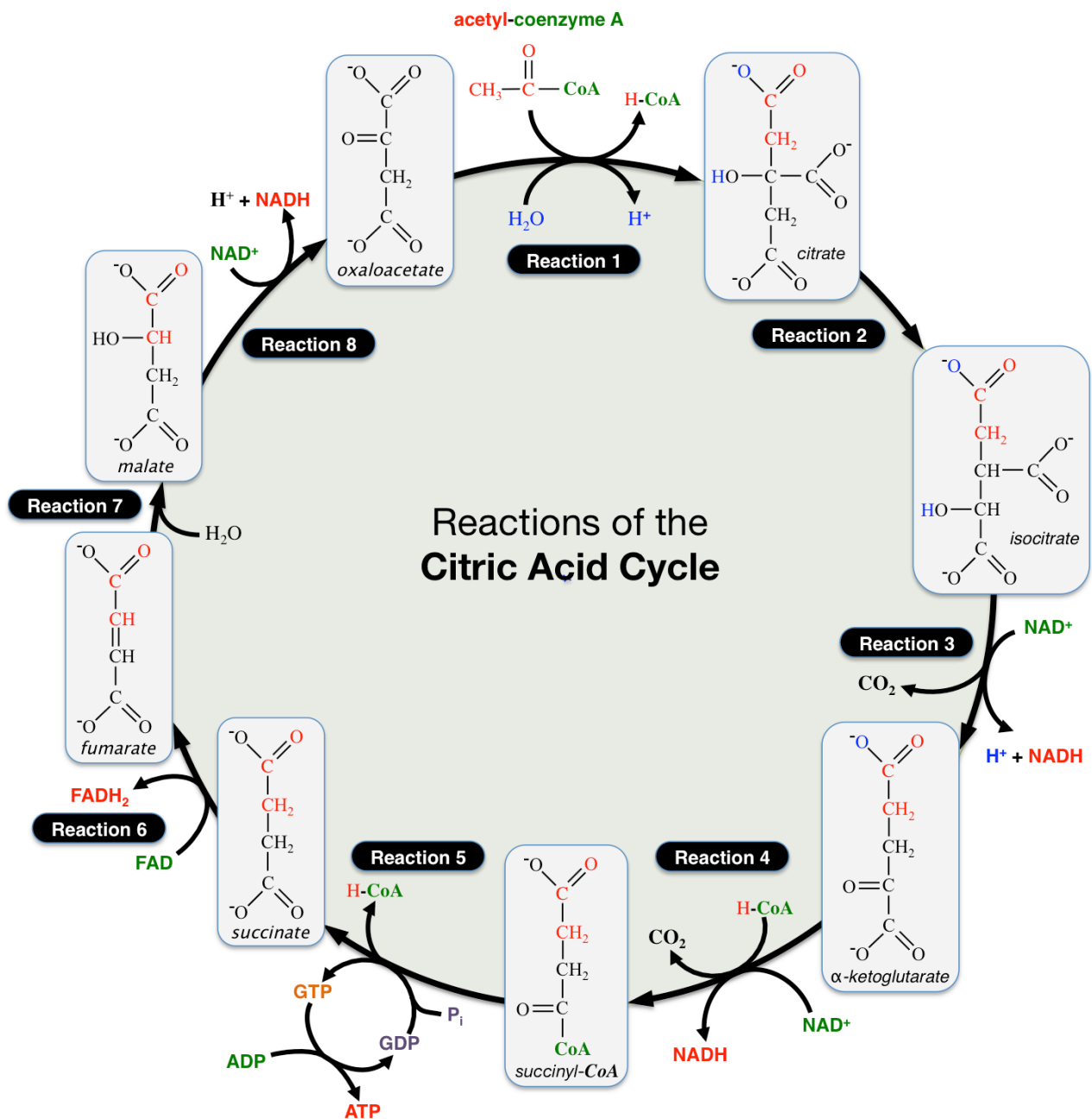
The *citric acid cycle* is characterized as a _____ **metabolic pathway**.

- A *circular pathway* is a repeating series of reactions in which the final product is _____ an *initial* reactant.

- In the first reaction, acetyl-coenzyme A (acetyl-CoA) reacts with oxaloacetate. In the citric acid cycle, *oxaloacetate* is not only a *reactant* in the first reaction; it is **also** the *product* of the last reaction.

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Acetyl-CoA brings two carbons in its acetyl group (these carbons are shown in red font in the video).

When one acetyl-CoA is completely processed in the citric acid cycle, _____ NADH, _____ FADH₂, _____ ATP, and *two* CO₂ molecules are produced.

In this process, energy that was originally contained in acetyl-CoA is converted to chemical potential energy within **NADH, FADH₂** and **ATP**.

Reactions of the Citric Acid Cycle

Reaction	Type of Reaction	Enzyme	Energy Transferred to:	Notes
1	acetyl group transfer	*citrate synthase*		An **acetyl group** is transferred to oxaloacetate.
2	isomerization	*aconitase*		The product and reactant are *constitutional isomers*.
3	oxidation/reduction and decarboxylation	*isocitrate dehydrogenase*	**NADH**	This reaction is irreversible. **Isocitrate** is decarboxylated and its hydroxyl group is oxidized to a carbonyl group. A *hydride ion* (**H:·**) is transferred from *isocitrate* to **NAD⁺**, thereby reducing **NAD⁺** to **NADH**. This reaction is the body's main regulation point for the citric acid cycle. When cells are "energy rich," **ATP** and **NADH** concentrations are high. **ATP** and **NADH** *inhibit* the *isocitrate dehydrogenase* enzyme. When energy is in demand, **ADP** and **NAD⁺** concentrations are high. **ADP** and **NAD⁺** *activate* *isocitrate dehydrogenase*.
4	oxidation/reduction and decarboxylation	*α-ketogulutarate dehydrogenase*	**NADH**	This irreversible process has multiple steps (not shown). Two electrons are transferred from α-ketogulutarate to an intermediate species. Ultimately, the two electrons and a **H⁺** ion are transferred from an intermediate to **NAD⁺** to form **NADH**.
5	acyl group transfer and phosphorylation	*succinyl-CoA synthase*	**ATP**	Humans have a *succinyl-CoA synthase* enzyme that produces **GTP** (*guanosine triphosphate*). Energy in **GTP** is used to produce an **ATP**. We have another *succinyl-CoA synthase* enzyme that produces **ATP** directly.
6	oxidation/reduction	*succinate dehydrogenase*	**FADH₂**	-CH₂-CH₂- is *oxidized* to -CH=CH- **FAD** is *reduced* to **FADH₂**. The **FAD/FADH₂** coenzyme is permanently bound to the succinate dehydrogenase enzyme.
7	hydration	*fumarase*		Hydration of an alkene.
8	oxidation/reduction	*malate dehydrogenase*	**NADH**	**Malate's** 2° alcohol is *oxidized* to a ketone. **NAD⁺** is *reduced* to **NADH**.

Summary of the Citric Acid Cycle

The *overall* chemical equation for the *citric acid cycle* metabolic pathway is:

acetyl-**CoA** + **3 NAD⁺** + **FAD** + **ADP** + **Pᵢ** + **2 H₂O** ⇌ **2 CO₂** + **3 NADH** + **FADH₂** + **ATP** + **H-CoA** + **3 H⁺**
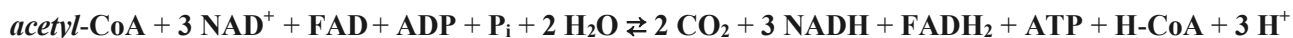
Potential energy from an acetyl-CoA that undergoes the citric acid cycle is converted to potential energy in *three* **NADH**, *one* **FADH₂**, and *one* **ATP**. Some energy is lost as *heat*.

The CO₂ produced in the *citric acid cycle* and in **stage 2** of metabolism, is one of the end-products of food metabolism.

- CO₂ is the most-oxidized form of carbon in organic compounds, and therefore has a very low energy content.
- Energy that was present in the food and food metabolites that contained these carbons has been extracted in the catabolism process.

Stage 4: Oxidative Phosphorylation

Glycolysis occurs in the _____ of the cell.

The reactions of the citric acid cycle occur in the _____.

The Structure of the Cell and a Magnification of an Individual Mitochondrion.
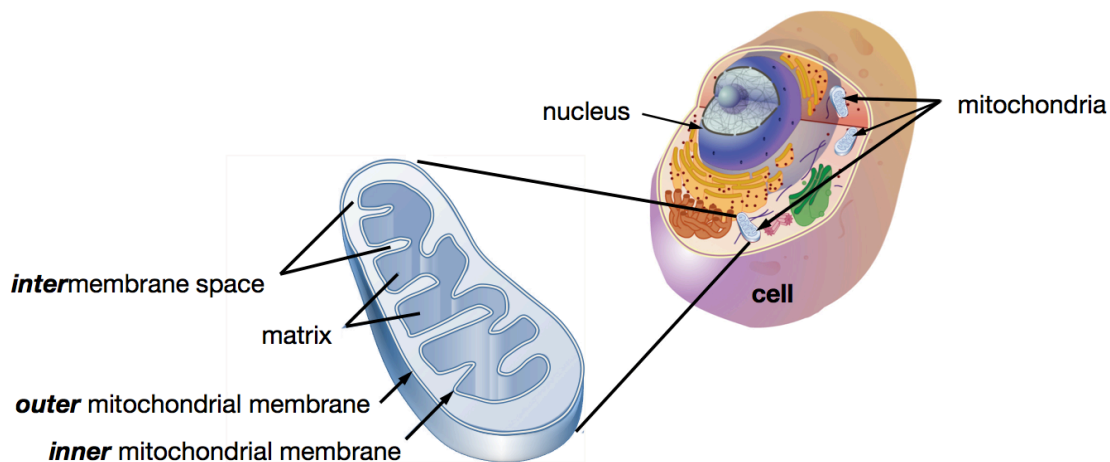
A mitochondrion consists of an _____ **membrane** bilayer and an _____ **membrane** bilayer.

The region **between** the *outer* and *inner membranes* is called the _____ _____.

The region within the inner membrane is called the _____.

Pyruvate oxidation/decarboxylation and *the reactions* of the citric acid cycle occur in the *matrix* region.

The pyruvate that is produced in **glycolysis** is able to pass from the cytoplasm, through both the inner *and* outer mitochondrial membranes, into the *matrix* region.

The next stage of carbohydrate catabolism, **oxidative phosphorylation (stage 4)**, requires that _____ be located *within the mitochondrial matrix*.

- Since pyruvate oxidation/decarboxylation *and* the reactions of the citric acid cycle occur in the *mitochondrial matrix*, the **NADH** created in those processes can immediately undergo oxidative phosphorylation.

- The **NADH** *that is produced by glycolysis* is able to pass through the *outer* mitochondrial *membrane* and enter the *intermembrane space*; however, it is *not* able to pass through the *inner mitochondrial* membrane to enter the *matrix* region.

  o In order for the energy from these **NADH** to be utilized, they must be processed through an "**NADH** _____."

The two most important **NADH** shuttles are the **malate-aspartate shuttle** and the **glycerol 3-phosphate shuttle**.

- The **malate-aspartate shuttle** works by oxidizing the **NADH** to **NAD$^+$** in the intermembrane space, then transferring the electrons through the inner mitochondrial matrix to an **NAD$^+$** that *is _____ inside the matrix,* *thereby producing an* **NADH** that *can undergo oxidative phosphorylation*.

- In the **glycerol 3-phosphate shuttle**, **NADH** is oxidized in the intermembrane space by transferring electrons to an inner mitochondrial membrane-bound **FAD**, *thereby producing an* **FADH$_2$** that *can undergo oxidative phosphorylation*.
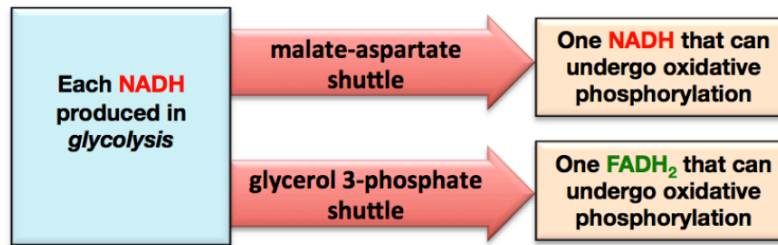
Example Problem: From one glucose molecule, determine how many **NADH** and **FADH$_2$** would be available for *oxidative phosphorylation* (stage 4 of metabolism). Assume that both **NADH** formed in glycolysis use the **malate-aspartate shuttle**.

> **Solution:** Start this problem with the amount of **NADH** and **FADH$_2$** that are formed ***from one glucose*** molecule in stages 1 to 3 of glucose catabolism. In the previous **UNDERSTANDING CHECK** problem (**chapter 15, part 5**), you found that **10 NADH**, and **2 FADH$_2$** are produced from one glucose molecule.
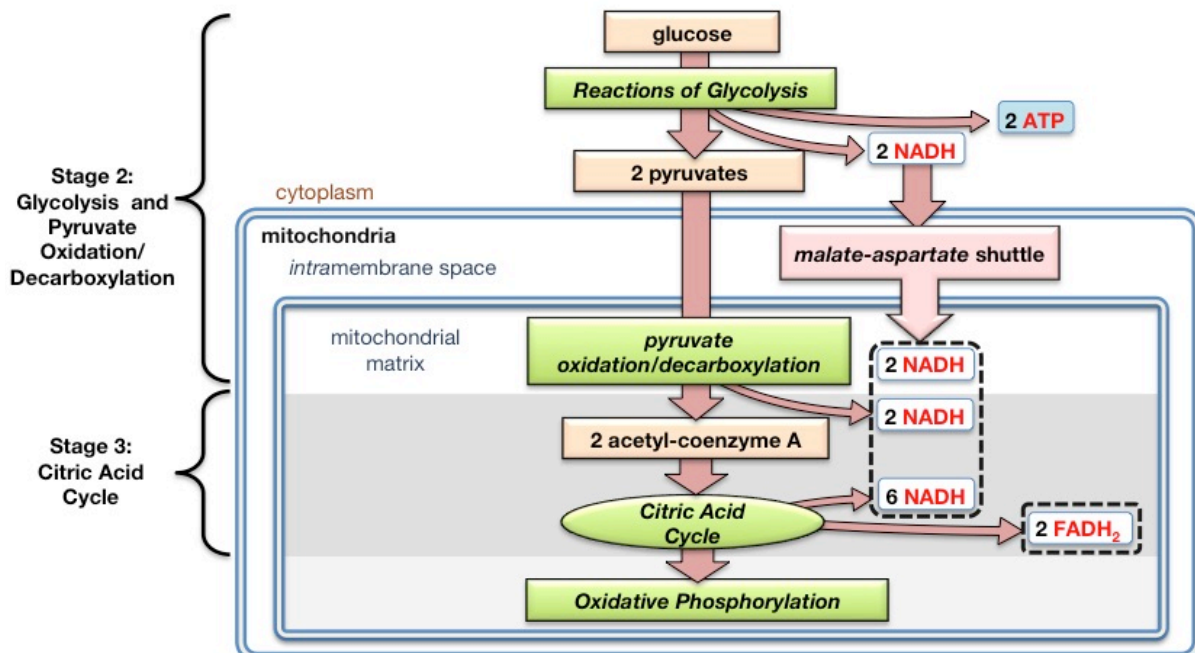
> The ***two* NADH** that are produced in ***glycolysis*** cannot pass through the inner mitochondrial membrane and enter the matrix region where oxidative phosphorylation takes place. Therefore, it is necessary that "**NADH** *shuttles*" be used. In the **malate-aspartate shuttle**, each NADH produced in *glycolysis* results in one **NADH** that can undergo oxidative phosphorylation. In this case, there would be **10 NADH** and **2 FADH$_2$** available for oxidative phosphorylation.

You try one: From one glucose molecule, determine how many NADH and FADH$_2$ would be available for *oxidative phosphorylation* (stage 4 of metabolism). Assume that both NADH formed in glycolysis use the **glycerol 3-phosphate shuttle**.

The primary goal of food catabolism is the production of **ATP**.
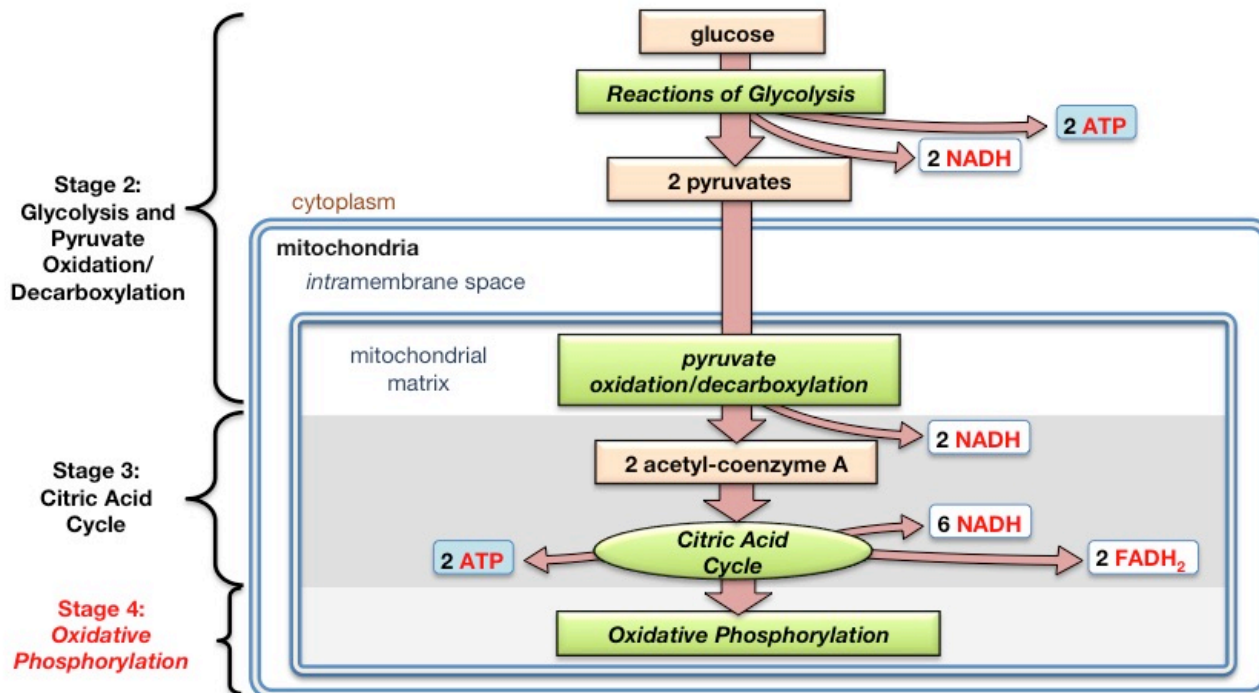
At this point in my narrative of carbohydrate catabolism:

- Only *four* ATP have been produced from one glucose **so far**.
- Most of the chemical potential energy that has been extracted from glucose is still in the form of

  _____ _____(**NADH** and **FADH₂**).

In **stage 4** of catabolism (*oxidative phosphorylation*), chemical potential energy contained in the *reduced coenzymes* is _____ to **ATP**.

Oxidative phosphorylation is the process in which _____ from **NADH** or **FADH₂** are transferred, through a series of electron transfer intermediates, to dissolved oxygen (O₂) in order to provide the energy required to produce **ATP**.

In this process, **ADP** and an inorganic phosphate (P$_i$) are converted to **ATP**.

The formation of **ATP** from **ADP** and P$_i$ would *not* occur spontaneously without the input of energy that is provided when electrons are transferred to O₂.

Because of the availability of H$^+$ in solution (from H₂O, H₃O$^+$, or the *acid form* of any other species present), when electrons are transferred to oxygen, the following reaction occurs:

$$O_2 + 4H^+ + 4 \text{ electrons} \rightarrow 2H_2O$$

In the reaction above, O$_2$ is_____; it gains electrons

O$_2$ is the *final* _____ of electrons in food catabolism.

The energy released by the transfer of electrons from **NADH** or **FADH₂**, through the electron transfer intermediates, to O₂ is not immediately used to drive the production of **ATP**.

Instead, this energy is used to move hydrogen ions from a region of lower hydrogen ion concentration (the mitochondrial matrix) to a region of higher hydrogen ion concentration (the intermembrane space).

By doing so, the energy that is released by the transfer of electrons is converted to

_____ *potential energy*.

- Physically, this is very similar to "charging" a battery

Oxidative phosphorylation does not happen in exactly the same way for **NADH** as it does for **FADH₂**.

Electron Transfers and Hydrogen Ion Transport From NADH Oxidation

The process begins with the _____ of **NADH** in the matrix region.
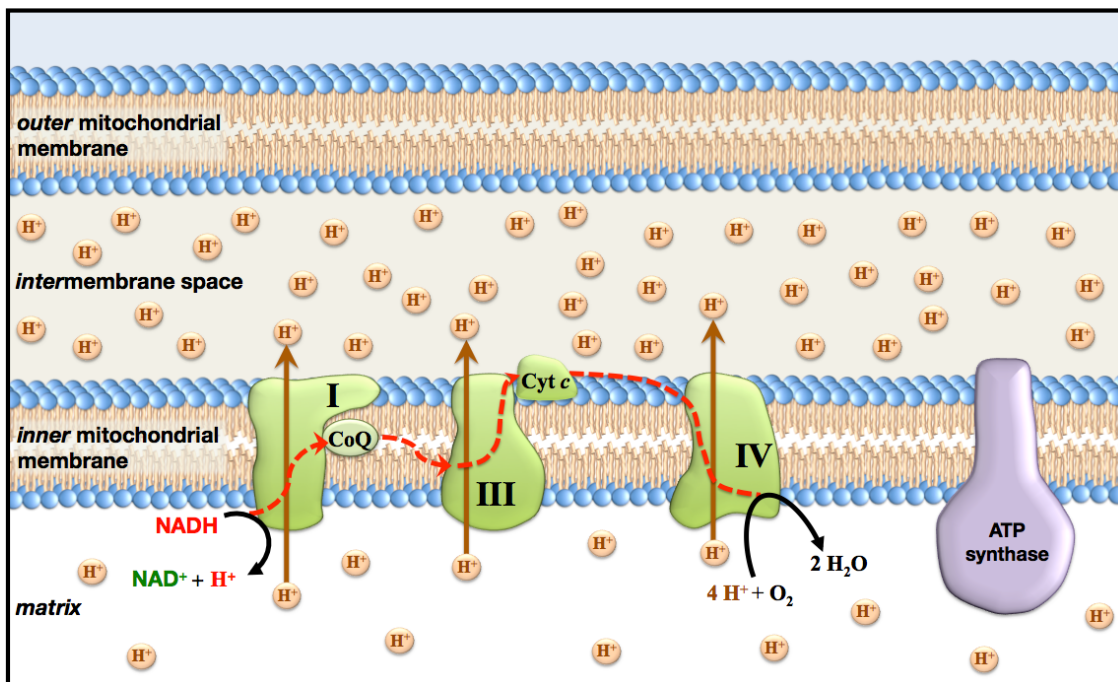
The electrons that are released in the oxidation of **NADH** are sequentially passed between electron transfer intermediates (shaded green) along the path that is indicated by the dashed red curve.

- Two of the electron transfer intermediates, *coenzyme Q* (**CoQ**) and *cytochrome C* (**Cyt c**), are quite *mobile*.
- The other electron transfer intermediates are *transmembrane* **proteins complexes** (labeled **I**, **III**, and **IV**).

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In order for the electrons to "move through" these protein complexes, they are transferred *within the complexes* by sequential oxidations and reductions of neighboring prosthetic groups or cofactors (not shown in the figure).

The movement of electrons through the protein complexes releases energy (analogous to water being released from a dam).

This energy is used by the complexes to _____ _____ *hydrogen ions* from a region of _____ hydrogen ion concentration (the mitochondrial matrix) to a region of _____ hydrogen ion concentration (the *inter*membrane space), as indicated in the figure by the arrows in the figure on the previous page.

Electrons are ultimately transferred to, and thereby *reduce* O_2.

Electron Transfers and Hydrogen Ion Transport from FADH₂ Oxidation

FADH₂ is produced in _____ of the *citric acid cycle*.

- The enzyme that catalyzes this reaction is part of an electron transfer intermediate called **complex II**.
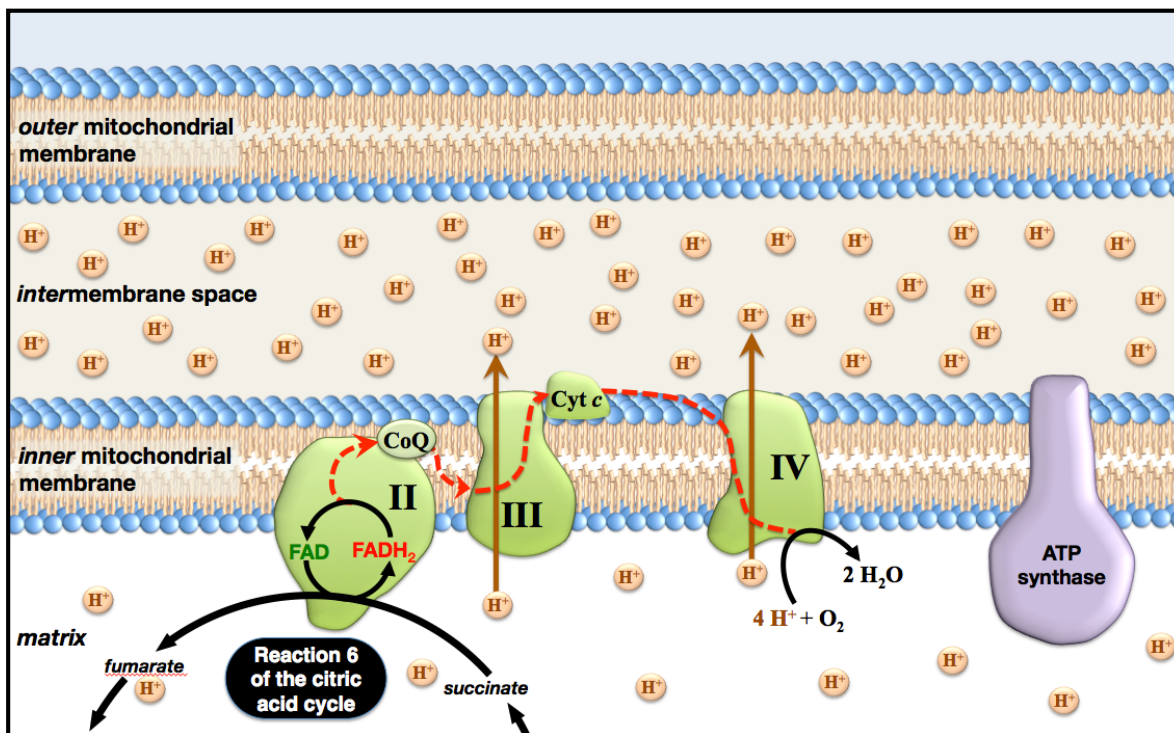
In oxidative phosphorylation, **FADH₂** is *oxidized* and its electrons are sequentially passed between electron transfer intermediates, along the path that is indicated by the dashed curve, and then finally transferred to O_2.

The movement of electrons through protein complexes **III** and **IV** releases energy.

This energy is used by these complexes to *actively transport* hydrogen ions through the inner mitochondrial membrane into the intermembrane space.

Summary of the Oxidation of NADH and FADH₂ During Oxidative Phosphorylation

When **NADH** and **FADH₂** are oxidized, their electrons are transferred, through intermediates, to O_2.

As electrons move through complexes I, III, and IV, energy is released.

This energy is used by the complexes to **actively transport** hydrogen ions from a region of *lower* hydrogen ion concentration (the mitochondrial matrix) to a region of *higher* hydrogen ion concentration (the intermembrane space).

In doing so, the *energy* from **NADH** and **FADH₂** (that was originally in food) is converted to *electrochemical energy* within mitochondria.

This part of oxidative phosphorylation is often referred to as _____ _____.

The electron transfer intermediates (shaded green in the previous figures) that are involved in *electron transport* are sometimes called "***the electron transport chain***."

Next, you will learn how electrochemical energy within mitochondria is used to drive the production of **ATP**.

ATP Production in Oxidative Phosphorylation

When there are *unequal* concentrations of a species on opposite sides of a membrane, we say that a "***concentration*** _____" exists.

The creation of *electrochemical potential energy* in the form of an H^+ concentration gradient was like charging a battery.

As with any dissolved species, hydrogen ions will _____ diffuse from areas of high concentration to areas of low concentration.

- It is lower in energy for the hydrogen ions to be in the matrix region (low concentration) than it is for them to be in the intermembrane space (higher concentration).

The **only** path between these regions in which hydrogen ions can passively diffuse is through the _____ enzyme, as illustrated below.
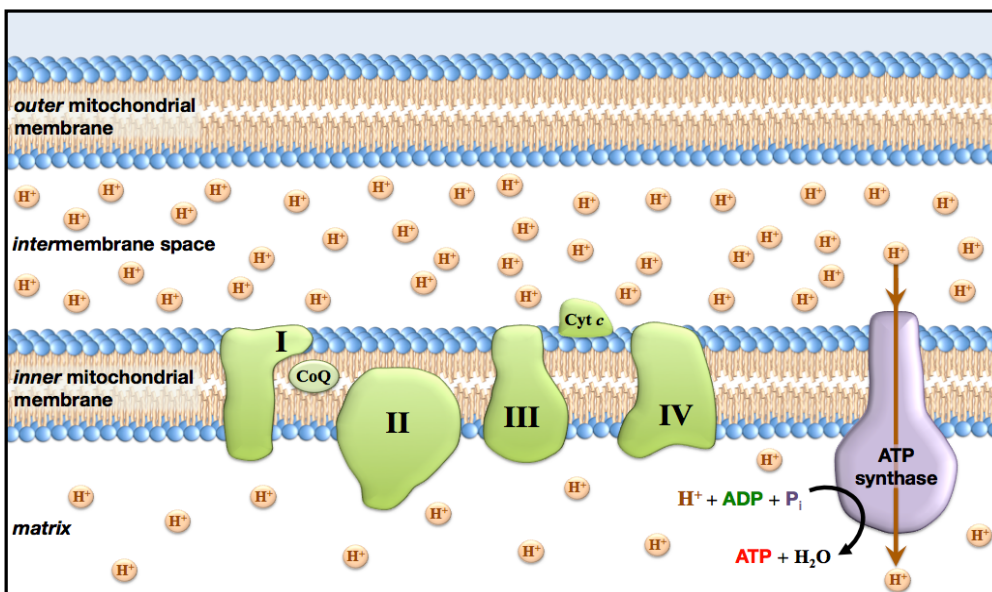
Much like electrical current passing through an electric motor does work, the passing of hydrogen ion current through an *ATP synthase* does work.

- This work is done by forcing the enzyme to change its shape and thereby supply the energy needed to form a bond between an inorganic phosphate (**P$_i$**) and **ADP**, to produce **ATP**.

The *ATP synthase* enzyme not only catalyzes the reaction for the synthesis of **ATP**, it also plays a role in delivering the energy needed to make **ATP** synthesis occur ***spontaneously***.

The number of **ATP** that can be produced from **NADH** or **FADH₂** depends on the cell and its current conditions.

The latest research indicates that, ***on average***,
one **NADH** produces about _____ **ATP**, and
one **FADH₂** produces about _____ **ATP**.

Let's calculate how many **ATP** can be produced from the catabolism of ***one glucose molecule***.
- For this calculation, we will assume that each **NADH** produces 2.5 **ATP**, and each **FADH₂** produces 1.5 **ATP**, and that **NADH** produced in glycolysis use the ***malate-aspartate shuttle***.

Solution:

Stage 2: In *glycolysis*, glucose is converted to two pyruvate ions. In this process, two **NADH** and two **ATP** are formed. The two **NADH** undergo the ***malate aspartate shuttle*** and result in the formation of two **NADH** within the mitochondrial matrix.

The pyruvate ions can diffuse past both mitochondrial membranes, and enter the matrix region. There, the pyruvate ions undergo an oxidation/decarboxylation reaction. In this process, two **NADH** and two acetyl-CoA are formed.

Stage 3: In the c*itric acid cycle*, the two acetyl-CoA produce a total of six **NADH**, two **FADH₂**, and two **ATP**.

Stage 4: In *oxidative phosphorylation,* the ten **NADH** and two **FADH₂** produced in **stages 2** and **3** are oxidized in order to produce **ATP**.

This gives total of 32 ATP, as shown in the illustration below.

25
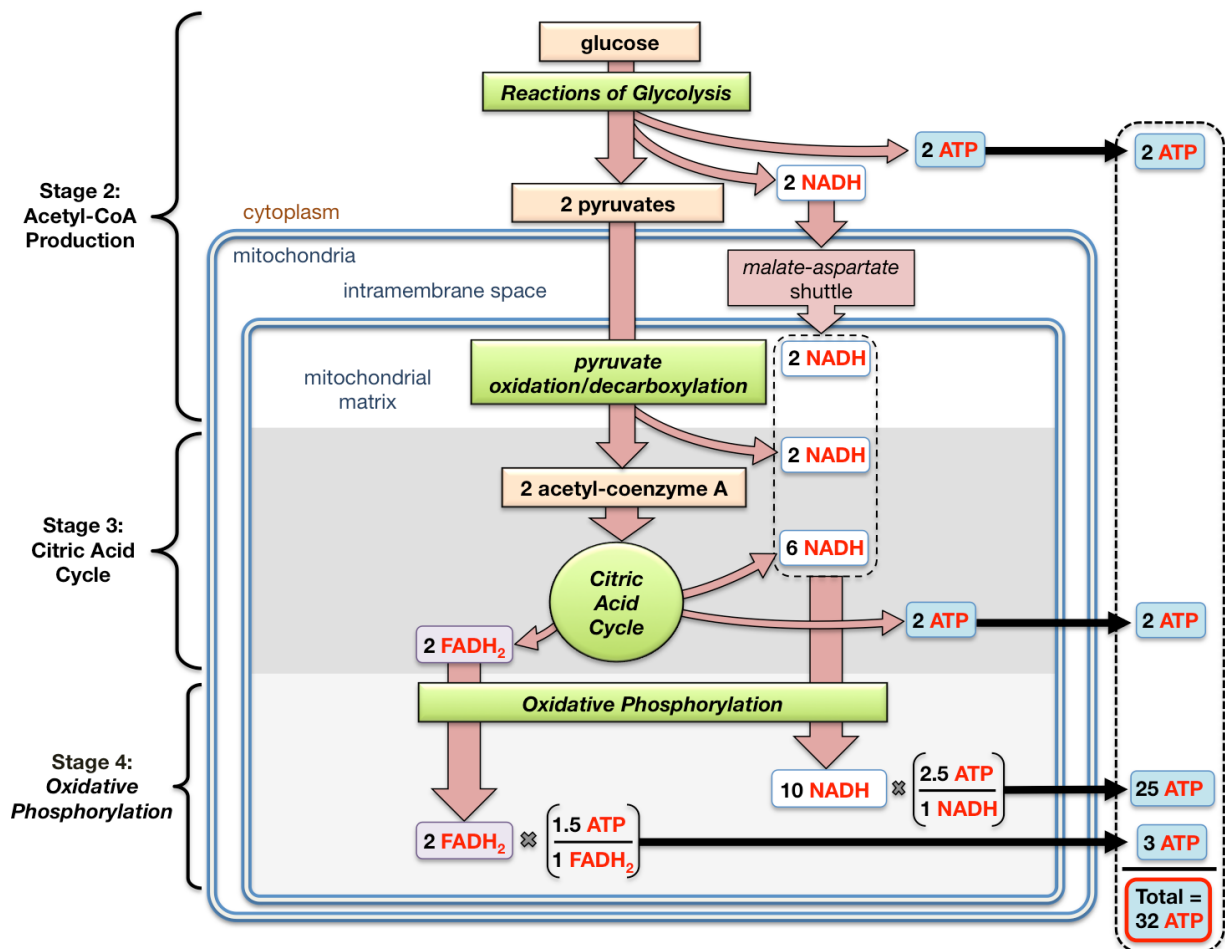
> **Understanding Check:** Calculate how many **ATP** can be produced from the catabolism of **one glucose molecule** when the two NADH from glycolysis use the ***glycerol 3-phosphate shuttle***.
> - Assume that each NADH that undergoes oxidative phosphorylation produces 2.5 ATP, and each $FADH_2$ produces 1.5 ATP.

Summary of Carbohydrate Catabolism

In the four stages of carbohydrate catabolism, chemical potential energy in carbohydrates is converted to chemical potential energy in **ATP**, a substance that can be used immediately by all cells to do cellular work.

The carbon, hydrogen, and oxygen atoms in carbohydrates, along with the oxygen we inhale, are converted to H_2O and CO_2.

Regulation of Blood Glucose Concentration

It is important for human **blood glucose concentration** (sometimes called blood sugar level) to remain within a "normal" range.
- The normal range of glucose concentration in the blood is about 80 to 110 mg per dL of blood.

Long term effects of having higher than normal blood glucose concentration (_____) can include damage to kidneys, the neurological system, the cardiovascular system, eyes, feet, and legs.

Between meals or during starvation, blood glucose levels fall below the normal range (_____).

- This can result in confusion, loss of coordination, difficulties in speaking, a loss of consciousness, seizures, and even death. Symptoms can come on quite quickly and include hunger, shaking, sweating, and weakness.

In the "***fed***" state, which occurs *soon after a meal* when blood glucose levels are high, ***liver*** and ***muscle cells*** (primarily) take in *extra* glucose and store it in the form of _____.

- The chemical structure of glycogen is very similar to that of *amylopectin*; the only exception is that *glycogen* branches more frequently. For a review of glycogen and amylopectin structures, see chapter 12, section 6.
- The conversion of *glucose* to glycogen is called _____.
- *Glycogenesis* is an *anabolic pathway* in which glucose residues, with the help of enzymes, are connected to each other through glycosidic bonds to form *glycogen*.

In the "***fasting state***," which occurs several hours after a meal, blood glucose levels become low, and glycogen is converted back to glucose in a process called _____.

- ***Glycogenolysis*** occurs primarily in ***liver*** and ***muscle*** cells.
- It is the opposite of *glycogenesis*. In *glycogenolysis*, the glycosidic bonds between glucose residues are hydrolyzed.

Roles of Glycogenesis and Glycogenolysis in the Regulation of Blood Glucose Concentration

The body regulates blood glucose levels by releasing hormones that result in the production of compounds that ***inhibit <u>and</u> activate key enzymes in the glycogenesis and glycogenolysis pathways***.

In response to increased blood glucose concentration (in the fed state), the pancreas releases a protein hormone called _____ into the blood stream.

- When insulin binds to liver and muscle cell receptors, it triggers a series of events that result in the ***activation*** of an enzyme in the *glycogenesis* pathway and the ***inhibition*** of an enzyme in the *glycogenolysis* pathway.

  o *Accelerating glycogenesis* will result in **decreasing** the blood glucose concentration by increasing the rate of the conversion of glucose to glycogen.

  o *Suppressing glycogenolysis* helps in maintaining normal blood glucose concentration as the conversion of glycogen to glucose is inhibited.

- Another way that insulin is involved in lowering blood glucose concentration is by initiating a process that increases facilitated diffusion of glucose from the bloodstream into **all cell types**.

causes a ***decrease*** in blood glucose levels
- accelerated by *insulin*
- suppressed by *glucagon*

glycogenesis

glucose   **glycogen**

glycogenolysis

causes an ***increase*** in blood glucose levels
- accelerated by *glucagon*
- suppressed by *insulin*
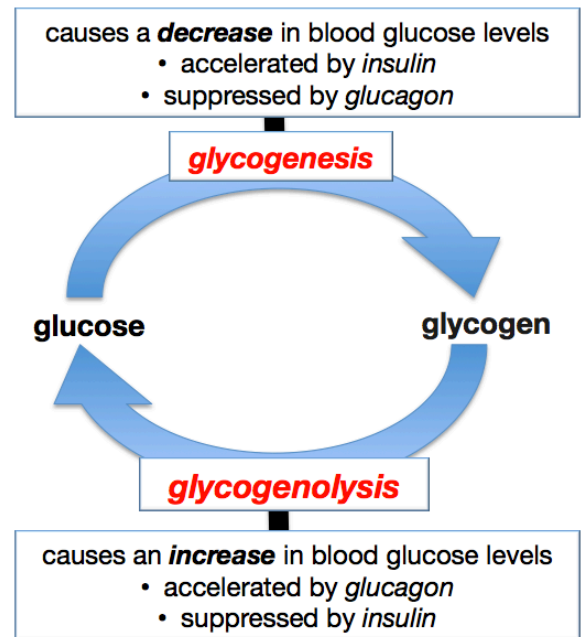
In response to decreased blood sugar levels (in the "fasting state"), the pancreas releases a protein hormone called _____ into the blood stream.

- Glucagon has the _____ ***effect of insulin*** on liver cells; it *accelerates* glycogenolysis and *suppresses* glycogenesis.

  o *Accelerating glycogenolysis* will result in **increasing** the blood glucose concentration as glucose produced during glycogenolysis is transported from liver cells into the bloodstream.

  o *Suppressing glycogenesis* helps in maintaining normal blood glucose concentration by suppressing the conversion of glucose to glycogen.

- Glucagon also increases blood glucose concentration by accelerating ***gluconeogenesis*** (the production of glucose from non carbohydrate species).

Diabetes

Diabetes Mellitus (DM), commonly referred to as **diabetes**, is a disease caused by *chronic* _____.

There are **three** types of **diabetes mellitus**: type I, type II, and gestational diabetes.

o In **diabetes type I**, also called ***insulin-dependent diabetes***, the pancreas produces too little _____. This can be a result of genetic disease, viral infection, or damage to the pancreas. Diabetes type I can be treated with insulin injections. Individuals must use a *glucometer* to frequently measure the concentration of glucose in their blood, and then inject insulin when elevated glucose levels are observed. Because diabetes type I often begins in childhood, it is sometimes referred to as _____ ***diabetes***.

o **Diabetes type II**, also called ***insulin-_____ diabetes***, occurs when sufficient insulin is produced, however the insulin receptors are unable to respond appropriately. About 90% of diabetes cases are type II. This type of diabetes can be even more difficult to manage than type I diabetes because it does not respond to insulin injections. Diabetes type II occurs after childhood and is therefore sometimes referred to as _____-*onset diabetes*.

o **Gestational diabetes** occurs during _____ in individuals without a previous diagnosis of diabetes. It is thought to be caused by pregnancy-related factors that affect insulin receptors. It is usually manageable with special diets and exercise; however, some individuals require antidiabetic drugs.

Triglyceride Metabolism

Dietary triglycerides, regardless of whether they came from plant or animal sources, are often referred to as _____.

When triglycerides are catabolized, their chemical potential energy is converted to chemical potential energy in **ATP**.

- This process begins with the digestion of triglycerides.
- Triglycerides are also used in the formation of phospholipids and glycolipids, and as cellular signaling compounds.

The body can store significant amounts of triglycerides, mostly in _____ **cells** (also called **fat cells**).

Digestion of Triglycerides

In order for triglycerides to pass through the intestine wall so that they can be used by the body, they must first undergo *partial* hydrolysis to produce _____ _____ and _____.

Triglycerides are first hydrolyzed to _____, then to _____.

Each one of these reactions produces a ***fatty acid*** (as shown below).

a **tri**glyceride   a **di**glyceride   a **mono**glyceride
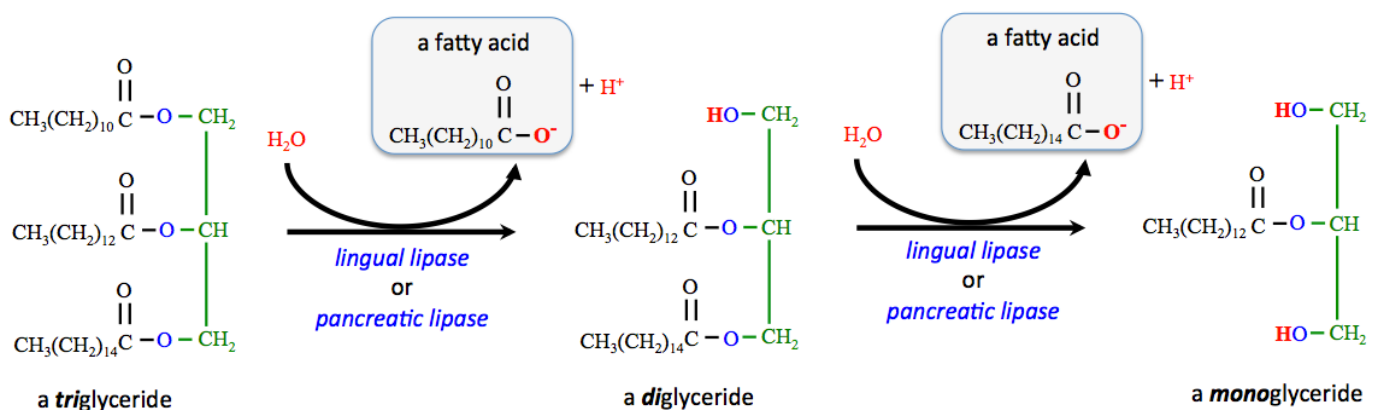
This is referred to as " _____ ***hydrolysis***" because one of the fatty acid residues *remains bound* to carbon number **2** of glycerol in the monoglyceride.

Triglyceride digestion begins in the _____ where *lingual lipase* catalyzes the partial hydrolysis of a *very small percentage* of triglycerides.

The **majority** of dietary triglycerides are digested in the _____ _____.

Large hydrophobic (insoluble) globules, that are composed mostly of triglycerides and a small amount of diglycerides, monoglycerides, and fatty acids, enter the **small intestine**. In the small intestine, bile salts disassemble these large hydrophobic globules and emulsify them into small micelles.

When emulsified by bile salts, the ester bonds of the glycerides are oriented toward the surface of the micelle. This enables *pancreatic lipase* to catalyze the *partial* hydrolysis of emulsified triglycerides and diglycerides to produce **fatty acids** and **monoglycerides**.

The fatty acids and monoglycerides that are formed inside the intestine can pass into the walls of the intestine. After being absorbed into the intestine walls, the fatty acids and monoglycerides are then re-assembled **back into triglycerides**.

Since lymph, blood, and intercellular fluids are *aqueous mixtures,* and triglycerides are hydrophobic, the triglycerides must be **emulsified** in order to be transported throughout the body. This is done by **chylomicrons**. Chylomicrons are small *lipoproteins* that are composed of a core that contains emulsified triglycerides (and some cholesterol and hydrophobic vitamins) surrounded by a lipid monolayer.

Triglycerides are emulsified in chylomicrons while in the wall of the intestine. The chylomicrons are then transferred into the lymph system, and then into the bloodstream. Triglycerides are released by the chylomicrons, and once again hydrolyzed to monoglycerides and fatty acids upon the inner surface of blood vessels. This occurs **primarily at blood vessels located in adipose (fat) tissue and muscles**. The monoglycerides and fatty acids can enter cells, where they are, once again, reassembled to triglycerides.
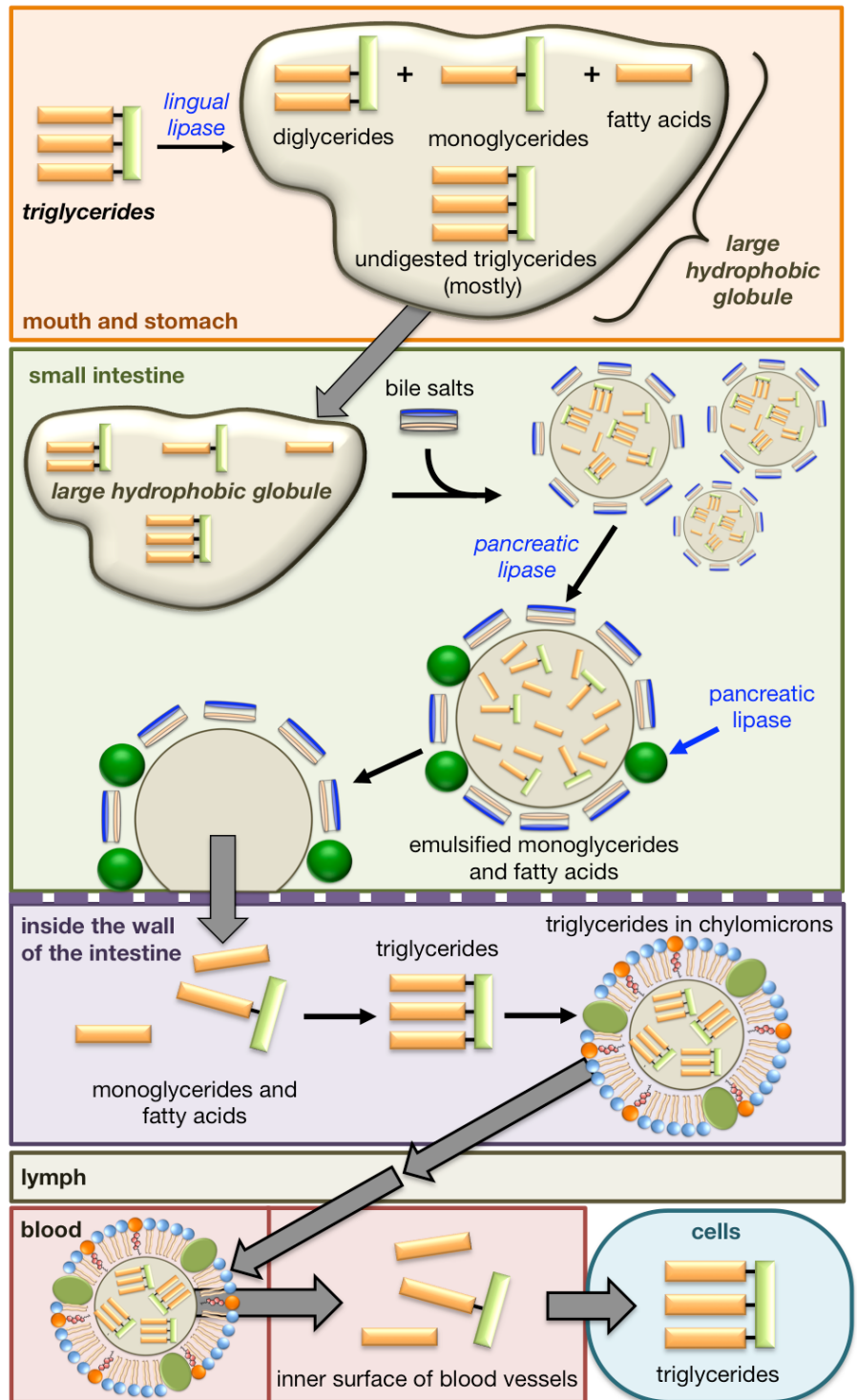
Adipose (fat) cells are the *major repository* for triglycerides; their primary function is to _____ triglycerides.

Peripheral (other) cells/tissues can access this stored energy, as needed, when adipose cells **completely** *hydrolyze* the triglycerides to **fatty acids** and **glycerol** in a process called _____.

The fatty acids are released from the adipose cells into the blood, and carried by *serum albumin protein* to other cells.

These **fatty acids** can then be _____ to produce **ATP**.

Catabolism of Fatty Acids

Fatty acids are catabolized in order to convert their potential energy into potential energy in **NADH**, **FADH₂**, and acetyl-CoA.

The first reaction in the catabolism of fatty acids is called _____.

- In this reaction, the _____ *group* of a fatty acid is transferred to *coenzyme* A.
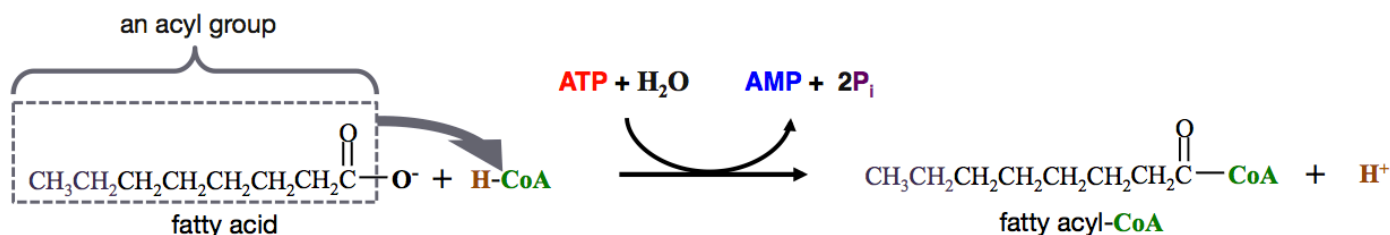
The fatty acid is converted to a _____ _____.

This reaction does not occur spontaneously without the external energy input provided from the hydrolysis of two inorganic phosphates from **ATP**.

- In this case, **ATP** is converted to **AMP** and two inorganic phosphate (**P**$_i$) ions.

The *activation* reaction is necessary in order for the acyl group from fatty acids to pass through the inner mitochondrial membrane and enter the matrix, where the subsequent reactions of fatty acid catabolism occur.

When fatty acyl-CoA enters the *mitochondrial matrix*, it undergoes a catabolic pathway called
_____ - _____ (*ß-oxidation*).

In *ß-oxidation*, a fatty acyl-CoA, goes through a *repeated* series of *four* reactions, *each time* losing two of its _____.
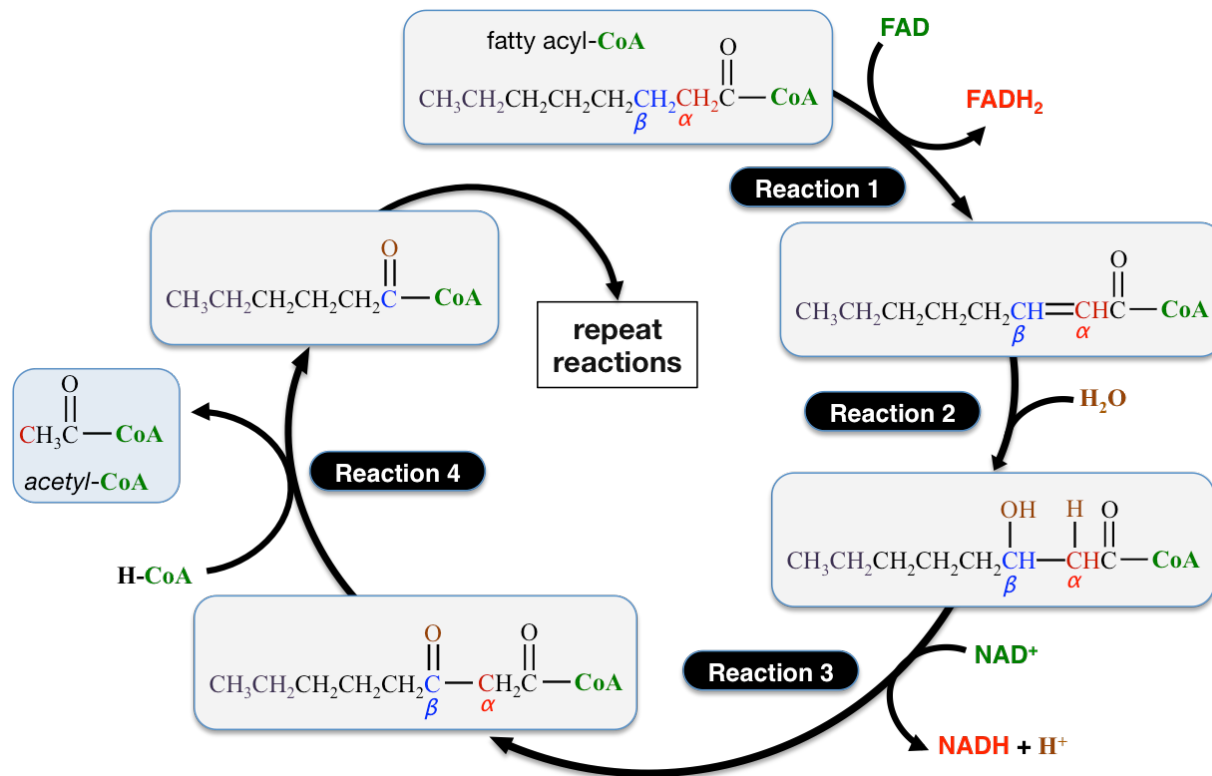
The carbon that is *next to* a fatty acyl's carbonyl group is designated as the "**α**-carbon," and the carbon that is two carbons away from the carbonyl group is designated as the "**ß**-carbon."

In **reaction 1** of **ß**-oxidation, the **α**- and **ß**-carbons are _____ (they lose hydrogens and electrons).
  - The hydrogens and electrons are transferred to **FAD** to produce **FADH₂**.

In **reaction 2** the double bond between the **α**- and **ß**-carbons is *hydrated*.

In **reaction 3**, the **ß**-carbon is oxidized.
  - In this oxidation, a hydrogen and electron are transferred to **NAD⁺**, reducing it to **NADH**.

In **reaction 4**, the bond between the **α**- and **ß**-carbon is broken.
  - A hydrogen forms a bond to what was formerly the **α**-carbon, **thereby** producing acetyl-CoA.
  - The *acyl group*, containing what was formerly the **ß**-carbon, is transferred to coenzyme A, thereby forming a _____ fatty acyl-CoA.

The *new* fatty acyl-CoA is _____ *carbons shorter* than the original one.

The *new* fatty acyl-CoA can undergo the **ß**-oxidation reactions.

For example, a *eight-carbon* fatty acyl-CoA will undergo *three* cycles of the *β-oxidation* reactions.
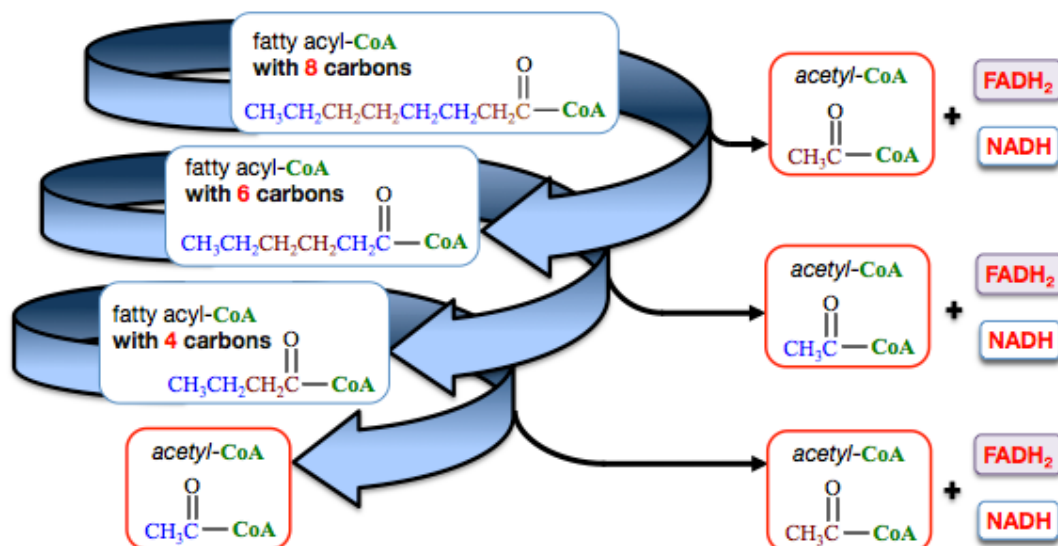
When the *original* fatty acyl-CoA undergoes the *β*-oxidation reactions series, one acetyl-CoA, one **NADH**, and one **FADH₂** are produced.

A *new* fatty acyl-CoA is also produced.

Each successive (new) fatty acyl-CoA undergoes the series of four reactions to produce more acetyl-CoA, **NADH**, and **FADH₂**.

The acyl group's length is decreased by *two carbons* with each successive *β*-oxidation reaction series.

When the fatty acyl-CoA contains _____ carbons, then it will undergo the reaction series *one final time*.

- In the final cycle, **reaction 4** produces two *acetyl*-CoA.

If "**N**" equals the number of carbons that are contained in a fatty acyl-CoA, then it will undergo **[(N/2) -1]** *β-oxidation* cycles.

β- oxidation is classified a "_____" **metabolic pathway**.

- A **spiral pathway** is a metabolic pathway in which a *series of repeated reactions* is used to break down (or build up) a compound.

> **Understanding Check:** How many cycles of the *β-oxidation* spiral will occur for a **twelve-carbon** fatty acyl-CoA?

> **Understanding Check:** For the **twelve-carbon** fatty acyl-CoA in the previous problem:
> - How many acetyl-CoA are produced after all of the *β-oxidation* cycles?
> - How many NADH are produced after all of the *β-oxidation* cycles?
> - How many FADH₂ are produced after all of the *β-oxidation* cycles?

ATP Production from Fatty Acids

As was the case for carbohydrate catabolism, the catabolism of triglycerides converts potential energy in food into the form of chemical potential energy that is most useful in cells - **ATP**.

Because *β*-oxidation occurs in the mitochondrial matrix, each acetyl-CoA that is produced can undergo the reactions of the citric acid cycle to produce an **ATP**, three **NADH**, and one **FADH₂**.

More **ATP** is produced when the **NADH** and **FADH₂** formed in the *β*-oxidation cycles, along with the **NADH** and **FADH₂** formed in the citric acid cycle, undergo oxidative phosphorylation.

Let's consider how many **ATP** are produced from the catabolism of a typical fatty acid, *myristate*, which contains **14** carbon atoms (assume that *oxidative phosphorylation* produces, *on average*, 2.5 **ATP** per **NADH** and 1.5 **ATP** per **FADH₂**).

First, *myristate* is activated to produce a 14-carbon fatty acyl-CoA. The activation *consumes* one **ATP**.

The net gain of **ATP** from can be calculated as shown in the illustration below.
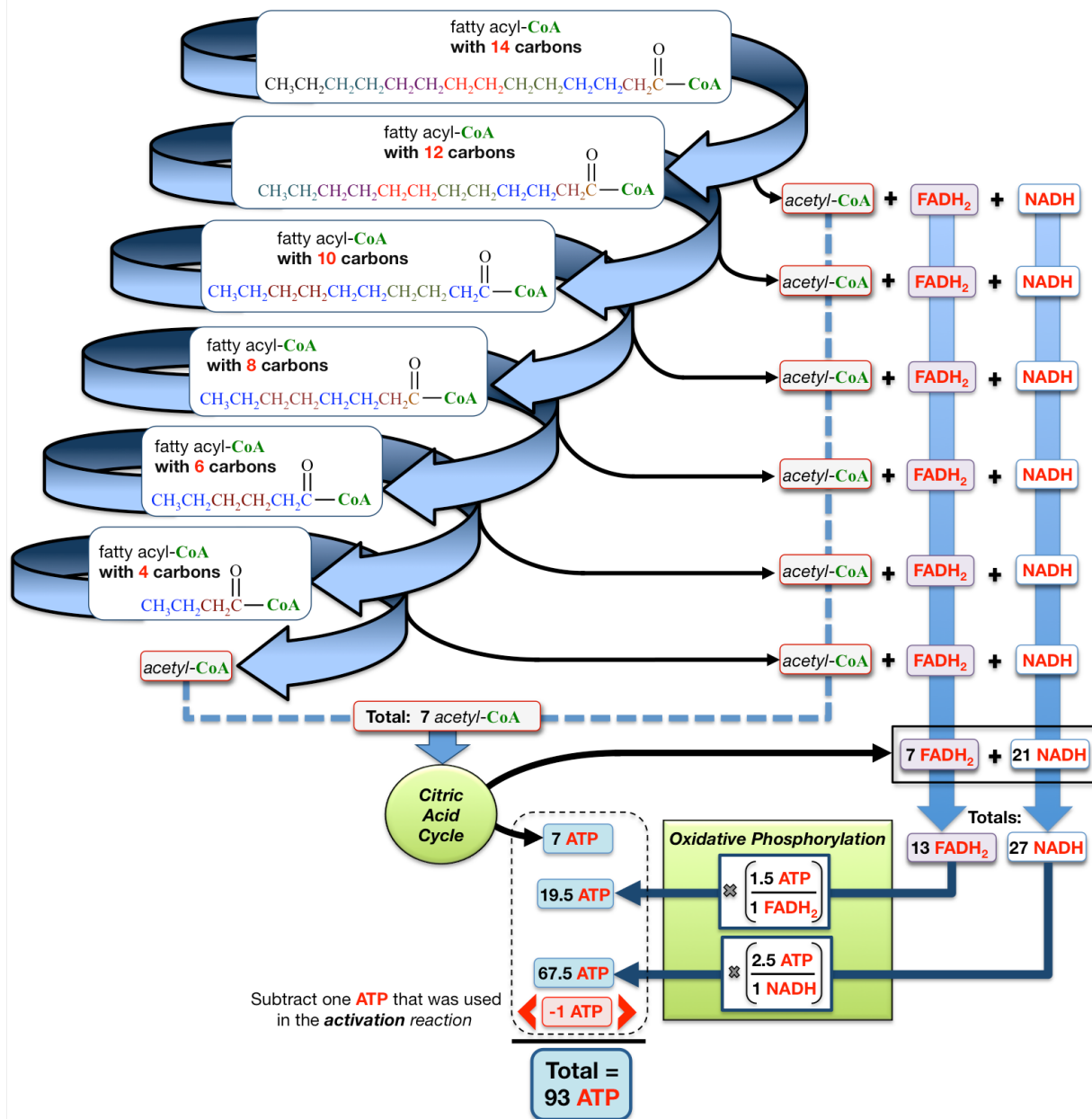
Each of the first *five* cycles of the *β*-oxidation spiral produces one acetyl-CoA, one **NADH**, and one **FADH₂**. The *final cycle* of the spiral produces *two* acetyl-CoA, one **NADH**, and one **FADH₂**. The acetyl-CoA are processed through the citric acid cycle, producing **ATP** and *more* reduced coenzymes. The **NADH** and **FADH₂** formed in *β*-oxidation and the **NADH**, and **FADH₂** formed in the citric acid cycle undergo oxidative phosphorylation. Since one **ATP** was consumed in the activation reaction, it is subtracted when calculating the *net gain* of **ATP**. *β*-oxidation of myristate, *on average*, results in a net gain of **93 ATP**.

Catabolism of Unsaturated Fatty Acids

Unsaturated fatty acids (derived from unsaturated fat) have ***double bonds*** in their hydrocarbon tails. Depending on the location of these double bonds, extra steps may be required to transform the double bonds in order to produce fatty acyl-CoA that can undergo **β**-oxidation.

Ketone Bodies

Catabolism of large quantities of triglycerides will result in high concentrations of acetyl-CoA.

Acetyl-CoA that is produced in excess of the amount that can be metabolized in the citric acid cycle results in a high concentration of acetyl-CoA in the mitochondrial matrix.

When this occurs, acetyl-CoA reacts with *other* acetyl-CoA to produce the three compounds that are referred to as _____ _____.
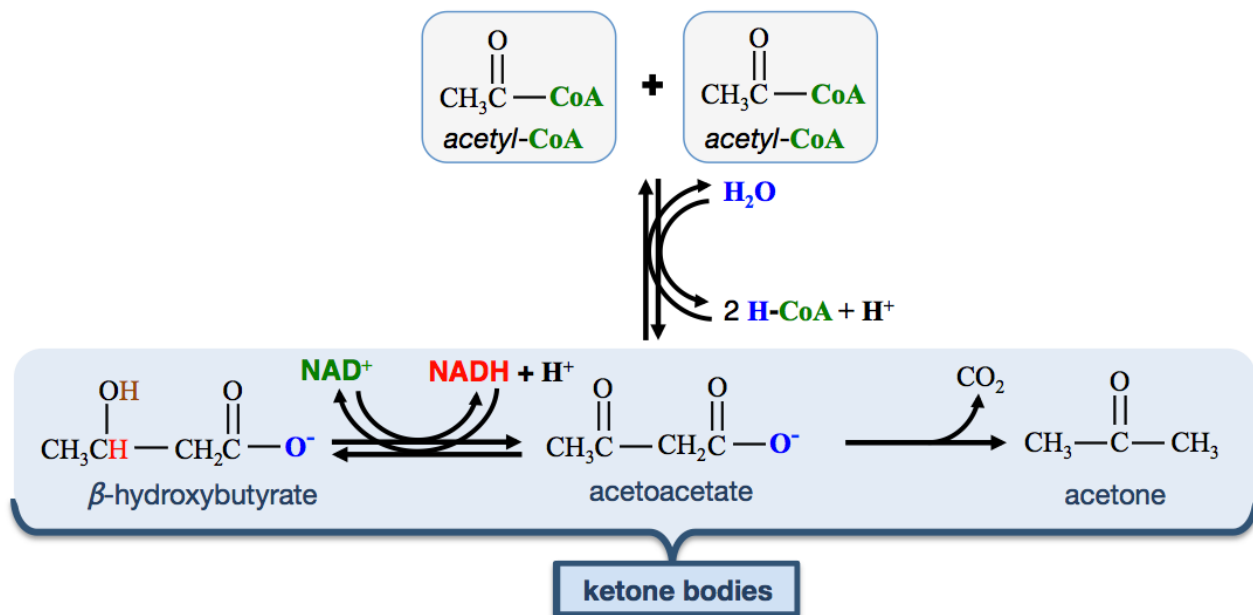
This process is referred to as _____.

Ketone bodies are water-soluble, therefore easily dispersed from the liver to other parts of the body. Most cells, with liver cells being the notable exception, are capable of converting ketone bodies back into acetyl-CoA, and then metabolizing it in the citric acid cycle. Converting ketone bodies back to acetyl-CoA is the *reverse of ketogenesis* (different enzymes are involved). Some cell types rely on ketone bodies for **ATP** production more than others. Heart muscles and the renal cortex use ketone bodies more readily than glucose. The brain's primary energy source is glucose, but it is unable to store glucose and does not allow fatty acid salts (or amino acids) to enter. In the case of starvation, when there is very little glucose present, the brain gets 75% of its energy from ketone bodies.

When individuals diet, they begin to metabolize the triglycerides that are stored in fat cells. This leads to *ketogenesis*.

In cases of starvation, poorly treated diabetes, and conditions related to alcoholic binge drinking, the cells cannot get glucose and extremely high rates of fatty acid salt catabolism results in dangerous, and even fatal levels of ketone bodies.

- *β-hydroxybutyric acid* and *acetoacetic acid* (the acid forms of *β-hydroxybutyrate* and acetoacetate, respectively) have significant acid strength.

- Their production results in a higher concentration of H_3O^+, which can overcome the blood's buffering capacity.

- When this occurs, the blood becomes acidic.

When blood pH is less than the normal range (7.35-7.45), the condition is called _____.

- *Acidosis* can result in tissue dysfunctions and is especially damaging to the central nervous system.

- When *acidosis* is caused by excess *ketone bodies*, the condition is called _____.

Fatty Acid Anabolism

Fatty acids are **produced** by a *spiral metabolic pathway* that operates in the **opposite** direction as *β*-oxidation; it builds-up fatty acyl-CoA by a repeating series of reactions that **add** acetyl-CoA to a growing fatty acyl-CoA structure.

This **anabolic** process of synthesizing fatty acids from acetyl-CoA is called **fatty acid** _____.

Fatty acid synthesis occurs primarily in adipose and liver cells.

The body can synthesize almost all of the fatty acids it needs *except for linoleic and linolenic acid*.

- Linoleic and linolenic acid can **only** be obtained through dietary triglycerides, and are therefore classified as **essential fatty acids**.

Protein Metabolism

When *dietary proteins* are digested, they are converted to *amino acids*. The *amino acids* are then used in various metabolic pathways.

- In an *anabolic* process, they are used to build proteins and peptides according to the body's needs. You learned about this process in chapter 14 when I discussed how proteins are synthesized in the *translation* process.
- *Amino acids* are also used as nitrogen sources for the biosynthesis of other amino acids and other nitrogen-containing compounds, such as nucleotide bases.

Amino acids that are ingested in excess of what is needed for these biosynthesis needs are catabolized to produce **ATP**.

Digestion of Proteins

In the digestion process, dietary proteins are converted to **amino acids** by the *hydrolysis* of their

_____ _____.

When a peptide bond is hydrolyzed, the peptide bond is broken and an oxygen is added to the carbonyl carbon and two hydrogens to the nitrogen.
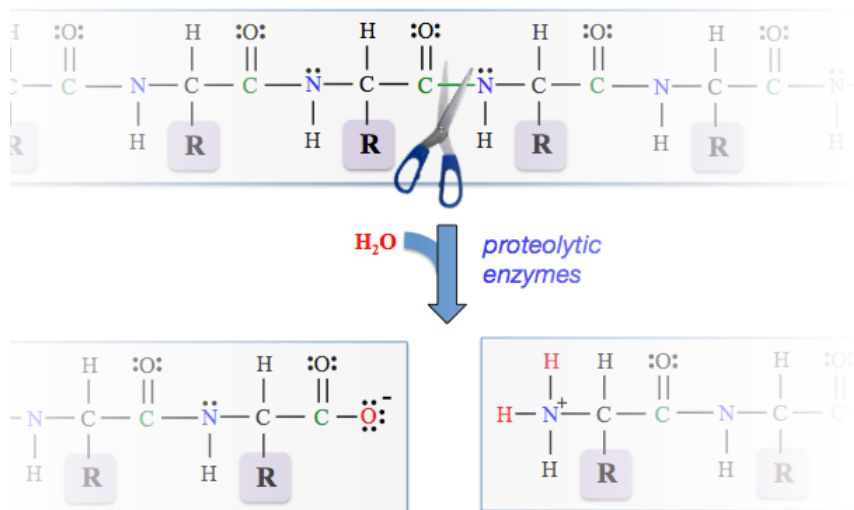
Protein digestion begins in the _____ and continues in the **small intestine**.
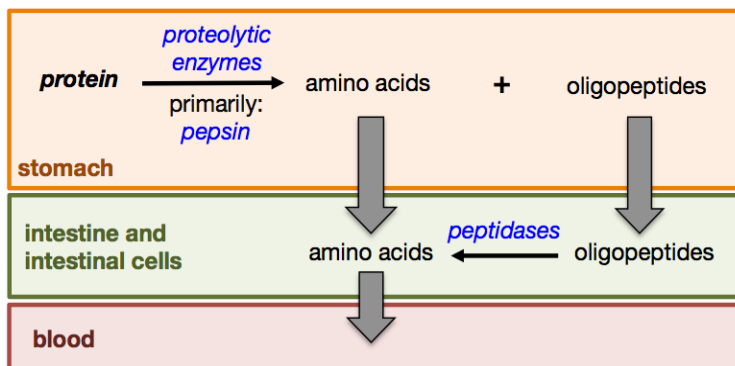
In the stomach, an acidic environment and proteolytic enzymes (primarily *pepsin*) catalyze the hydrolysis of proteins to *amino acids* and *oligopeptides*.

As these species move though the small intestine and enter the intestinal cells, the oligopeptides are further hydrolyzed to amino acids. This is done with the help of dietary enzymes called *peptidases*.

The amino acids are released from the intestinal cells into the blood stream, and then transported to other cells.

Understanding Check: Draw the structural formulas of the three amino acids that are produced when all of the peptide bonds in the tripeptide shown below are hydrolyzed.
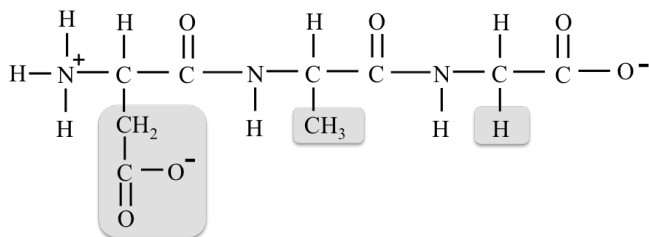
Catabolism of Amino Acids

Some of the amino acids produced in digestion are used for the synthesis of **proteins**, the synthesis of *other* **amino acids**, and the synthesis of *other* **nitrogen-containing compounds**.

Amino acids that are ingested in surplus of these biosynthesis needs are _____ as fuel for the production of **ATP**.

This is done by transforming them into intermediate metabolites that can be converted to _____, _____ _____, *or* undergo the _____ _____ _____.

The entry points of amino acids into the various metabolic pathways are indicated in the figure below.
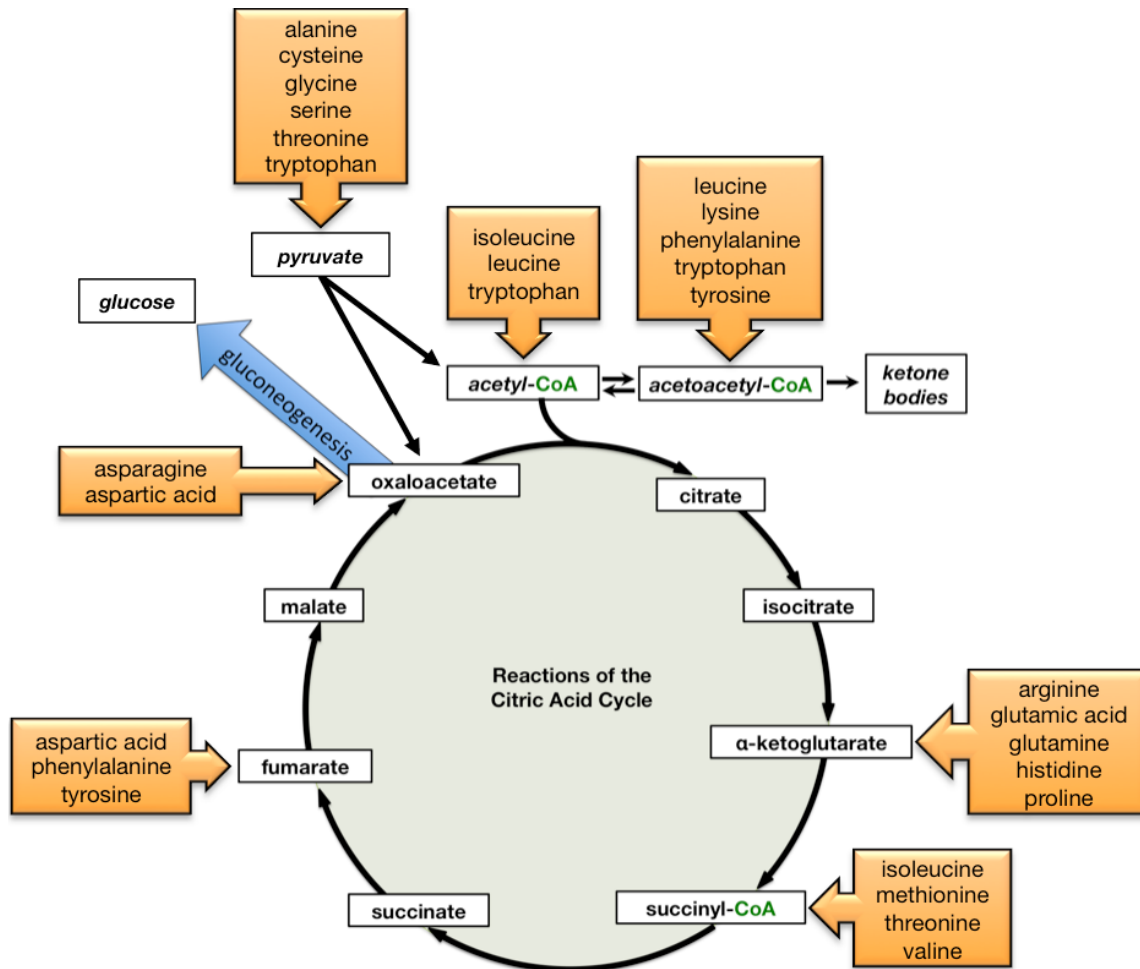
I do not expect students to memorize this table; however, there are a couple of important concepts that I want you to know:

1) Amino acids can be converted to pyruvate, acetyl-CoA, acetoacetyl-CoA, or some citric acid cycle intermediates. These compounds are then converted to glucose, ketone bodies, *or* undergo the citric acid cycle.

2) All *twenty common amino acids* can be converted into either pyruvate, acetyl-CoA, acetoacetyl-CoA, or a citric acid cycle intermediate.

   • The details of *how* the twenty common amino acids are converted into the metabolic intermediates are far beyond the scope of this course.

   • What is important to understand is that these conversions involve one or both of two important amino acid reactions: _____ and _____ _____.

Transamination

Transamination involves the _____ of a quaternary ammonium group (NH_3^+).

The NH_3^+ that is bound to the **α-carbon** of an amino acid is transferred to an **α-keto acid**.

- An **α**-keto acid is a *carboxylic acid* that has a **carbonyl group** ($C = O$) at the **α**-carbon.

In a *transamination reaction*, an amino acid and an **α**-keto acid are converted to a **new** amino acid and a **new α**-keto acid. The general form of the transamination reaction is shown below.

| an amino acid | an *α–keto* acid | | a new *α–keto* acid | a new amino acid |
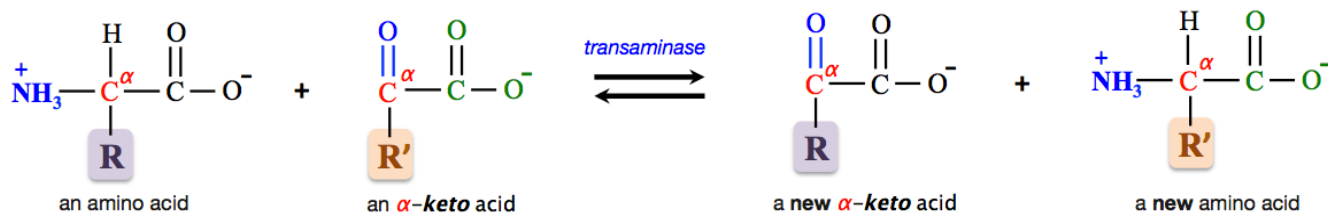
In *transamination reactions*, the NH_3^+ from an amino acid is **usually** transferred to **α-ketoglutarate** (an **α**-keto acid).

Example:

| alanine (Ala) (an amino acid) | α–ketoglutarate (an *α–keto* acid) | | pyruvate (a new *α–keto* acid) | glutamic acid (Glu) (a new amino acid) |
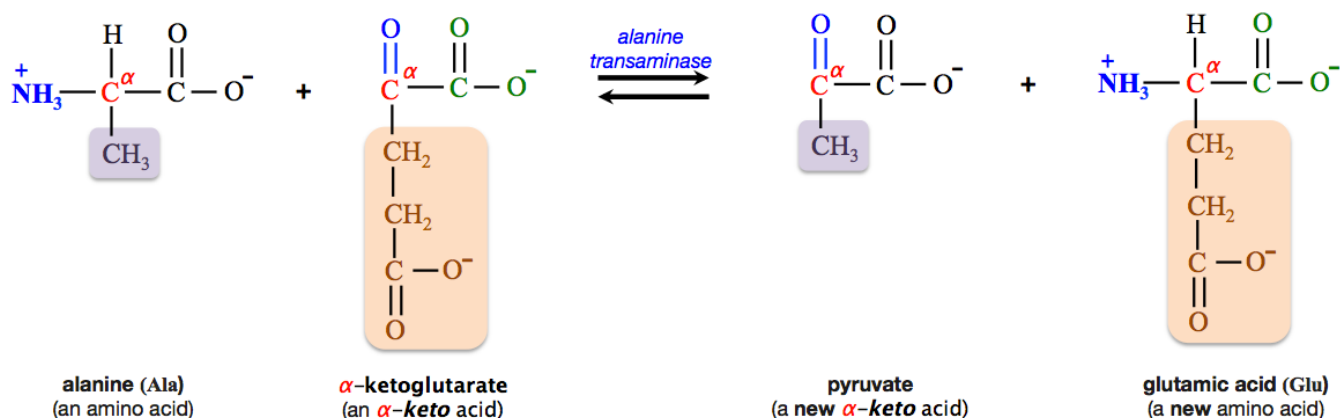
In this reaction, alanine is converted to pyruvate.

Another example of a *transamination reaction* is the conversion of aspartic acid to oxaloacetate, as shown below.

| aspartic acid (Asp) an amino acid | α–ketoglutarate an *α–keto* acid | | oxaloacetate a new *α–keto* acid | glutamic acid (Glu) a new amino acid |
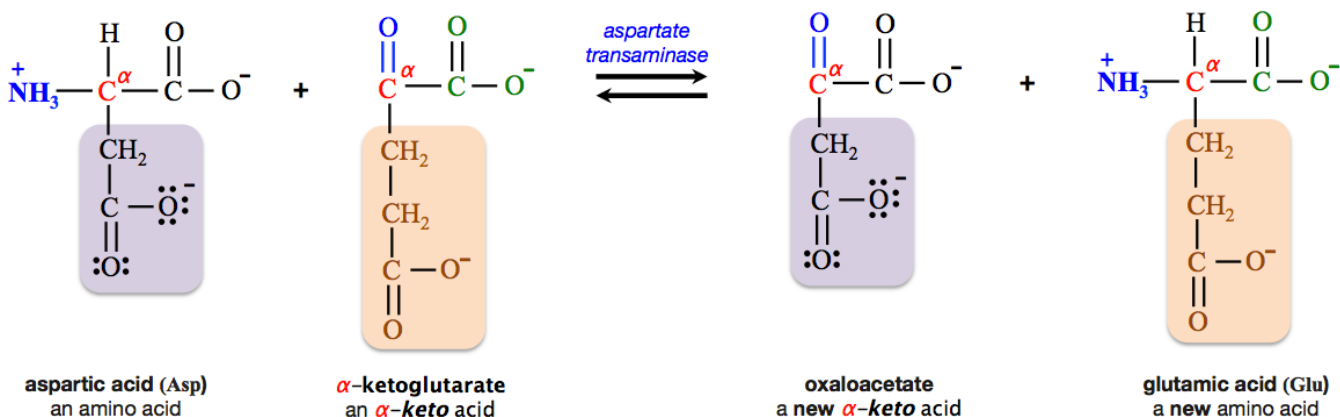
In transamination reactions, **α**-ketoglutarate is converted to *glutamic acid*. We will now take a look at how *glutamic acid* is recycled back to **α**-ketoglutarate in the **oxidative deamination** reaction.

Oxidative Deamination

In *oxidative deamination*, a *quaternary ammonium group* (-NH$_3^+$) is _____ from *glutamic acid,* thereby producing an ammonium ion (NH$_4^+$) and *α*-ketoglutarate.

glutamic acid (Glu)   α-ketoglutarate
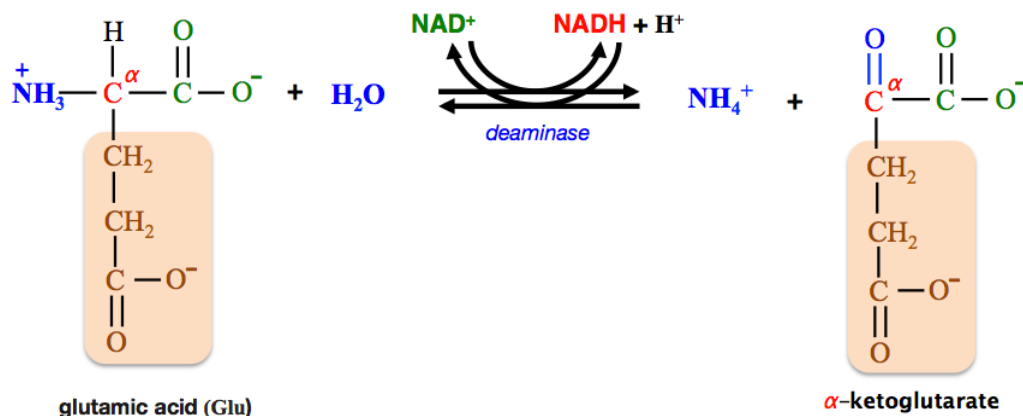
In addition to the removal of a *quaternary ammonium group*, *glutamic acid's* *α*-carbon is oxidized (gains an oxygen *and* loses a hydrogen). This oxidation is accompanied by the reduction of **NAD**$^+$.

The *α*-ketoglutarate that is produced in the reaction is now free to accept a _____ *quaternary ammonium group* from another amino acid in a *transamination reaction,* as illustrated below.
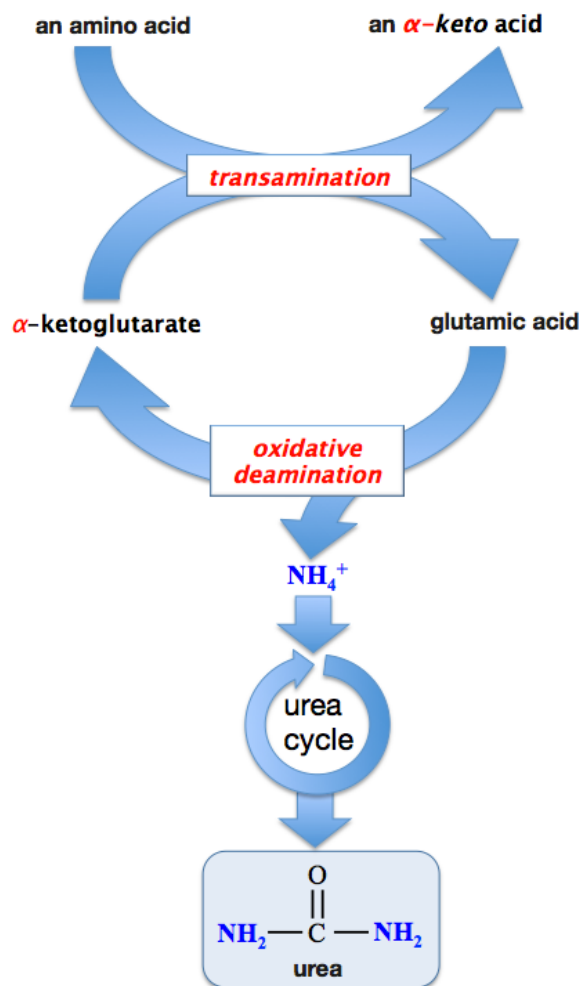
The free ammonium ions (NH$_4^+$) that are produced in oxidative deamination are ***toxic*** at elevated concentrations.

Humans and most other terrestrial vertebrates are capable of converting the ammonium ions to_____.

- This occurs in a series of reactions called the **urea cycle**.

Urea is filtered, by the _____, into the urinary track and then removed from the body during urination.

Kidney disease can result in the build up of dangerous amounts of urea.

In cases of ***end-stage renal (kidney) failure***, safe blood urea levels are exceeded, and patients must undergo _____ **treatments**.

Dialysis involves artificial methods of urea removal.

The most common of these is called **hemodialysis**. Hemodialysis takes several hours and is usually done multiple times per week. This process is not only time-consuming, but far from ideal because of many complications and side effects. Bedside nocturnal dialyzers are now available.

In otherwise healthy patients with kidney failure, kidney transplants are possible. Kidney donations are fairly common since most humans have two kidneys, and one kidney is usually sufficient to eliminate urea.

Understanding Check: Identify the following reaction as either a **transamination** _or_ an **oxidative deamination** reaction.

| valine (Val) an amino acid | α-ketoglutarate an α-keto acid | a new α-keto acid | glutamic acid (Glu) a new amino acid |
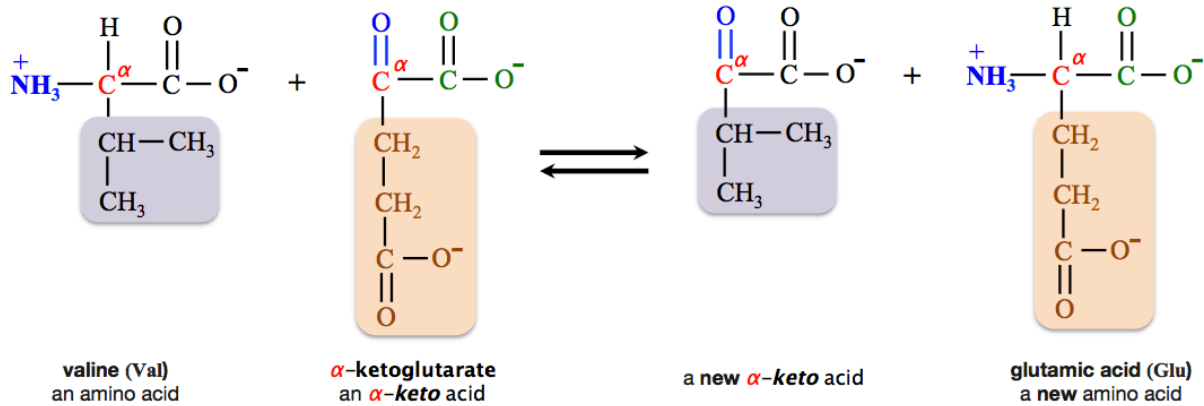
Summary of Metabolism

The body is able to build proteins, carbohydrates, and triglycerides from smaller organic compounds in anabolic processes.

- Anabolic processes generally require the input of external energy.
- This energy often comes from chemical potential energy in **ATP**.

The body is able to break down proteins, carbohydrates, and triglycerides into smaller organic compounds in catabolic processes.

- Catabolic processes typically release energy.
- This energy is often used by the body to produce **ATP**.

The metabolic strategy behind the production of **ATP** is that **ATP** is an energy source that can be instantaneously used by organisms to do cellular work and to provide the energy required for life-sustaining reactions that would otherwise not occur spontaneously.

The metabolic strategies of catabolism and anabolism are summarized in the illustration below.

40
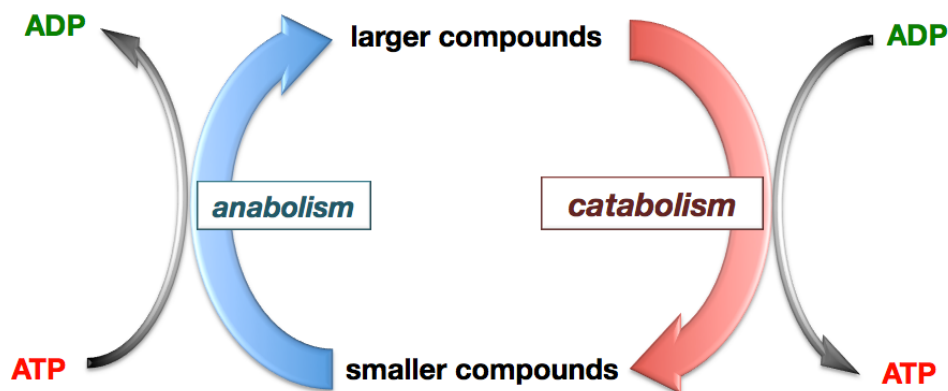
Catabolism

The catabolism of food is summarized in the image below:
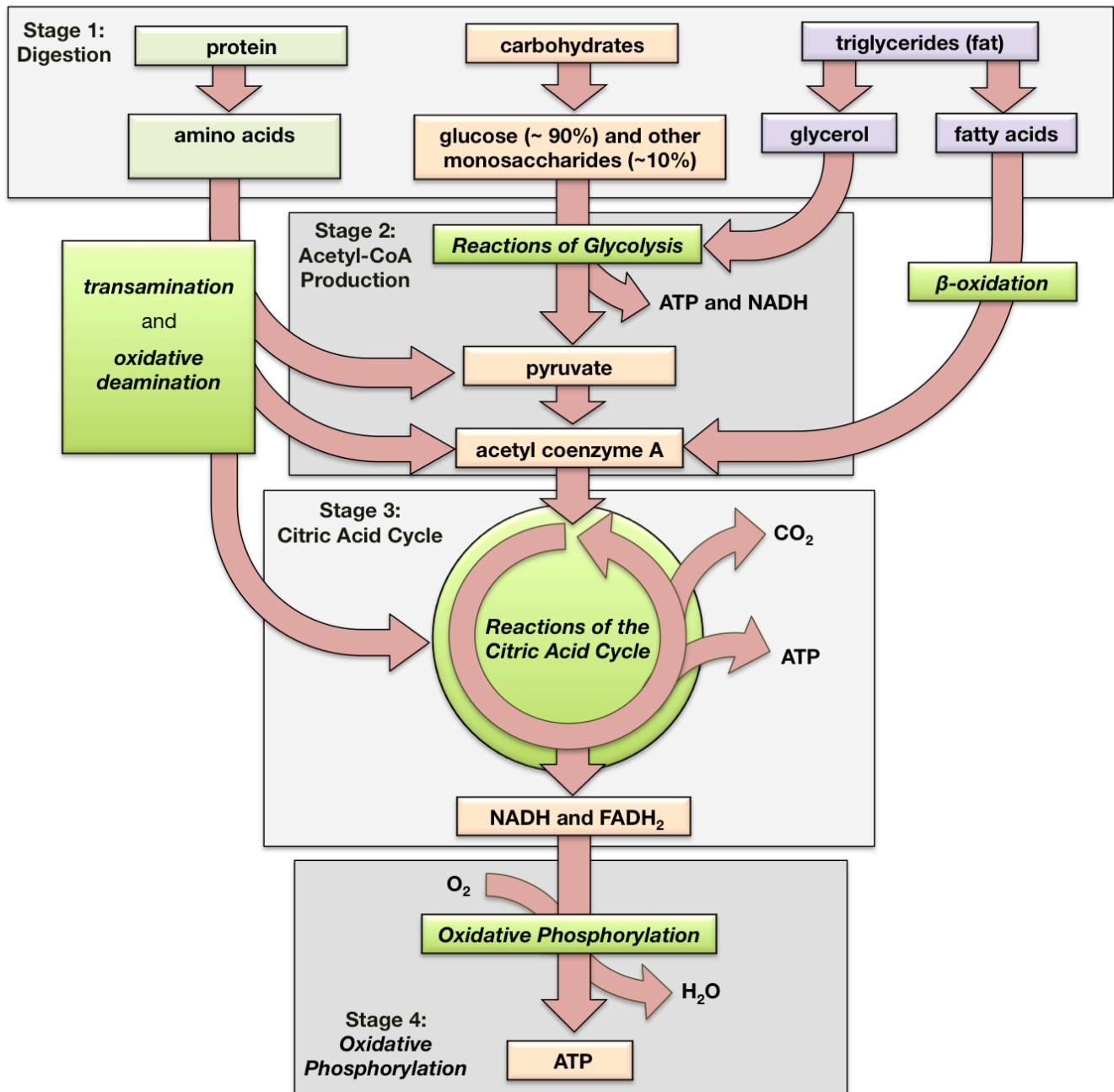
In the four stages of food catabolism, chemical potential energy in food is converted to chemical potential energy in ATP, NADH, and $FADH_2$.

- The NADH and $FADH_2$ can then be converted to electrochemical energy in the form of a hydrogen ion gradient.

- The electrochemical potential in this gradient is used to drive the production of ATP.

The **catabolic processes** discussed in this chapter are digestion, glycolysis, pyruvate oxidation/decarboxylation, the citric acid cycle, glycogenolysis, lipolysis, β-oxidation, and oxidative deamination.

These *catabolic processes* are listed and briefly described in the table below.

The Catabolic Processes in Chapter 15

Name	Description	Notes
digestion	**Carbohydrates** are *hydrolyzed* to **monosaccharides**. **Triglycerides** are "**partially**" *hydrolyzed* to **fatty acid salts** and **monoglyceride**. **Proteins** are *hydrolyzed* to **amino acids**.	
glycolysis	A **linear metabolic pathway** in which *glucose* is converted into **two** *pyruvate ions*.	**High** concentrations of **ATP**, *pyruvate*, or *other pathway products* suppress this process.
pyruvate oxidation/ decarboxylation	*Pyruvate* is oxidized and decarboxylated to produce *acetyl*-**CoA**.	
citric acid cycle	A **circular metabolic pathway** in which *acetyl*-**CoA** is metabolized to produce **ATP**, **NADH**, and **FADH$_2$**.	
glycogenolysis	*Glycogen* is converted to *glucose*. Glycogenolysis occurs primarily in **liver** and **muscle** cells. Liver cells will release the glucose into the bloodstream so that it can be taken in by other types of cells.	*Low blood glucose* and **glucagon** accelerate this process. **High blood glucose** and **insulin** suppress this process.
β-oxidation	A **spiral metabolic pathway** in which *fatty acids are converted to acetyl*-**CoA, NADH** and **FADH$_2$**.	
lipolysis	*Triglycerides* that are stored primarily in adipose (fat) cells and muscle cells are broken down into *fatty acids* and *glycerol*. Liver cells can release the fatty acids and glycerol into the bloodstream so that they can be taken in by other types of cells.	
oxidative deamination	A *quaternary ammonium group* (-**NH$_3^+$**) is removed from *glutamic acid*, thereby producing ammonium (**NH$_4^+$**) and *α*-ketoglutarate.	

Anabolism

The ***anabolic processes*** discussed in this chapter are gluconeogenesis, glycogenesis, fatty acid synthesis, and protein synthesis.

These *anabolic processes* are listed and briefly described in the table below.

The Anabolic Processes in Chapter 15

Name	Description	Notes
gluconeogenesis	The conversion of ***non-carbohydrate species into glucose***. This process is *similar* to the reverse of glycolysis. Gluconeogenesis occurs primarily in the liver. It increases blood glucose levels because liver cells can release the glucose that is produced into the bloodstream.	***Low blood glucose*** and ***glucagon*** accelerate this process.
glycogenesis	*Glucose* is converted to *glycogen.* Glycogenesis occurs primarily in **liver** and **muscle** cells. Glycogenesis lowers blood glucose levels because glucose is taken up by liver and muscle cells and then converted to glycogen.	***High blood glucose*** and ***insulin*** accelerate this process. ***Low blood glucose*** and ***glucagon*** suppress this process.
fatty acid synthesis	Fatty acids are produced by a spiral pathway that works in the opposite direction of **β**-oxidation; it builds up fatty acyl-CoA by a repeating series of reactions that add acetyl-CoA to a growing fatty acyl-CoA structure. Fatty acid synthesis occurs primarily in adipose and liver cells.	
protein synthesis	*Amino acids* are converted to *proteins.*	This process was mentioned briefly in this chapter; however, it was ***thoroughly discussed chapter 14***.

Chapter 15 Review Worksheet and Key

NOTE: You can view the key in the back of the document

1.   *Define the term* metabolic pathway.

2.   *Explain how it is possible that the initial reactant in glycolysis (glucose) has six carbons, but the product (pyruvate) has three carbons.*

3.   *What effect will an enzyme have on the value of ΔG for the reaction?*

4.   *What provides the energy used to produce ATP from ADP and P$_i$, anabolism or catabolism?*

5.   *Define the term reduction and explain how it applies to the difference in the structures of NAD$^+$ and NADH.*

6.   *How does anabolism differ from catabolism in terms of the relative size of the reactants that enter a particular pathway and the products that leave it?*

7.   *Write a reaction equation for the hydrolysis of ATP to produce P$_i$.*

8.   *Where (in the mouth, the stomach, or the small intestine) does digestion of each begin?*

        a.   polysaccharides

        b.   triglycerides

        c.   proteins

9.   *How do the structures of amylose and amylopectin, the two homopolysaccharides that make up starch, differ?*

10.   *What is the role of glycolysis?*

11.   *What compound acts as an inhibitor of glycolysis?*

12.   a. *What products are formed when pyruvate undergoes alcoholic fermentation?*

13.   a. *Is the conversion of pyruvate to lactate an oxidation or a reduction?*

        b. *When this reaction takes place in a cell, what is the oxidizing agent?*

        c. *What is the reducing agent?*

14.   *Is the conversion of pyruvate into acetyl-CoA an oxidation or a reduction?*

15.   *Glycolysis can be described as a process in which energy is invested "up front" in exchange for a greater return of energy later on. Which steps in glycolysis involve investment of energy?*

16. *Which three steps in glycolysis cannot be directly reversed during gluconeogenesis?*

17. *In the citric acid cycle, is the alcohol group in isocitrate oxidized, or reduced? Explain.*

18. *What is the net change in ATP, NADH, and $FADH_2$ from the passage of two acetyl-CoA through the citric acid cycle?*

19. a. *Which two compounds donate their electrons to electron transport chain?*

    b. *Which molecule is the final electron acceptor of the electron transport chain?*

20. *H^+ moves from the intermembrane space, through ATP synthase, and into the mitochondrial matrix. Which term best describes this process: facilitated diffusion or active transport?*

21. *Oxidative phosphorylation typically generates how many ATP from 1 NADH?*

22. *Account for the 30-32 ATPs generated when one glucose molecule is catabolized by glycolysis and the citric acid cycle.*

23. *Describe how fatty acid salts are activated in order to undergo β oxidation.*

24. *In one pass through the β oxidation spiral a fatty acyl-CoA is shortened by two carbon atoms. What other products are formed?*

25. *Calculate the net number of ATPs produced when one 18-carbon fatty acid salt is activated, enters the mitochondrion, and undergoes complete β oxidation.*

Include the ATP formed from acetyl-CoA in the citric acid cycle, and ATP from all of the reduced coenzymes that are produced.

26.   a. *Name the three ketone bodies.*

        b. *Are they all ketones?*

27.   *What is the source of NH_4^+ produced during amino acid catabolism?*

38.   *Oxidative deamination of glutamate produces which compound besides NH_4^+?*

Chapter 15 Review Worksheet KEY

1. *Define the term* metabolic pathway.

   A metabolic pathway is a series of biochemical reactions.

2. *Explain how it is possible that the initial reactant in glycolysis (glucose) has six carbons, but the product (pyruvate) has three carbons.*

   Because glucose is split into two 3-carbon compound in steps 4 and 5 of glycolysis. Ultimately, two pyruvate ions are formed.

3. *What effect will the enzyme have on the value of ΔG for the reaction?*

   No effect. An enzyme increases the rate of a reaction, but it has no effect on ΔG.

4. *What provides the energy used to produce ATP from ADP and P_i, anabolism or catabolism?*

   Catabolism

5. *Define the term reduction and explain how it applies to the difference in the structures of NAD^+ and NADH.*

   Reduction is the gain of electrons. In organic and biochemical molecules, a gain of hydrogen and /or a loss of oxygen is indication that reduction has taken place. NADH, the reduced form of the coenzyme, has one more hydrogen atom than NAD^+, the oxidized form of the coenzyme.

6. *How does anabolism differ from catabolism in terms of the relative size of the reactants that enter a particular pathway and the products that leave it?*

   During anabolism small molecules are combined to make larger ones. In catabolism larger molecules are broken down into smaller ones.

7. *Write a reaction equation for the hydrolysis of ATP to produce P_i.*

   $ATP + H_2O \rightarrow ADP + P_i + H^+$
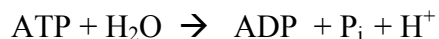
8. *Where in the body does the digestion of each begin?*

   a. polysaccharides

   Mouth

b. triglycerides

Mouth

c. proteins

Stomach

9.   *How do the structures of amylose and amylopectin, the two homopolysaccharides that make up starch, differ?*

Amylopectin contains α-$(1 \rightarrow 6)$ glycosidic bonds. Amylose does not.

10. *What is the role of glycolysis?*

Glycolysis converts a glucose molecule into 2 pyruvate ions with accompanying production of 2 ATP and 2 NADH.

11. *What compound acts as an inhibitor of glycolysis?*

ATP

12.   a. *What products are formed when pyruvate undergoes alcoholic fermentation?*

Ethanol and CO_2.

13.   a. *Is the conversion of pyruvate to lactate an oxidation or a reduction?*

In Figure 15.9, the conversion of pyruvate to lactate shows a ketone being converted to an alcohol by addition of hydrogen. This indicates reduction has occurred.

Reduction

b. *When this reaction takes place in a cell, what is the oxidizing agent?*

The oxidizing agent in a reaction is the substance that is reduced. Therefore, pyruvate is the oxidizing agent.

Pyruvate

c. *What is the reducing agent?*

The NADH is losing hydrogen and an electron. In doing so, it reduces the pyruvate and it is therefore the reducing agent.

NADH

14. *Is the conversion of pyruvate into acetyl-CoA an oxidation or a reduction?*

Oxidation: Organic oxidation is observed as the loss of hydrogen or the gain of oxygen. The conversion of pyruvate to acetyl-CoA results in the pyruvate losing hydrogen and an electron to NAD^+. Therefore the pyruvate is oxidized.

15. *Glycolysis can be described as a process in which energy is invested "up front" in exchange for a greater return of energy later on. Which steps in glycolysis involve investment of energy?*

Steps 1 and 3 involve "investment" or input of energy through coupling of the reaction with ATP hydrolysis.

16. *Which three steps in glycolysis cannot be directly reversed during gluconeogenesis?*

Steps 1, 3, and 10.

17. *In the citric acid cycle, is the alcohol group in isocitrate oxidized, or reduced?*

The alcohol is oxidized; it loses hydrogens.

18. *What is the net change in ATP, NADH, and FADH$_2$ from the passage of two acetyl-CoA through the citric acid cycle?*

The passage of two acetyl-CoA through the citric cycle creates 2 ATP, 6 NADH, and 2 FADH$_2$.

19. a. *Which two compounds donate their electrons to electron transport chain?*

NADH and FADH$_2$

b. *Which molecule is the final electron acceptor of the electron transport chain?*

The O_2 molecule.

20. *H^+ moves from the intermembrane space, through ATP synthase, and into the mitochondrial matrix. Which term best describes this process: facilitated diffusion or active transport?*

Facilitated diffusion is the process of ions or molecules moving through a membrane assisted by a protein. The hydrogens move through this enzyme because of the concentration gradient. No additional external energy is required.

Facilitated diffusion

21. *Oxidative phosphorylation typically generates how many ATP from 1 NADH?*

2.5 ATP

22. *Account for the 30-32 ATPs generated when one glucose molecule is catabolized by glycolysis and the citric acid cycle.*

In glycolysis, one glucose molecule yields 2 pyruvates, 2 ATP and 2 NADH. Depending on the system used to shuttle the electrons from NADH into mitochondria, these 2 NADH become 2 NADH or 2 $FADH_2$. Converting the 2 pyruvates into 2 acetyl-CoA's produces 2 NADH.

Two passes through the citric acid cycle starting with acetyl-CoA produces 2 ATP, 2 $FADH_2$, and 6 NADH.

In the electron transport chain, each $FADH_2$ generates 1.5 ATP and each NADH generates 2.5 ATP.

23. *Describe how fatty acid salts are activated in order to undergo β oxidation.*

Fatty acid salts are activated by the attachment of a coenzyme A (CoA) residue to produce fatty acyl-CoA.

24. *In one pass through the β oxidation spiral a fatty acyl-CoA is shortened by two carbon atoms. What other products are formed?*

One acetyl-CoA, one $FADH_2$, and one NADH

25. *Calculate the net number of ATPs produced when one 18-carbon fatty acid salt is activated, enters the mitochondrion, and undergoes complete β oxidation. Include the ATP formed from acetyl-CoA in the citric acid cycle, and ATP from all of the reduced coenzymes that are produced.*

Activation in the first step **consumes** on ATP. Each step in the spiral produces one $FADH_2$, one NADH and one acetyl-CoA. The number of passes = (number of carbons – 2)/2 so for an 18-carbon fatty acid salt there are (18-2)/2 = 8. The NADH and $FADH_2$ produced in these passes produces ATP as follows:

.

$FADH_2$	NADH
8 x 1.5 = 12 ATP	8 x 2.5 = 20 ATP

Total from β oxidation reactions = 32 ATP

Then, since two ATPs are generated in the final cycle, a total of 9 acetyl-CoA enter the citric cycle.

The ATP produced as these 9 acetyl-CoA undergo the reactions of the citric acid cycle is calculated as follows:

9 Acetyl-CoA (1 ATP per citric acid cycle) = 9 ATP

NADH	$FADH_2$
(9 x 3) x 2.5 = 67.5 ATP	9 x 1.5 = 13.5 ATP

Total ATP produced from acetyl CoA = (9 + 67.5 + 13.5) = 90 ATP
Total ATP for reaction =
Total from β oxidation reactions + Total of citric cycle - Activation
$$= 32\ ATP\ + 90\ ATP - 1\ ATP$$
$$= 121\ ATP$$

Total ATPs produced = 121

26. a. *Name the three ketone bodies.*

Acetoacetate, 3-hydroxybutyrate, and acetone

b. *Are they all ketones?*

No. 3-Hydroxybutyrate contains does not contain the ketone bonding pattern.

27. *What is the source of NH$_4^+$ produced during amino acid catabolism?*

The release of NH$_4^+$ from amino acids commonly requires two reactions. The first is transamination, wherein an amino group from an amino acid is transferred to an α-keto acid. The second is oxidative deamination, wherein the amino group is replaced by a carbonyl group. The amino group is released as NH$_4^+$.

Oxidative deamination

38. *Oxidative deamination of glutamate produces which compound besides NH$_4^+$?*

α-ketoglutarate