Chapter 4 Lecture Notes

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

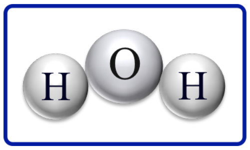
Step 1: Count the total number of ________________ _________________ from all the atoms in the molecule.

Example: H_2O

2 H atoms $2 \times 1e^- = 2e^-$

1 O atom $1 \times 6e^- = \underline{6e^-}$

Total number of valence e- $= 8e$-



The line bond structure of H_2O will have 8 electrons

Step 2: Draw the "Skeleton Structure"

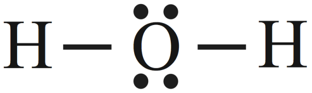
- Attach the atoms together with ___________ ___________in the most symmetric way possible.

H— O —H

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

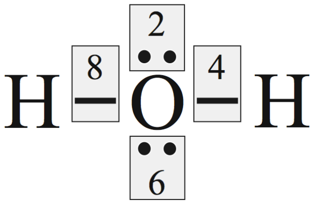
Total number of valence e^-	$8e^-$
Minus electrons used in skeleton	$\underline{-\ 4e^-}$
Electrons remaining **to be added** =	$4e$-

Step 4: Add the remaining electrons as ______________ _____________ as evenly as possible on all atoms except hydrogen.



Step 5: Check for ______________.

– Are there 8 electrons around all atoms (except hydrogen)?
If YES, you are finished!

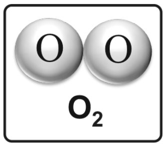


Step 6 (if needed): Use lone pairs to make ________________ or _________________ bonds until the octet rule is satisfied for *all atoms* in the molecule.

- 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?



2 O atoms 2 x $6e^- = 12e^-$
Total number of valence e^- $= 12e^-$

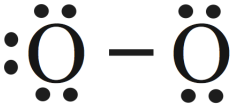
Step 2: Draw the "Skeleton Structure"
-Attach the atoms together with single bonds in the most symmetric way possible.

$$O - O$$

Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

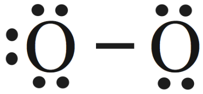
Total number of valence e^-	$12e^-$
Minus electrons used in skeleton	$\underline{-\ 2e^-}$
Electrons remaining *to be added* =	$10e$-

Step 4: Add the remaining electrons as lone pairs as evenly as possible on all atoms except hydrogen.



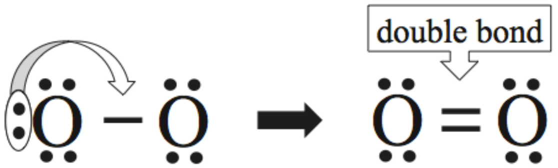
Step 5: Check for Octets

– Are there 8 electrons around all atoms (except hydrogen)?



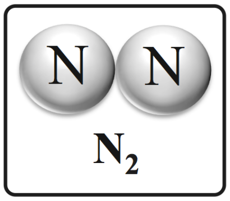
– If NO, use lone pairs to make double or triple bonds.

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.



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 $2 \times 5e^- = 10e^-$

Total number of valence e^- $= 10e^-$

Step 2: Draw the "Skeleton Structure"

-Attach the atoms together with single bonds in the most symmetric way possible.

N — N

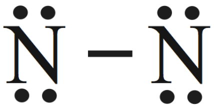
Step 3: Subtract the number of electrons used to make the skeleton structure from the total number of valence electrons.

Total number of valence e^- $10e^-$

Minus electrons used in skeleton $\underline{-\ 2e^-}$

Electrons remaining *to be added* = $8e$-

Step 4: Add the remaining electrons as lone pairs as evenly as possible on all atoms except hydrogen.

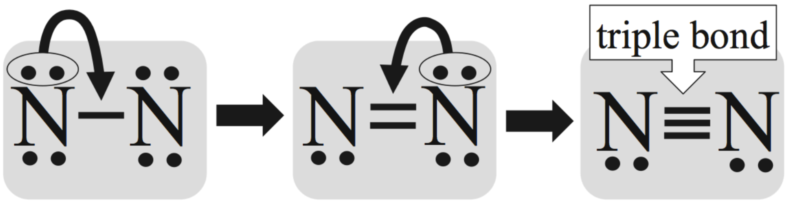


Step 5: Check for Octets

– 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.



Draw the line bond structure for ammonia: **NH_3**

Step 1: Count the total number of valence electrons from all the atoms in the molecule.

Molecular formula of molecule ________

Atom	Number of atoms		Number of valence electrons per atom	Totals
N	1	x		=
H	3	x		=

Total # of electrons in line bond structure =______

Step 2: Draw the "Skeleton 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: **SO_3**

Step 1: Count the total number of valence electrons from all the atoms in the molecule.

Molecular formula of molecule ________

Atom	Number of atoms		Number of valence electrons per atom	Totals
				=
				=

Total # of electrons in line bond structure =______

Step 2: Draw the "Skeleton 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**.

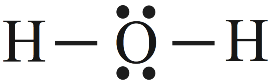
Step 6 (if needed): Use lone pairs to make **double** or **triple** bonds until the octet rule is satisfied for all atoms in the molecule.

Structural Formulas

A **molecular formula** shows us the number and types of atoms contained in a molecule.

- **Example** of a ***molecular formula***: H_2O

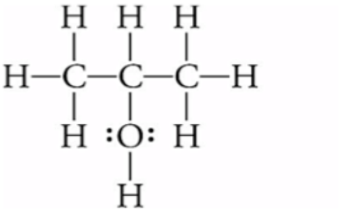
Drawings, such as *line bond structures*, that show the _________________of atoms within molecules are called _________________**formulas.**

- **Example** of a ***structural formula***: 

Structural Formulas vs. Molecular Formulas

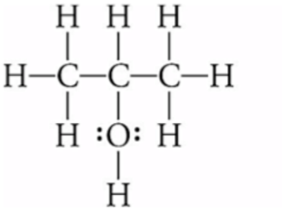
The **molecular formula** of *isopropyl alcohol* (often called rubbing alcohol) is C_3H_8O.

The **structural formula** of *isopropyl alcohol* is:

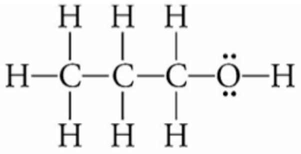


Which of these two types of formulas, the ***molecular formula*** or the ***structural formula***, do you think is more informative?

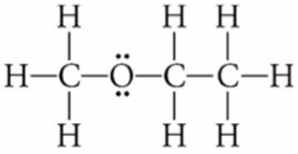
There are actually **three *completely different molecules*** that have this same molecular formula of **C_3H_8O**:



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***

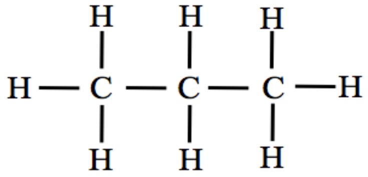
Condensed Structural Formulas (Condensed Structures)

When drawing **condensed structures**:

- Single bonds between carbon and hydrogen ***are omitted***.
    - **Example:** a carbon bonded to three hydrogen atoms is drawn as "**CH_3**"
- 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***.

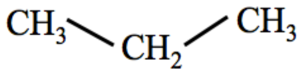
Example: Propane (C_3H_8)

The **connectivity** of the carbon and hydrogen atoms can be seen ___________ in propane's ***line bond structure***:



In ***condensed structures***, ____________bonds between carbon and hydrogen atoms ***are omitted***. We can draw the condensed structure of propane as:

$CH_3-CH_2-CH_3$ or

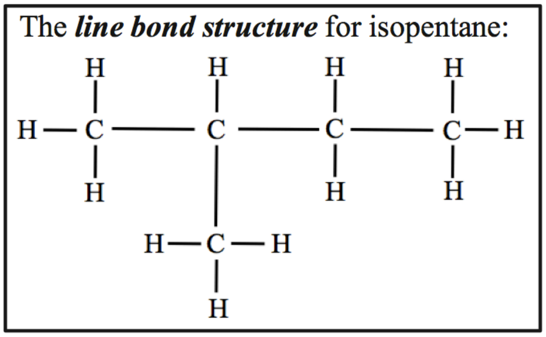


When drawing condensed structures, for ***non*** auto-graded use, carbon-carbon single bonds can be omitted when the carbon atoms are in a ____________ _______________ such as the three carbons in propane:

$$CH_3CH_2CH_3$$

Even though not all of the bonds are drawn in condensed structures, they are ____________and can be *unequivocally* known.

Example: Isopentane (C_5H_{12})

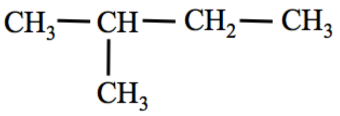


The ***line bond structure*** for isopentane:

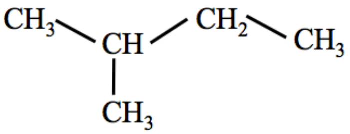
In isopentane, there are four carbons bonded in a ***linear sequence***.

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:

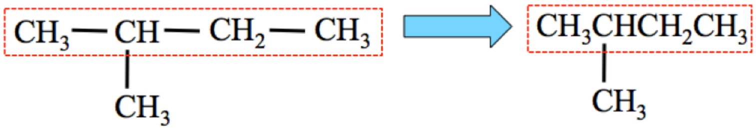


$CH_3-CH(CH_3)-CH_2-CH_3$ or



When you are asked to draw *condensed structures* for auto-graded, online problem sets you should draw **all of the carbon-carbon bonds** *as shown* ***above***.

- For **non auto-graded** use, 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).

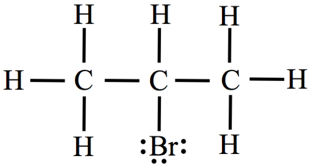


$CH_3-CH(CH_3)-CH_2-CH_3 \rightarrow CH_3CH(CH_3)CH_2CH_3$

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.

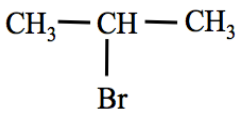
Example: Isopropyl bromide (C_3H_7Br)

The ***line bond structure*** of isopropyl bromide is:



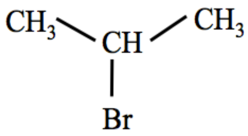
In ***condensed structures***, single bonds between atom pairs ***other than*** **C-C**, **C-H**, **O-H**, and **N-H** are ***always drawn***.

- Therefore the **C-Br** bond is drawn in the condensed structures:



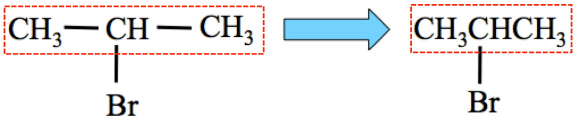
$CH_3-\underset{\underset{Br}{|}}{CH}-CH_3$

<u>or</u>



- Lone pairs ***can be omitted*** in condensed structures.

- For **non auto-graded** use, 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.



$CH_3-\underset{\underset{Br}{|}}{CH}-CH_3 \rightarrow CH_3\underset{\underset{Br}{|}}{CH}CH_3$

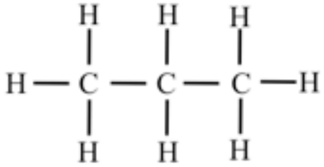
Skeletal Structural Formulas (Skeletal Structures)

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 (C_3H_8)



Line Bond Structure

$CH_3-CH_2-CH_3$

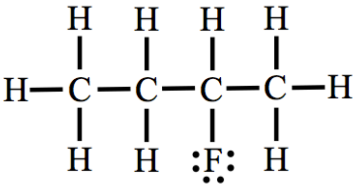
Condensed Structure

Skeletal Structure

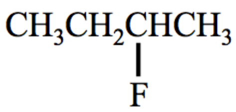
If the hydrogens bonded to carbon are omitted from skeletal structures, how do we determine how many hydrogens are bonded to each carbon? The answer to this is quite simple and is related to the octet rule:

- 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

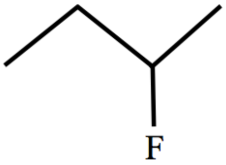


Line Bond Structure



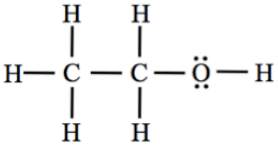
$CH_3CH_2\underset{F}{\underset{|}{C}}HCH_3$

Condensed Structure



Skeletal Structure

Example: Ethanol



Line Bond Structure

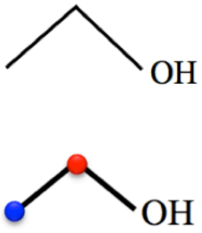
$CH_3—CH_2—OH$

online, auto-graded style

$CH_3CH_2—OH$ **or** CH_3CH_2OH

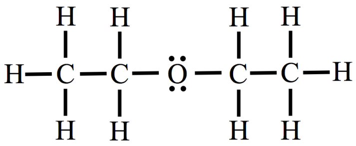
acceptable non auto-graded styles

Condensed Structure



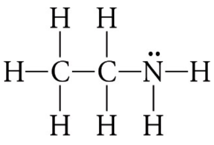
Skeletal Structure

Understanding Check: Draw **condensed *and* skeletal structur** of diethyl ether.



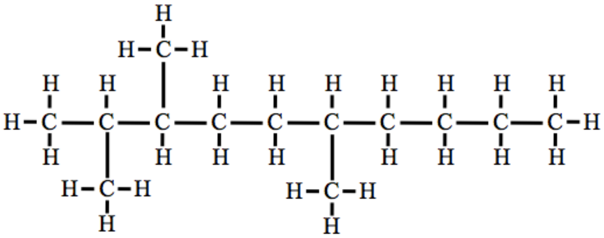
diethyl ether

Understanding Check: Draw **condensed *and* skeletal structure** of ethylamine.



ethylamine

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.

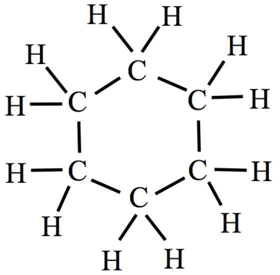


Structural Formulas of Cyclic Compounds

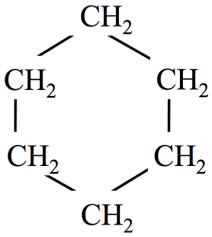
Many compounds contain atoms bonded, not in a *linear sequence*, but in a "**ring**" pattern.

Molecules that contain rings of atoms are called ______________ compounds.

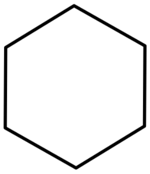
- An example of a *cyclic compound* is a molecule called cyclohexane. The three structural formulas for cyclohexane are:



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.

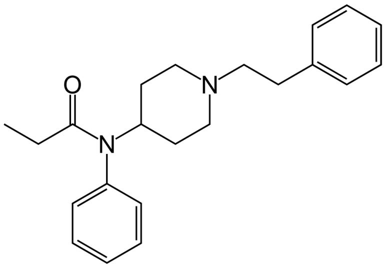
Structural formulas, whether line bond, condensed, or skeletal, are either **one-** or **two-dimensional**.

Most molecules are ____________ ***dimensional***.

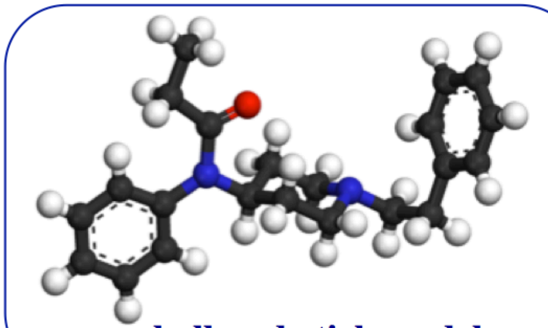
- Line bond structures are commonly drawn with the lines/bonds at 90° angles, but the **bond angles** in molecules (the angle between covalent bonds), with rare exceptions, are not at 90°.
- Skeletal and condensed structures often use bond angles of 90° or approximately 120° only for convenience in depicting the bonding pattern connectivity, not necessarily to represent the actual bond angles/geometry of the molecule.

Example: Fentanyl

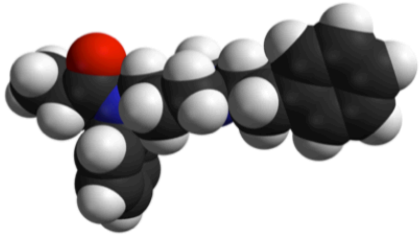
The ***skeletal structure*** of fentanyl is:



The "***geometry***" of the molecule can be depicted in two types of views:



ball-and-stick model

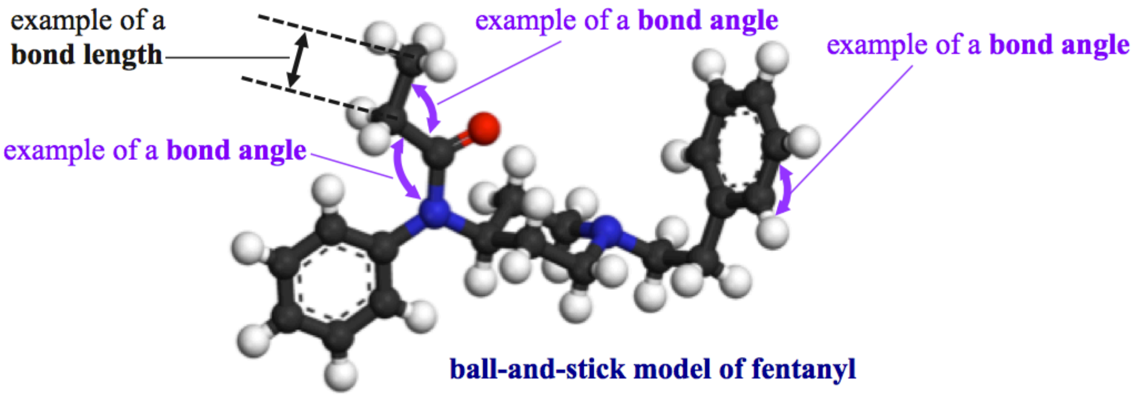


space-filling model

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.

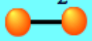
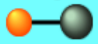
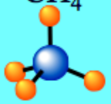
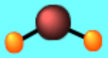


ball-and-stick model of fentanyl

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 **<u>one</u> central atom** with ***all other*** atoms bonded to the central atom	CH_4 	H_2O 
Large Molecule	Larger than *Small Molecule*; there **is <u>not</u> just one single, central atom** with **<u>all</u>** 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***.

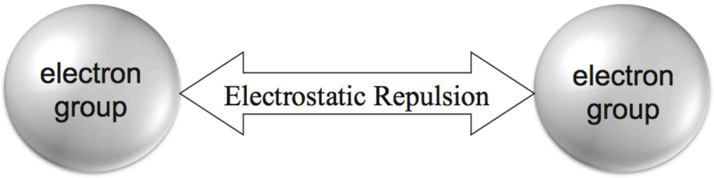
- Examples: H_2 and HCl

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**.*

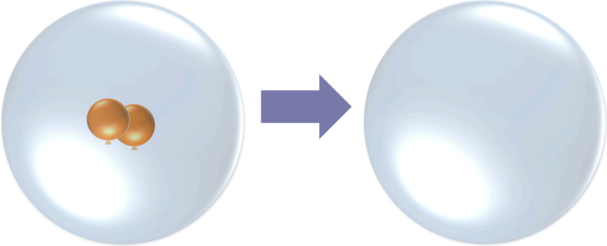
(2) **A** _________ __________ (**on** the *atom of interest*).

- 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 ______________ ________________.

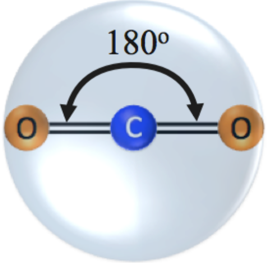
Draw the line bond structure for **CO_2**.

The central atom (C) goes in the _____________ of the sphere.

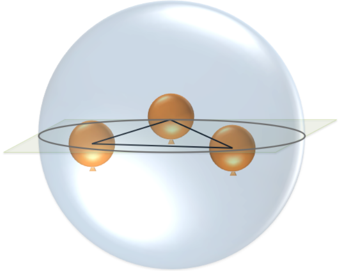
- There are _______ electron groups around the central atom!
- Each bonded atom counts as ______ electron group.

The electron groups are placed as _________ apart from each other as possible!

Both electron groups are on the same _______ and are at a ________ angle.



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.

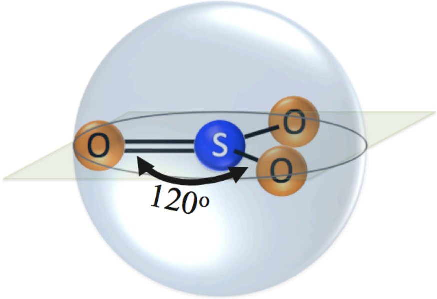
The same thing happens with ***electron groups***.

Draw the line bond structure for **SO_3**.

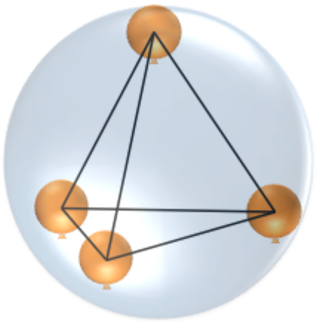
The central atom (S) goes in the middle of the sphere.

There are _______ electron groups around the central atom!

All electron groups are on the same ________ and are at _______ angles.



Example: 4 Electron Groups

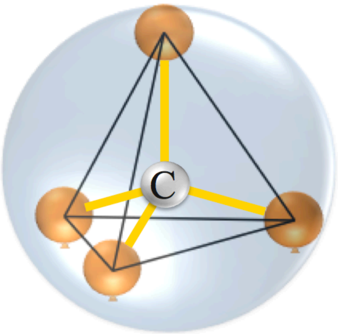


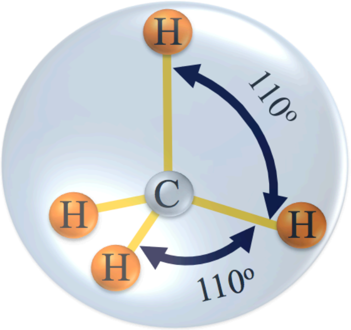
If 4 negatively charged balloons are placed into a hollow, clear plastic sphere, electrostatic repulsion will cause the balloons to move as far apart from each other as possible.

The same thing happens with ***electron groups***.

Draw the line bond structure for a methane molecule (**CH_4**).

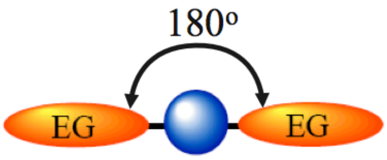
The central atom (C) goes in the middle of the sphere.
How many electron groups are around the central atom?
There are <u>**4**</u> electron groups around the central atom!
The electron groups are placed as far apart from each other as possible!



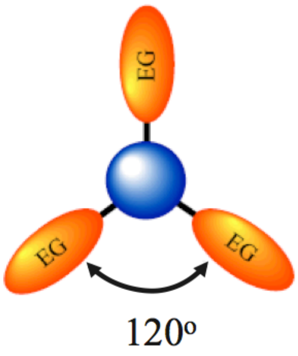


This arrangement is a 4-sided, 3-dimensional structure with electron groups at about __________ angles.

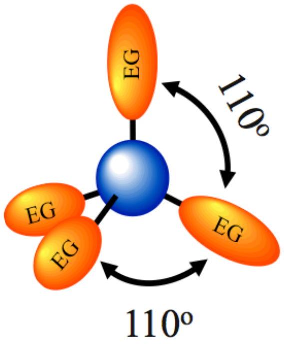
Electron Arrangement Review



2 Electron Groups



3 Electron Groups

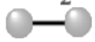
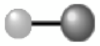


4 Electron Groups

For two or three electron groups, the angles will deviate slightly from **120º** and **110º** 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.

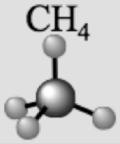
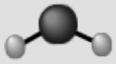
The Geometry of Diatomic Molecules

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 ***<u>all</u> 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

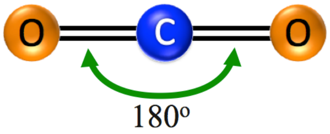
Step 1. Get the Electron Group Arrangement

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.



This molecular shape is called ________________________.

A very helpful tool for determining **molecular shape** is called the "**ABE Method**."

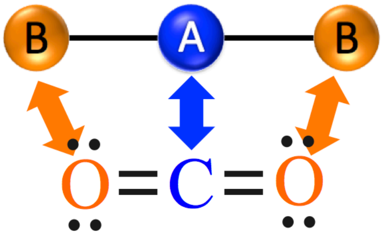
"**A**" represents the central atom (**carbon** in our **CO_2** example).

"**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***)

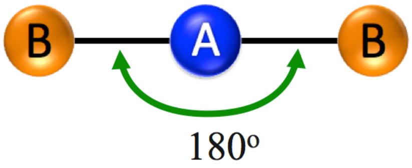


The **ABE** Method uses a "general notation" that indicates the type and number of __________ ___________ (**B** or **E**) that surround the central atom (**A**).

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 "$\mathbf{B_2}$."

All AB_2 molecules have _______ **bond angles** and are in the ______________ **molecular shape** category.



Molecular Shape Table

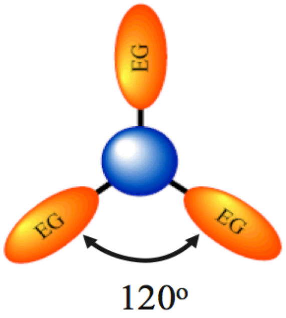
		Number of Lone Pairs		
		0 Lone Pairs	1 Lone Pair	2 Lone Pairs
Number of Electron Groups (EG)	2 EG			
	3 EG			
	4 EG			

Three Electron Groups

Example: Draw the line bond structure of **SO_3**

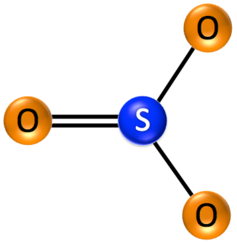
Step 1. Get the Electron Group Arrangement

- The number of electron groups *around the central atom* determines the **bond angles**.

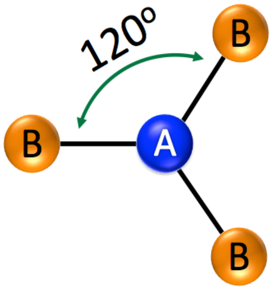


3 Electron Groups

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.



This molecular shape is called ______________ ___________________.



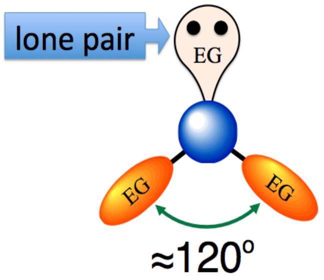
We write the **ABE** Method notation for SO_3 and ***all*** other small molecules that have ***three* bonded atoms** and ***no*** lone pair *on the central atom* as "________."

- There are three oxygens bonded to the central atom therefore we write "$\mathbf{B_3}$."

All AB_3 molecules have _______ **bond angles** and are in the ***trigonal planar*** molecular shape category.

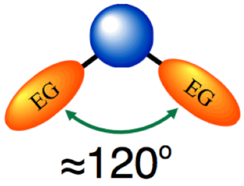
Example: Draw the line bond structure of **ozone gas (O_3).**

Step 1. Get the Electron Group Arrangement



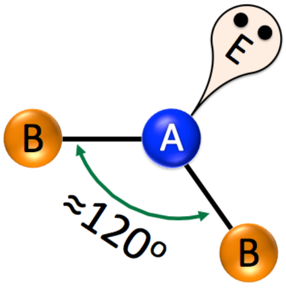
- The number of electron groups *around the central atom* determines the **bond angles**.
  - **Three electron groups:** 120° angles, all electron groups are on the same plane as the central atom. Angles will deviate **slightly** from 120° if *one of the electron groups* is a ***lone pair***.

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 "__________."

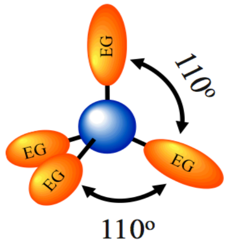
- There are two oxygens bonded to the central atom therefore we write "$\mathbf{B_2}$."
- There is **one lone pair** on the *central atom* therefore we write "**E**."

All AB_2E molecules have _________ **bond angles** and are in the ***bent*** molecular shape category.

Four Electron Groups

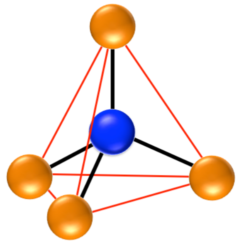
Example: Draw the line bond structure of **methane gas (CH_4).**

Step 1. Get the Electron Group Arrangement



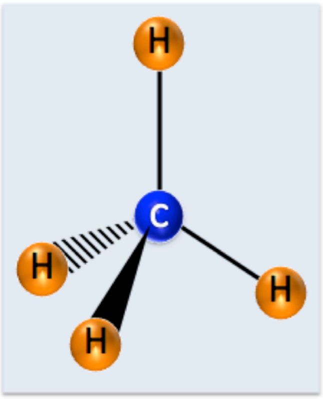
- The number of electron groups *around the central atom* determines the **bond angles**.
  - **Four electron groups:** 110° angles, occupies three dimensions in space

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

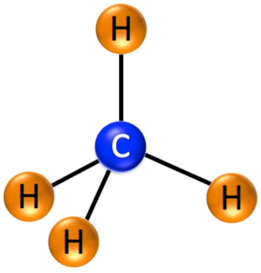


This molecular shape is called ________________________ .

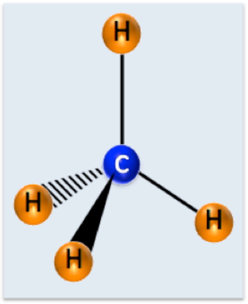
We often use a __________ _____ _________ representation in order to illustrate a three-dimensional molecule on a two-dimensional surface such as a page or computer screen.



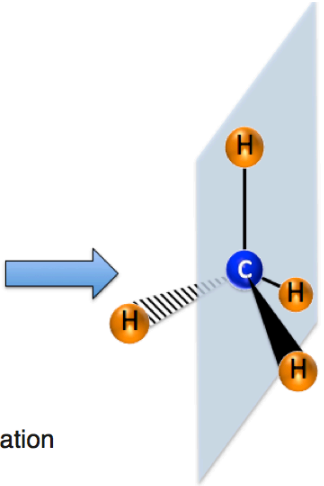
a wedge and dash representation



a perspective representation



a wedge and dash representation

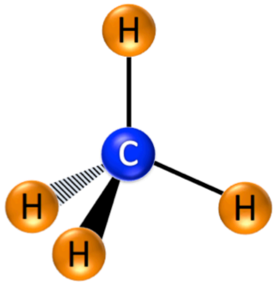


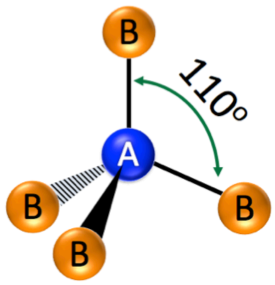
The implication of a wedge and dash representation

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.



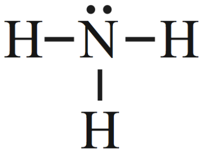


We write the **ABE** Method notation for CH_4 and ***all*** other small molecules that have ***four* bonded atoms** and ***no*** lone pair *on the central atom* as "__________."

- There are four hydrogens bonded to the central atom therefore we write "**B_4**."

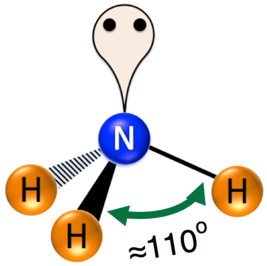
All AB_4 molecules have ________ **bond angles** and are in the ***tetrahedral*** molecular shape category.

Four Electron Group Example: Consider the line bond structure of **ammonia** (**NH_3**)**.**



$$\begin{array}{c} H-\ddot{N}-H \\ | \\ H \end{array}$$

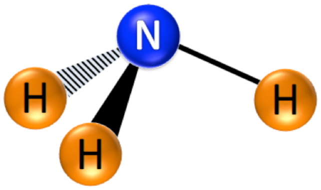
Step 1. Get the Electron Group Arrangement



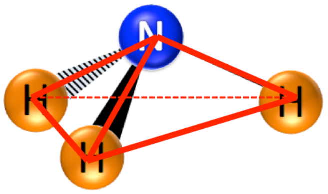
- The number of electron groups *around the central atom* determines the **bond angles**.
    - **Four electron groups:** 110° angles, occupies three dimensions in space. Angles will deviate **slightly** from 110° if *one or more of the electron groups* is a ***lone pair***.

Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

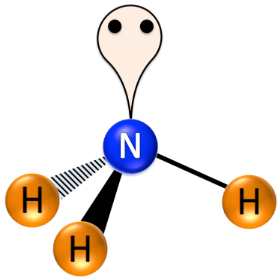
- When determining **molecular shape**, we treat lone pair(s) as if they were **invisible**!

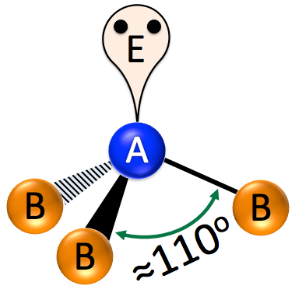


This molecular shape is called _______________.



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 "_________."

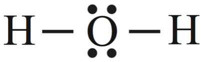




- There are three hydrogens bonded to the central atom therefore we write "**B_3**."
- There is **one lone pair** on the *central atom* therefore we write "**E**."

All AB_3E molecules have ________ **bond angles** and are in the ***pyramidal*** molecular shape category.

Four Electron Group Example: Consider the line bond structure of a **water molecule (H_2O):**

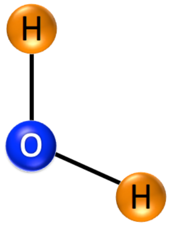


$\mathrm{H}-\ddot{\underset{\cdot\cdot}{\mathrm{O}}}-\mathrm{H}$

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***.

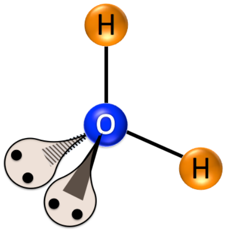
Step 2. Determine the Molecular Shape Category Based on the Arrangement of Atoms.

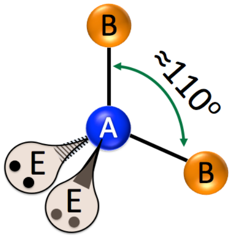


- When determining **molecular shape**, we treat lone pair(s) as if they were **invisible**!

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 "_________."





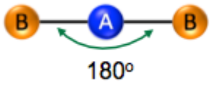
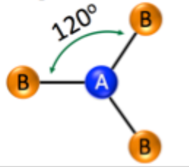
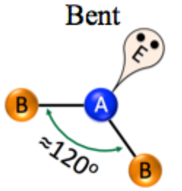
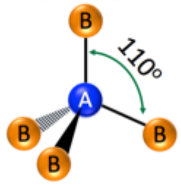
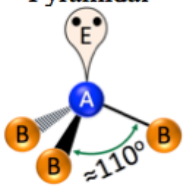
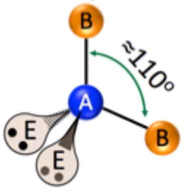
- There are two hydrogens bonded to the central atom therefore we write "$\mathbf{B_2}$."
- There are **two lone pairs** on the *central atom* therefore we write "$\mathbf{E_2}$."

All AB_2E_2 molecules have __________ **bond angles** and are in the ***bent*** molecular shape category.

Molecular Shape Table

Number of Lone Pairs

Number of Electron Groups (EG)

	0 Lone Pairs	1 Lone Pair	2 Lone Pairs
2 EG	AB_2 Linear 		
3 EG	AB_3 Trigonal Planar 	AB_2E Bent 	
4 EG	AB_4 Tetrahedral 	AB_3E Pyramidal 	AB_2E_2 Bent 

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

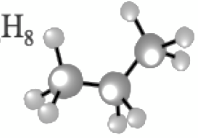
b) H_2S

c) SO_2

d) CS_2

e) carbon tetrachloride

The Molecular Geometry of Large Molecules

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 

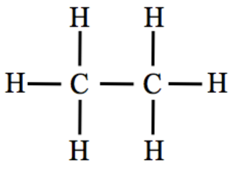
The **bond angles** around any _________ *of interest* in a **large molecule** can be predicted in the same manner that we used for small molecules.

- 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.

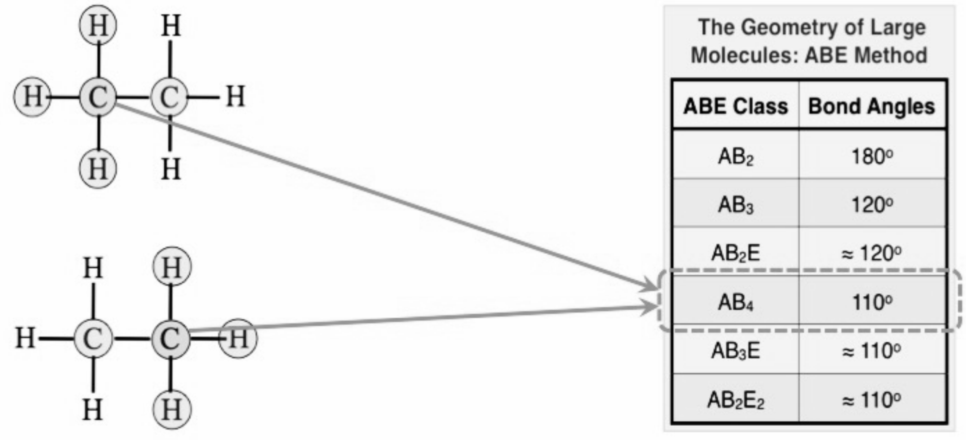
The Geometry of Large Molecules: ABE Method

ABE Class	Bond Angles
AB_2	180°
AB_3	120°
AB_2E	≈ 120°
AB_4	110°
AB_3E	≈ 110°
AB_2E_2	≈ 110°

Example: Consider the line bond structure of an ethane molecule:



What are the ***bond angles*** around **each** of the **carbon atoms** in an ethane molecule?



The Geometry of Large Molecules: ABE Method

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AB_2	180°
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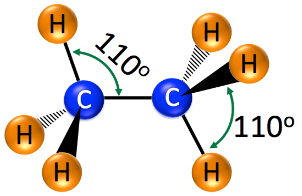
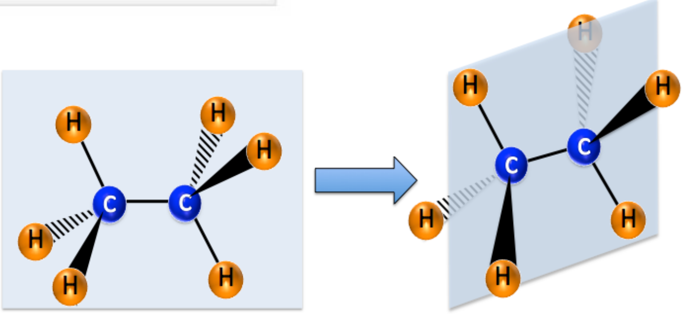
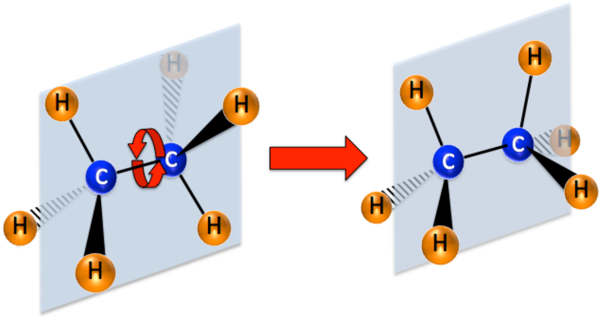
AB_2E_2	≈ 110°



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.

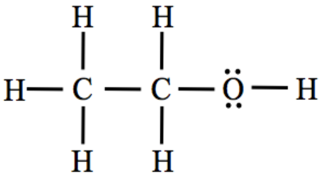


The reason for this is that _______bonds can "_________" and therefore large molecules are **always *changing their shape***.

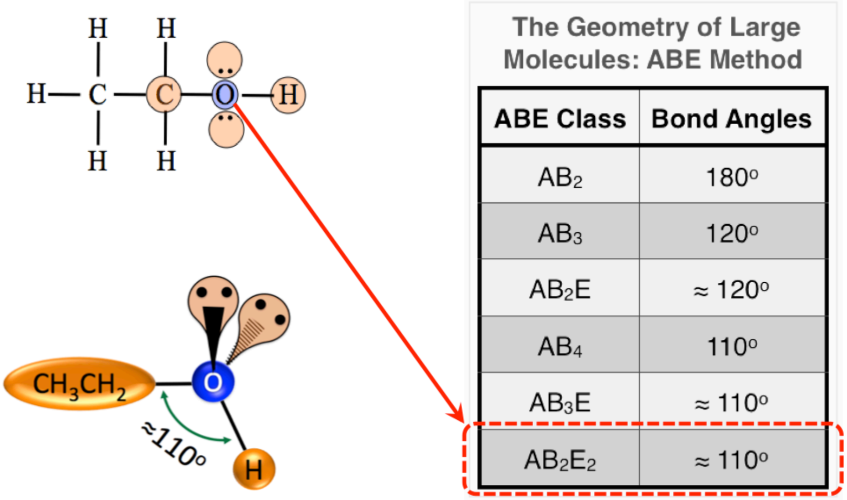
It is important to understand that although single bonds are capable of rotation, ***the bond angles around any particular atom do not change upon rotation***.

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?

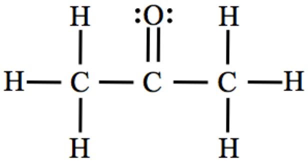


The Geometry of Large Molecules: ABE Method

ABE Class	Bond Angles
AB_2	180°
AB_3	120°
AB_2E	≈ 120°
AB_4	110°
AB_3E	≈ 110°
AB_2E_2	≈ 110°

Understanding Check: Predicting Bond Angles in Large Molecules

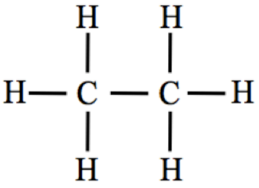
Consider the line bond structure of an acetone molecule:

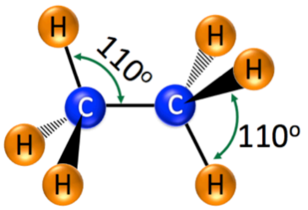


a) What are the bond angles around the left-most carbon atom?
b) What are the bond angles around the carbon atom in the middle of the molecule?
c) What are the bond angles around the right-most carbon atom?

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:





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.

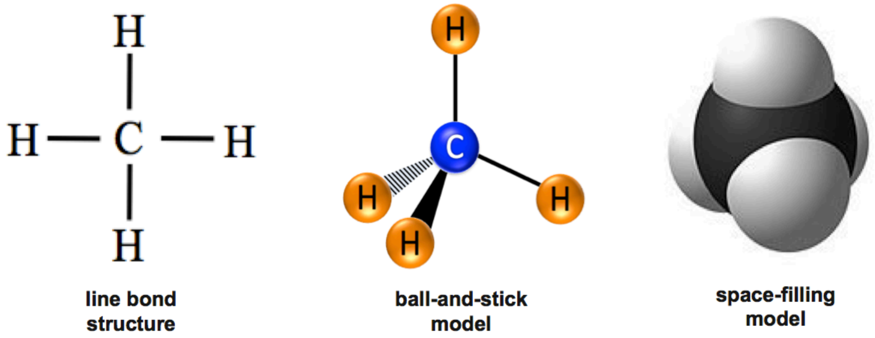
The Distribution of Electrons in Molecules

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)



line bond structure

ball-and-stick model

space-filling model

Space-filling models are images that show *molecular geometry* and also indicate the approximate *area that electrons occupy.*

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:

$H-\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}:$

The two electrons in the **H-Cl *bond*** are ***not*** shared ***equally*** by the chlorine and hydrogen atoms.

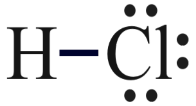
The shared electrons spend, on average, a bit more time nearer the chlorine than the hydrogen.

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.

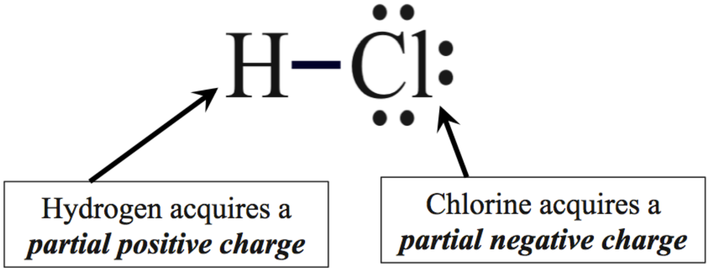
H – H

When electrons in bonds are **evenly** shared, as is the case for ***like** atoms* (such as H_2), we call the bond a _____________ _________.

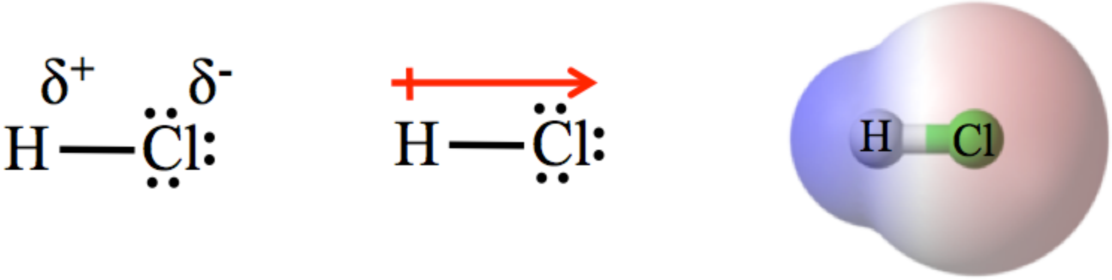


When electrons in bonds are not equally shared, as is the case for *un-like atoms*, we call the bond a _____________ _________.

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.



Representations of Bond Polarity in HCl



The line bond structure (above, left) uses the Greek lowercase letter delta (**δ**) to indicate a *partial positive charge* ($\boldsymbol{\delta}^+$) or a *partial negative charge* ($\boldsymbol{\delta}^-$) 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*.

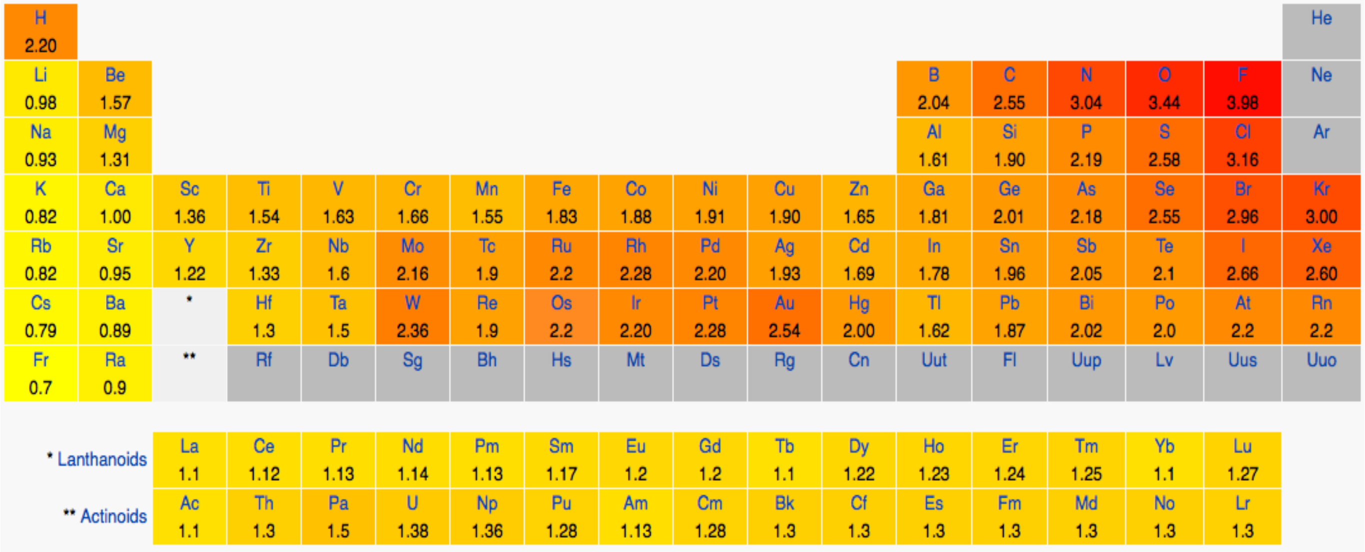
- The area where electrons spend more time and therefore has a partial negative charge is shaded red.
- The area that is electron deficient has a partial positive charge and is shaded blue.

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	

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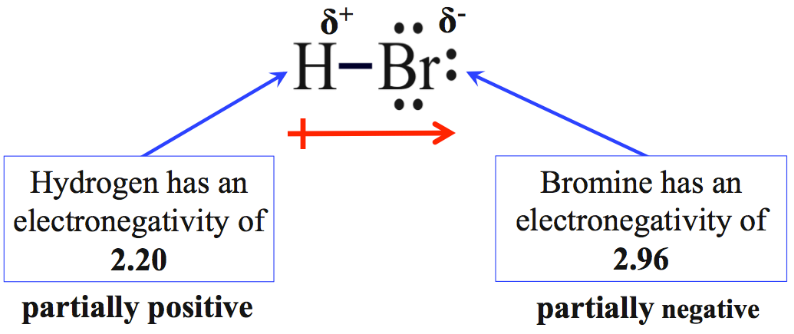
Note that there is a **periodic trend** in electronegativity values of the **s-** and **p-**block elements; electronegativity increases going from left to right (in a row) and bottom to top (in a column).

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).



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**

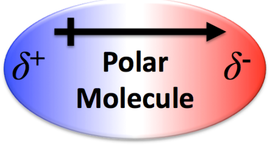
Since there is a greater difference in electronegativity between F and H vs. Br and H, **the H-F bond is __________ polarized than the H-Br bond.**

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.

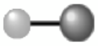
For example, one type of force responsible for attracting molecules ***to other molecules*** that is, in part, responsible for whether the molecules exist close to each other in the liquid or solid phase instead of the gas phase is called the **dipole-dipole force**.

- 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 _________________.

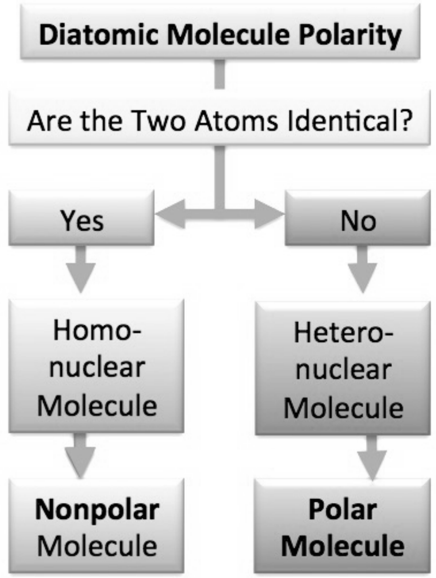
I will show you a method for determining the polarity of a molecules for each of our *molecular size categories* (diatomic, small, and large molecules).

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 ___________.



Understanding Check:
Determining the Polarity of Diatomic Molecules

Categorize each of the diatomic molecules listed below as **polar** or **nonpolar**.

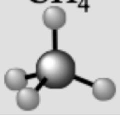
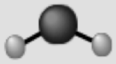
a) O_2

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.

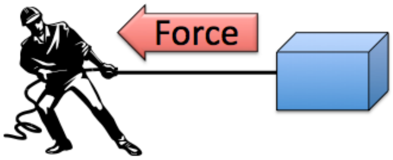
Just because a small molecule contains polar bonds does not necessarily mean that it is a polar molecule.

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.

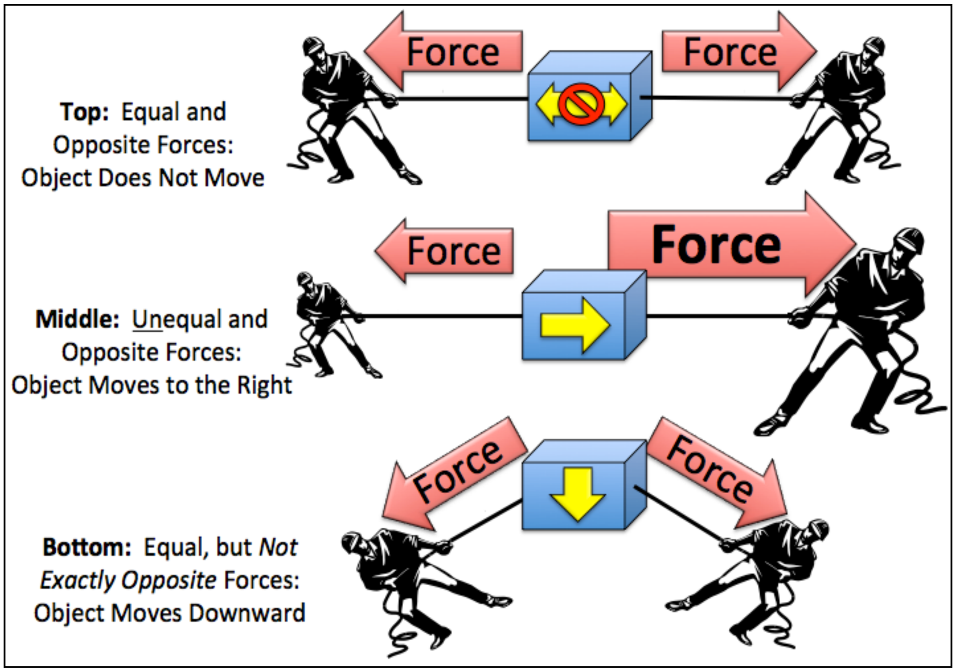
Another physical quantity with both magnitude and direction is a **force**. When you pull on an object, how fast and where the object moves depends on how hard you pull ***and*** in what *direction* you pull.



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*.

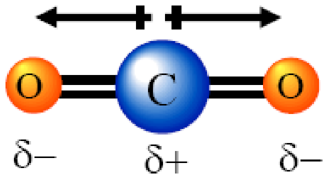
Middle: The two tension forces are in opposite directions, however the force pulling to the right is larger (represented by a larger vector arrow). The blue box moves to the right because the forces are not "balanced" and do not "cancel" - they ***do not** add up to zero*.

Bottom: The two tension forces are equal but they are *not 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___________________.

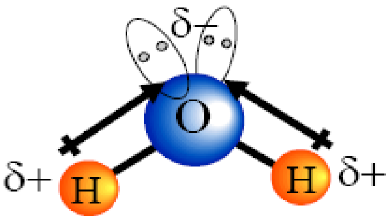
- The oxygens have a ________________ negative charge.
- The carbon has a partial positive charge.

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

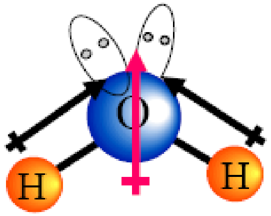


There are 2 polar bonds in an H_2O molecule.

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**.

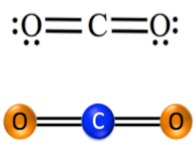
Nonsymmetric small molecules with polar bonds are **polar** molecules.

General Rule to Know if a molecule is Symmetric or Nonsymmetric:

Symmetric molecules have the *central atom* surrounded by _________________________electron groups.

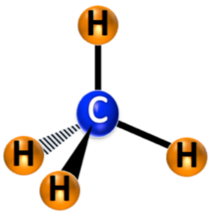
Examples of symmetric and *non*symmetric molecules:

CO_2



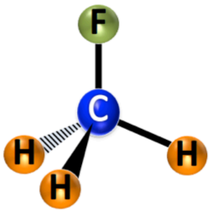
Symmetric
(Nonpolar)

CH_4



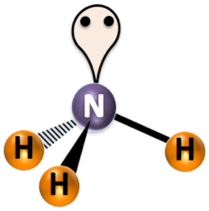
Symmetric
(Nonpolar)

CH_3F



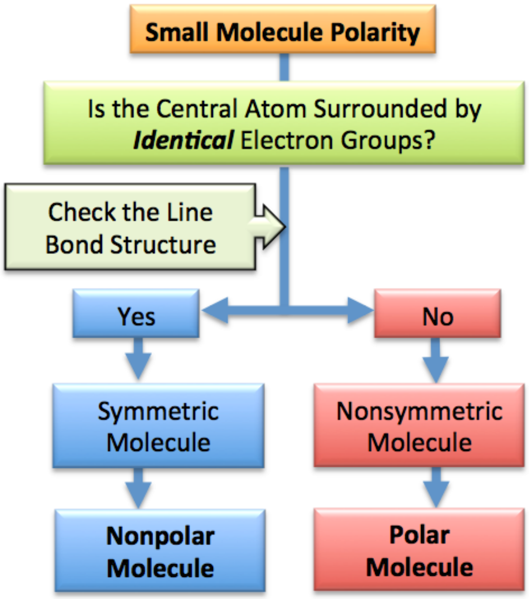
***Non*symmetric**
(Polar)

NH_3



***Non*symmetric**
(Polar)

Polarity of Small Molecules Summary

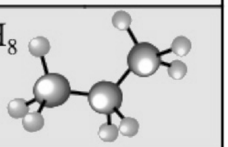


Understanding Check:
Determining the Polarity of Small Molecules

Categorize each of the diatomic 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

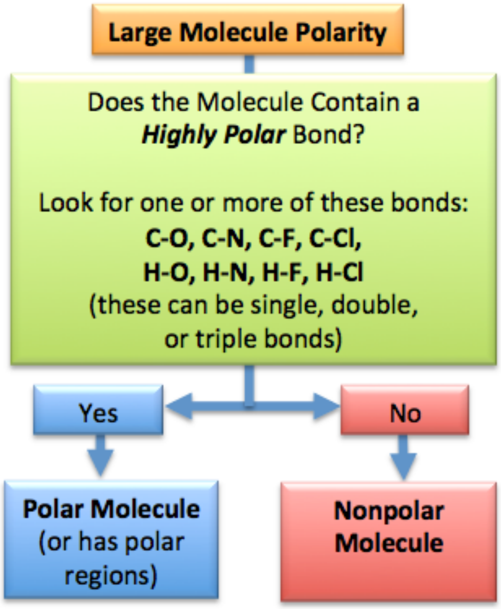
The Polarity of *Large* Molecules

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).

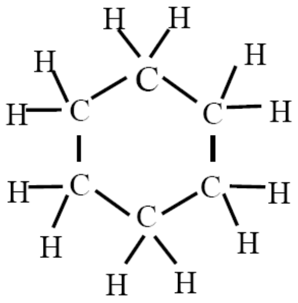
Large molecules will be considered polar (or have polar regions) if they have __________ ________ bonds.

- 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.



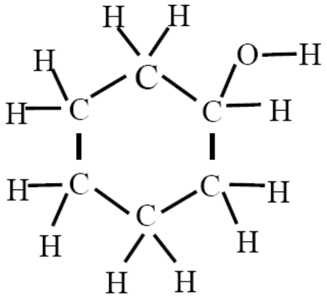
Example:

Cyclohexane vs. **Cyclohexanol**



No *highly polar* bonds

Nonpolar

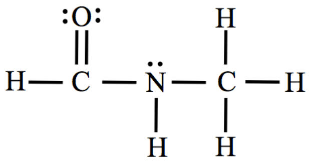


Two *highly polar* bonds
(C-O and O-H)

Polar

Understanding Check: Determining the Polarity of Large Molecules

The compound shown below has been used to kill any insect larvae present in cereal and dried fruit.



This molecule is ________.

a) polar
b) nonpolar

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.

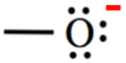
- In the compounds that you will come across in this course, *carbon* and *hydrogen* atoms *will never* have a formal charge.
- *Oxygen* and *nitrogen* ***may or may not*** have a formal charge.

I will only need you to be able to determine the formal charge on two elements -

_____________ and _____________**.**

1) The Formal Charge on Oxygen:

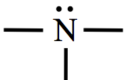
- Oxygen has a formal charge of **1-** when it has ***just*** ___________ ***single bond*** (three lone pairs).

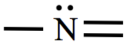


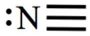
- In ***all other cases that we discuss in this course***, oxygen will **not** have a formal charge (formal charge = zero).
  - Examples:

2) The Formal Charge on Nitrogen:

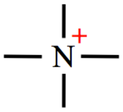
- Nitrogen will have ***no** formal charge* when it has ***one or more lone pairs on it***.

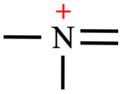


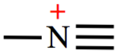




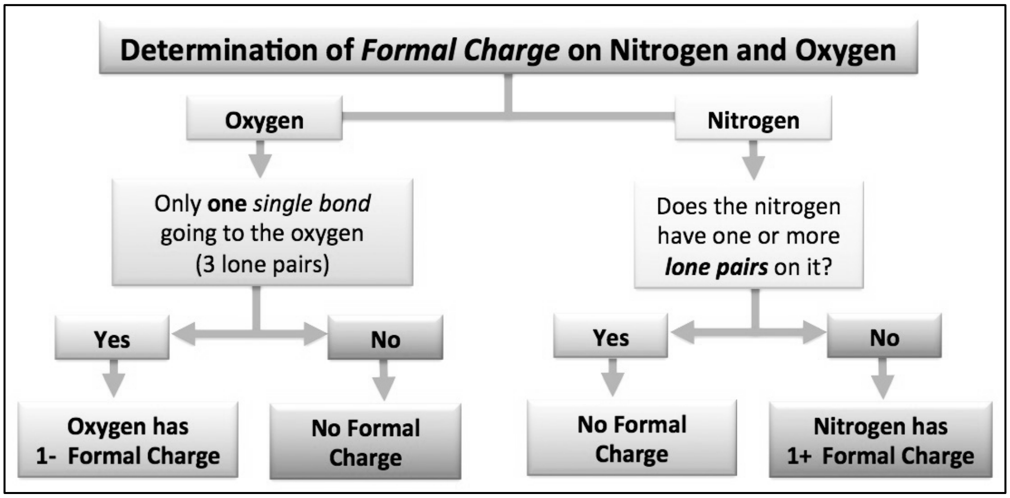
- In ________ ***other cases***, nitrogen has a **1+** formal charge.





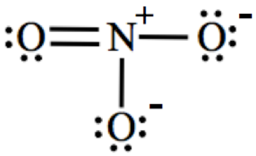


Determination of the formal charge of oxygen and nitrogen is summarized in the thought-map flowchart shown below.



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.

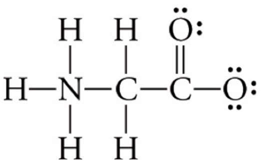


The nitrogen has ***no lone pairs***, therefore it has a formal charge of **1+** (or +).

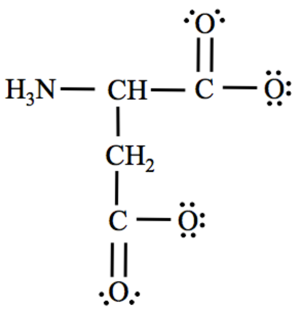
The oxygens below and to the right of the nitrogen have ***just one single bond***, therefore they have a formal charge of **1-** (or **-**).

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* ($\boldsymbol{\delta^+}$) or *partial negative charge* ($\boldsymbol{\delta^-}$).
>
> **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)

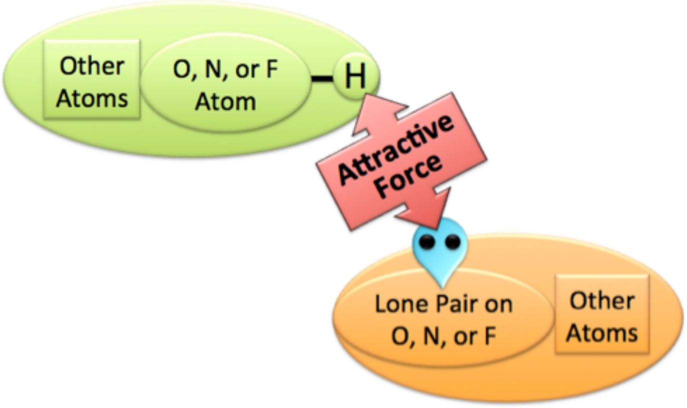
H_2O molecules are not ions, so ***what forces are responsible for holding H_2O molecules, or other molecules, together in their solid states***?

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**.

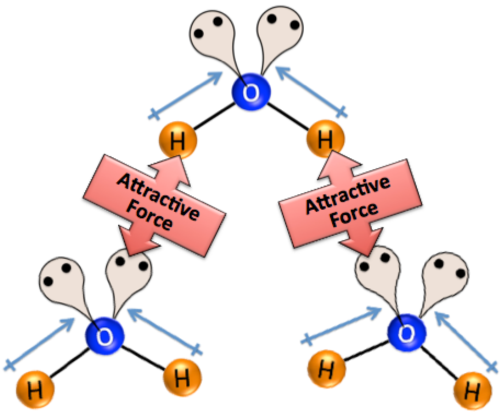
In this video, you will learn about **five** types of ***noncovalent interactions***.

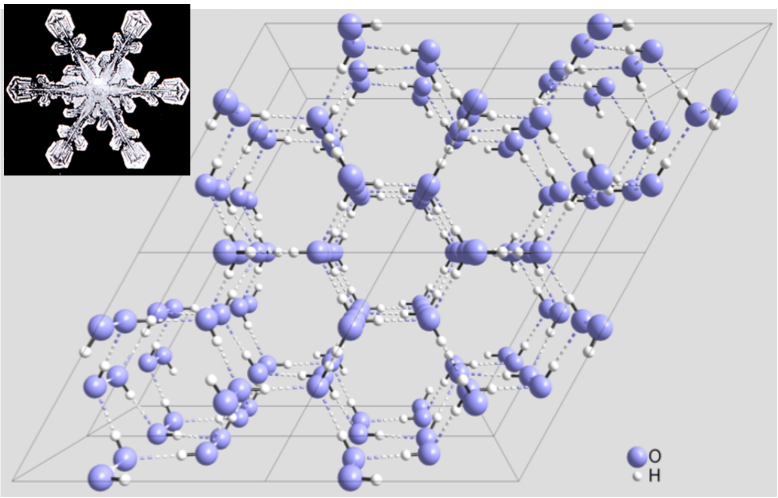


1) Hydrogen Bonding

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.

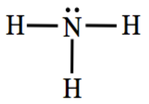




On the Left: Hydrogen bonds (as dashed lines) in a ball and stick model of an ice crystal.

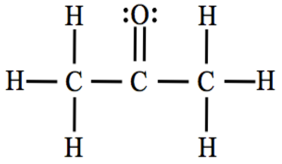
Understanding Check:

The line bond structures of ammonia and acetone are shown below:



$$\mathrm{H-\underset{\underset{\displaystyle H}{|}}{\ddot{N}}-H}$$

ammonia



$$\begin{array}{ccccccccc} & & \mathrm{H} & & :\mathrm{O}: & & \mathrm{H} & & \\ & & | & & \| & & | & & \\ \mathrm{H} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{H} \\ & & | & & & & | & & \\ & & \mathrm{H} & & & & \mathrm{H} & & \end{array}$$

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?

2) Dipole-Dipole Forces

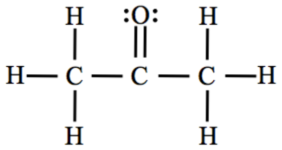
Polar molecules are attracted to other polar molecules by a type of noncovalent interaction called the ______________________________ **force**.

The partially positive ($\boldsymbol{\delta^+}$) end of one molecule's dipole is electrostatically attracted to the partially negative ($\boldsymbol{\delta^-}$) end of another molecule's dipole (and vice versa).

Example: Diethyl Ether

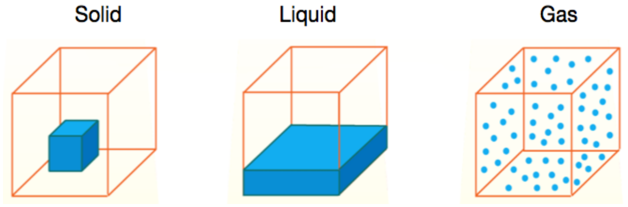
Understanding Check:

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.

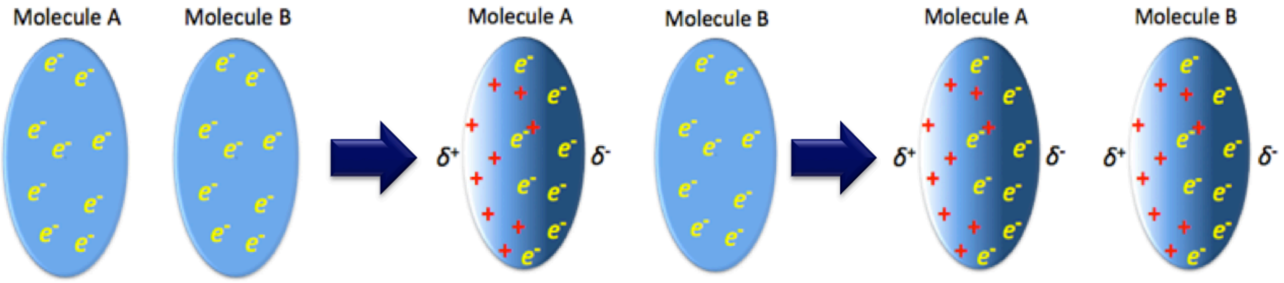
It was observed that nonpolar molecules such as CO_2, O_2, and N_2, which are ***not capable*** of interacting through dipole-dipole forces or hydrogen bonding, can be cooled to temperatures at which they exist in the liquid and solid phases.

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.

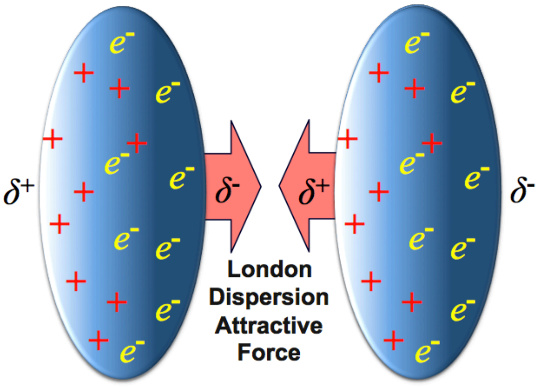
London dispersion forces are caused by an "instantaneous" dipole in one molecule _____________ the formation of a "temporary" dipole in another molecule.



_______ ***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 (ºC)	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

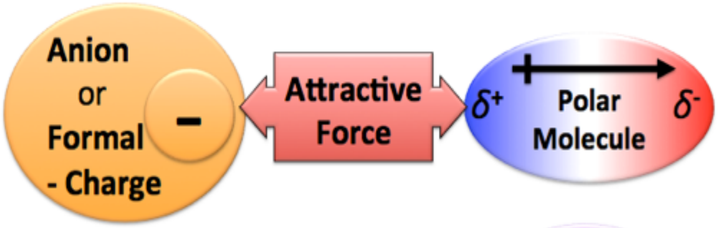
Understanding Check:

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

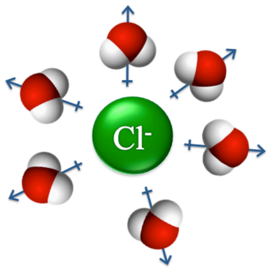
An **ion-dipole interaction**, as the name implies, is the electrostatic attractive interaction ***between*** an ***ion*** (or formal charge) ***and*** the ____________ of a polar molecule.

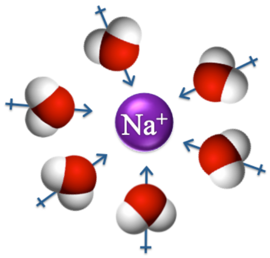


The attraction could be ***between*** an **anion** (or negative formal charge) ***and*** the partially positive end **(δ^+)** of a dipole, or vice versa, ***between*** a **cation** (or positive formal charge) ***and*** the partially negative end **(δ^-)** of a dipole.

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:

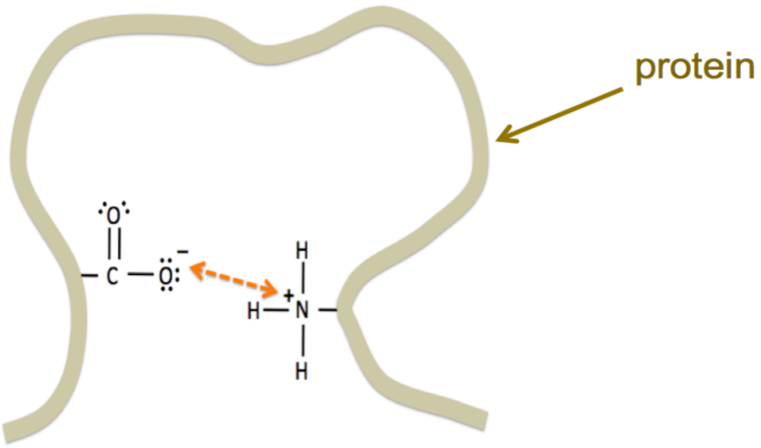
a. Can an ion-dipole interaction occur between ammonium (NH_4^+) and H_2O?

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.



Summary of Noncovalent Interactions

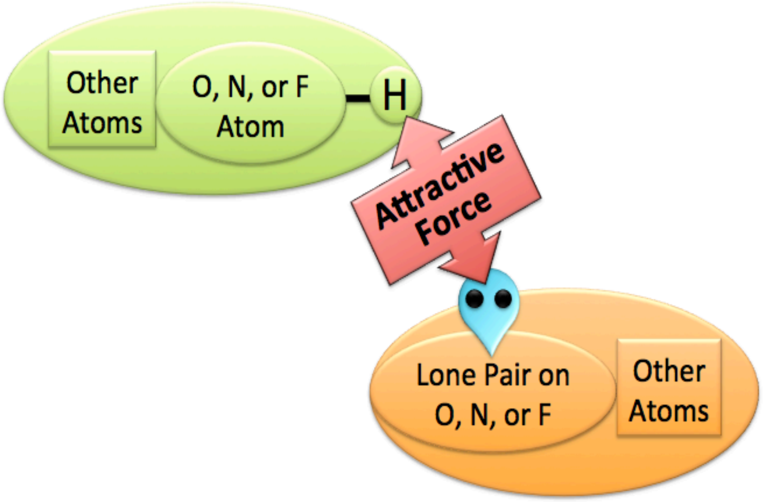
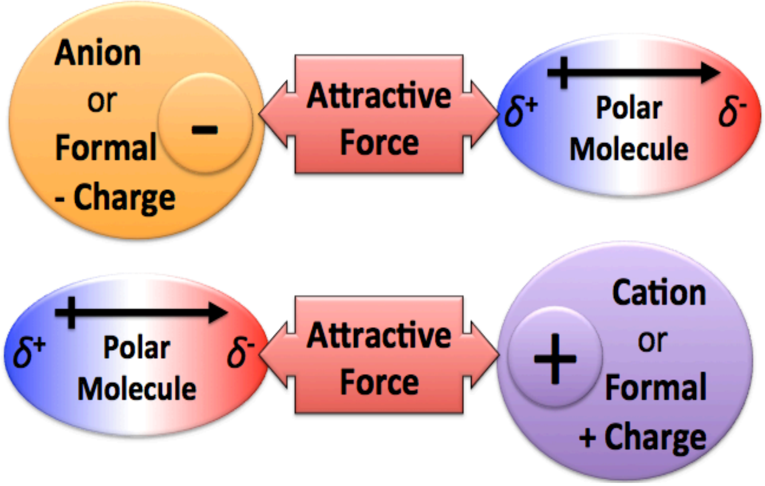
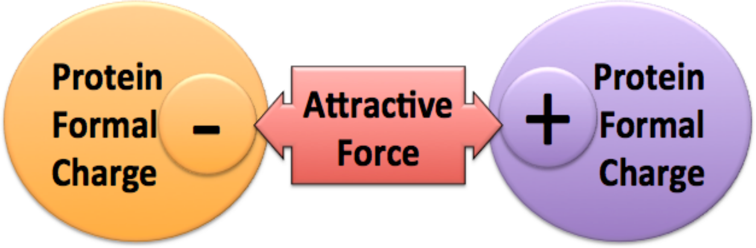
In this video, you learned about ***five*** types of **noncovalent interactions**.

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

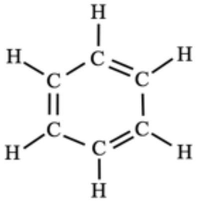
Hydrocarbons contain only ____________ and ________________ atoms.

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.

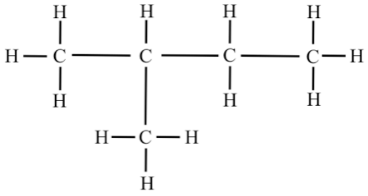
Hydrocarbons can be categorized into the four subcategories, shown in the table below, based on their chemical bonding patterns.

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 

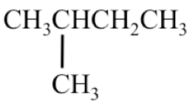
Hydrocarbons are also classified as being either _____________ (all single bonds) or _________________ (contains one or more carbon-carbon double or triple bonds).

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



$$\begin{array}{l}CH_3CHCH_2CH_3\\ \quad\;\; |\\ \quad\; CH_3\end{array}$$

Condensed Structure

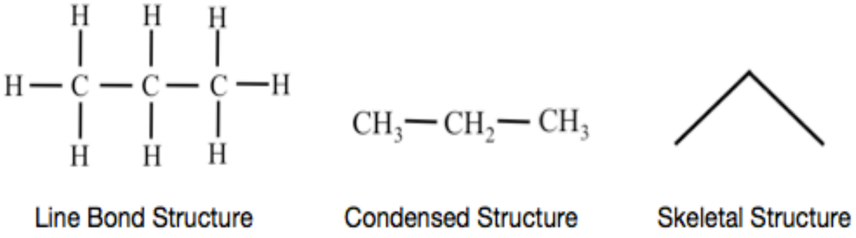
Skeletal Structure

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**.

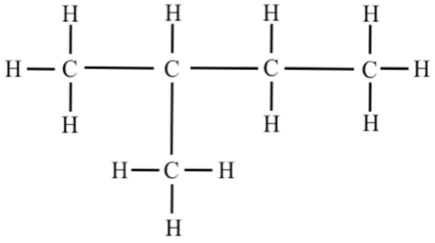
Example of a *normal* hydrocarbon:

The *line bond, condensed, and skeletal structures* for ***propane*** are shown below.



In *propane*, ________ **of the carbons** are bonded in a ***linear sequence***, therefore *propane* is classified as a **normal hydrocarbon**.

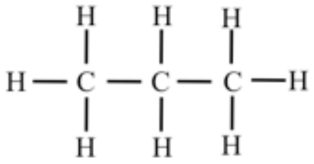
For both *normal and branched alkanes*, if "***n***" is the number of carbon atoms in the molecule, then the alkane will have the molecular formula of $C_nH_{(2n+2)}$.



"***n***" (the number of carbon atoms) = 5

The molecular formula is $C_5H_{(2.5+2)} = \mathbf{C_5H_{12}}$

isopentane
(a **branched** hydrocarbon)



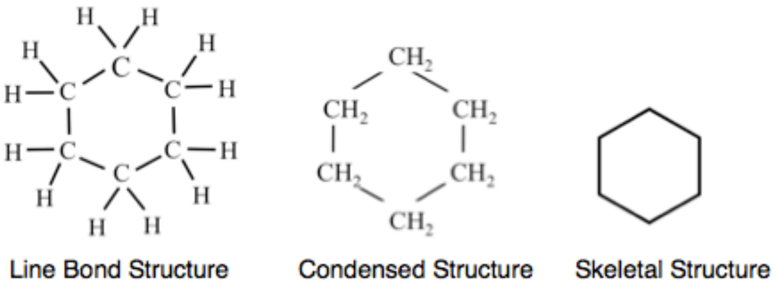
"***n***" = 3

The molecular formula is $C_3H_{(2.3+2)} = \mathbf{C_3H_8}$

propane
(a **normal** hydrocarbon)

Example of a *cyclic* hydrocarbon:

The *line bond, condensed, and skeletal structures* for ***cyclohexane*** are shown below.



When the carbons in a hydrocarbon molecule are bonded together such that they form a __________, we call it a **cyclic** hydrocarbon.

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.

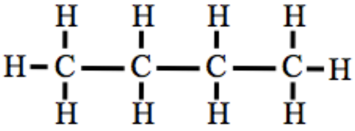
Example: If a linear or branched alkane has ***three carbon atoms*** in the parent chain, the parent chain name is ***prop**ane*

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

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**.

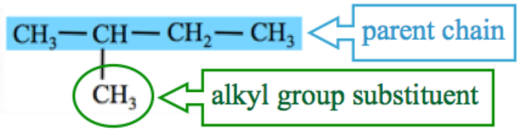


butane

Step 2. Name any alkyl group substituents.

Alkyl group substituents are comprised of the carbons and hydrogens that “branch” from the parent chain.

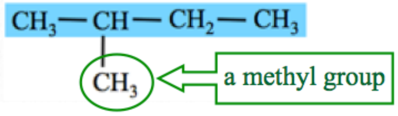
In the molecule drawn below (a branched alkane), the parent chain has four carbons and one **alkyl group substituent**.



$$\begin{array}{l} CH_3-CH-CH_2-CH_3 \\ \qquad\;\; | \\ \qquad CH_3 \end{array}$$

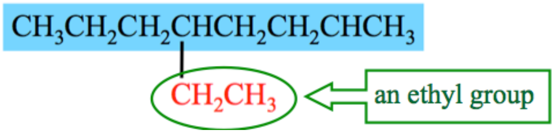
Alkyl group substituents are named based on the _____________ of _____________ in the substituent.

If there is ***one carbon*** in the substituent, we call it a _____________ group.



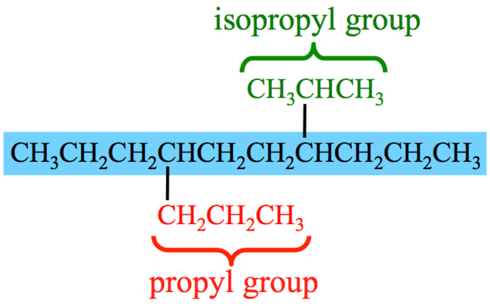
$$\begin{array}{l} CH_3-CH-CH_2-CH_3 \\ \qquad\;\; | \\ \qquad CH_3 \end{array}$$

If there are ***two carbons*** in the substituent, we call it an _____________ group.



$$\begin{array}{l} CH_3CH_2CH_2CHCH_2CH_2CHCH_3 \\ \qquad\qquad\quad\;\; | \\ \qquad\qquad\quad CH_2CH_3 \end{array}$$

When *three carbons* are contained in a substituent, then there are ***two*** distinct bonding patterns that are possible.

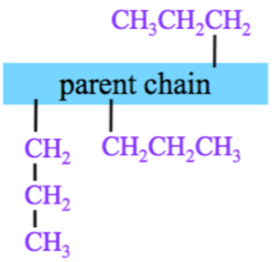


$$\begin{array}{l} \qquad\qquad\quad CH_3CHCH_3 \\ \qquad\qquad\qquad\;\; | \\ CH_3CH_2CH_2CHCH_2CH_2CHCH_2CH_2CH_3 \\ \qquad\qquad\; | \\ \qquad\quad CH_2CH_2CH_3 \end{array}$$

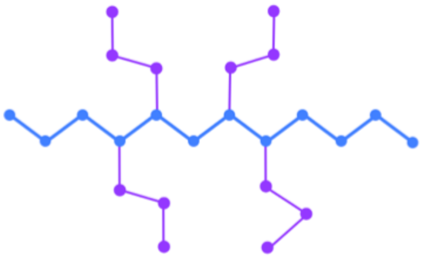
If a carbon on the ***end of the substituent*** is bonded to the parent chain, we call the substituent a _____________ group.

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.

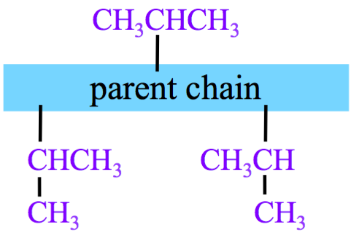


condensed formula

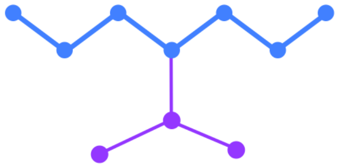


skeletal formula

There are multiple, ***correct*** ways to draw **<u>iso</u>propyl groups** in structural formulas.



condensed formula

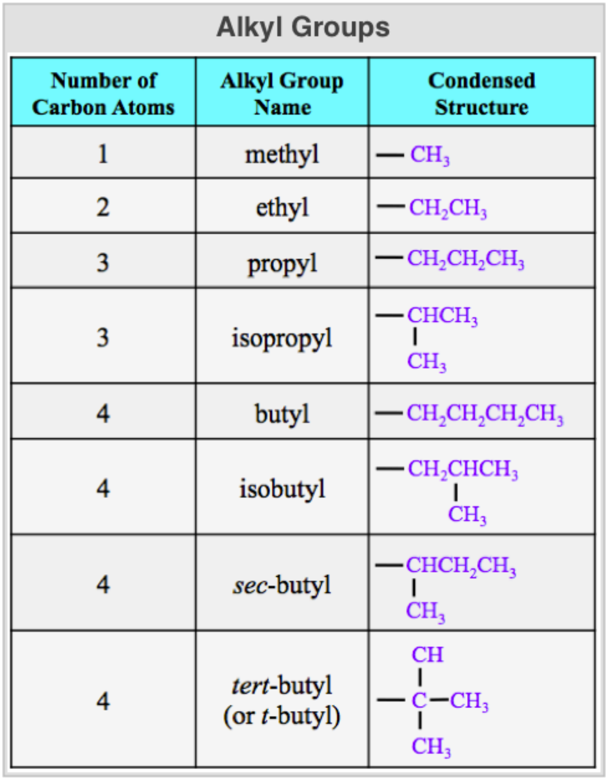


skeletal formula

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.



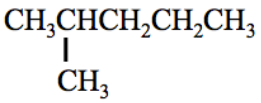
Alkyl Groups

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	$-\underset{\underset{CH_3}{\mid}}{CH}CH_3$
4	butyl	—$CH_2CH_2CH_2CH_3$
4	isobutyl	$-CH_2\underset{\underset{CH_3}{\mid}}{CH}CH_3$
4	*sec*-butyl	$-\underset{\underset{CH_3}{\mid}}{CH}CH_2CH_3$
4	*tert*-butyl (or *t*-butyl)	$-\overset{\overset{CH}{\mid}}{\underset{\underset{CH_3}{\mid}}{C}}-CH_3$

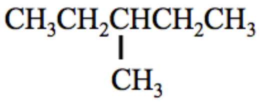
Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

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.



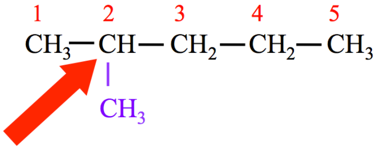
$CH_3\underset{\underset{CH_3}{\mid}}{CH}CH_2CH_2CH_3$



$CH_3CH_2\underset{\underset{CH_3}{\mid}}{CH}CH_2CH_3$

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.



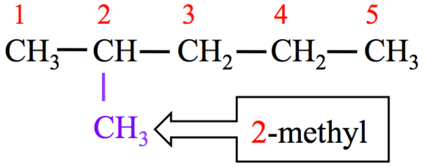
$$\overset{1}{CH_3}-\underset{\underset{CH_3}{\mid}}{\overset{2}{CH}}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{CH_3}$$

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**.



$$\overset{1}{CH_3}-\underset{\underset{CH_3}{\mid}}{\overset{2}{CH}}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{CH_3}$$

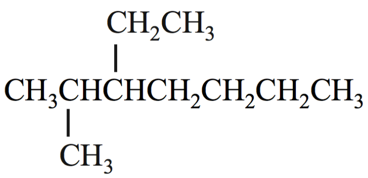
WHEN NEEDED: Add the labels di, tri, or tetra in front of the alkyl group name **if** two, three, or four (respectively) identical substituents are present. *Not needed in this example.*

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**.

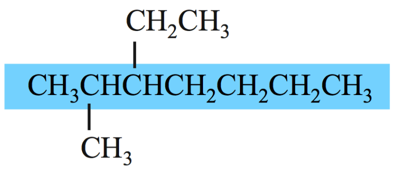
We write the IUPAC name of this molecule as: **2-methylpentane**.

Example: Give the IUPAC name for the alkane shown below.



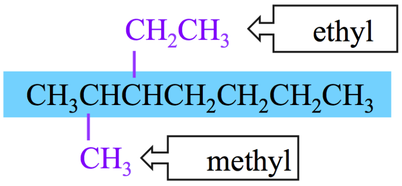
$CH_3\underset{CH_3}{C}H\overset{CH_2CH_3}{C}HCH_2CH_2CH_2CH_3$

Step 1. Name the *parent chain*.
The parent chain (seven carbons) is **heptane**.

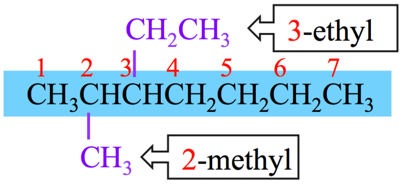


$CH_3\underset{CH_3}{C}H\overset{CH_2CH_3}{C}HCH_2CH_2CH_2CH_3$

Step 2. Name any alkyl group substituents.



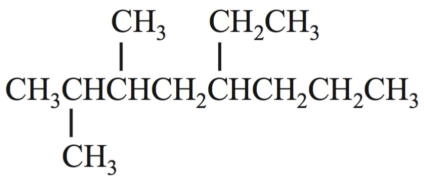
Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.



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.

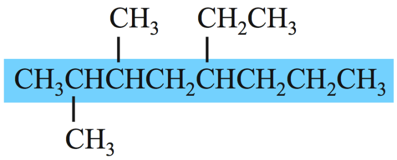
3-ethyl-2-methylheptane

Example: Give the IUPAC name for the alkane shown below.



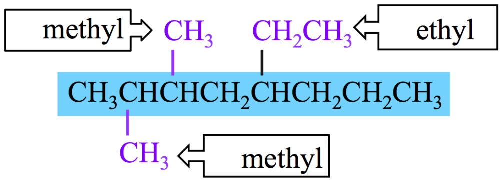
$CH_3\underset{CH_3}{C}H\overset{CH_3}{C}HCH_2\overset{CH_2CH_3}{C}HCH_2CH_2CH_3$

Step 1. Name the *parent chain*.
The parent chain (eight carbons) is **octane**.

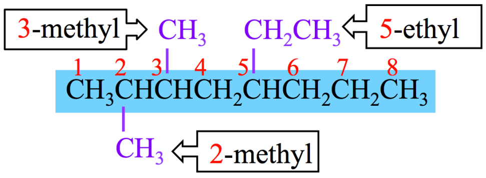


$CH_3\underset{CH_3}{C}H\overset{CH_3}{C}HCH_2\overset{CH_2CH_3}{C}HCH_2CH_2CH_3$

Step 2. Name any alkyl group substituents.

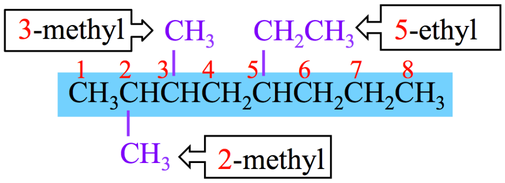


Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.



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.

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.



$CH_3CHCHCH_2CHCH_2CH_2CH_3$ with CH_3 on carbon 2, CH_3 on carbon 3, CH_2CH_3 on carbon 5

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**

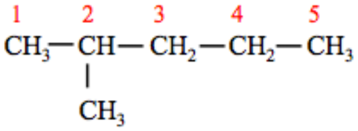
5-ethyl-2,3-dimethyloctane

Common Errors

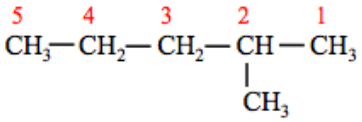
Do not assume that the parent chain position numbers always start with carbon number 1 as the left-most parent carbon.

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.



$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CH_2-CH_3$

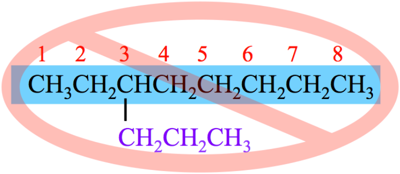


$CH_3-CH_2-CH_2-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_3$

There is no molecule called *4-methylpentane.*

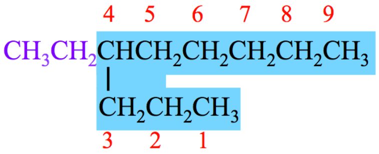
The ***parent chain is the longest, continuous chain of carbons atoms, NOT necessarily*** the carbon chain that is drawn horizontally in a single line.

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**.



$CH_3CH_2\underset{\displaystyle CH_2CH_2CH_3}{\underset{|}{C}}HCH_2CH_2CH_2CH_2CH_3$

The correct way to think about naming this molecule is shown below.



$CH_3CH_2\underset{\displaystyle CH_2CH_2CH_3}{\underset{|}{C}}HCH_2CH_2CH_2CH_2CH_3$

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.

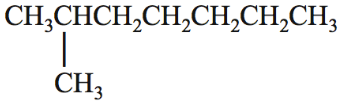
Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

- 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***.

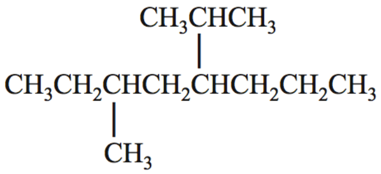
Step 4. Construct the name of the alkane by placing the alkyl groups in alphabetical order and specifying their position numbers, followed by the name of the parent chain.

- 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.

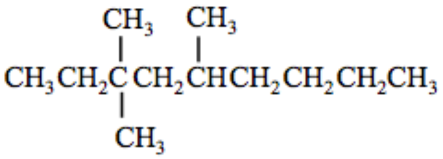


$CH_3\underset{\underset{CH_3}{|}}{C}HCH_2CH_2CH_2CH_2CH_3$



$CH_3CH_2\underset{\underset{CH_3}{|}}{C}HCH_2\overset{\overset{CH_3CHCH_3}{|}}{C}HCH_2CH_2CH_3$

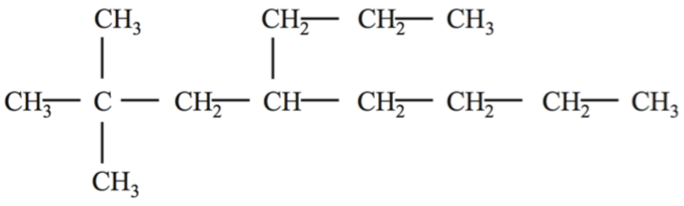
Understanding Check: Give the correct IUPAC name the alkane shown below.



$CH_3CH_2\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}CH_2\overset{\overset{CH_3}{|}}{C}HCH_2CH_2CH_2CH_3$

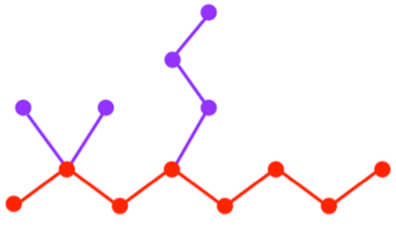
Drawing the Structure of an Alkane from its Name

Example: Draw the ***condensed and skeletal*** structure for 2,2-dimethyl-4-propyloctane.



$CH_3-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH_2-\overset{\overset{CH_2-CH_2-CH_3}{|}}{CH}-CH_2-CH_2-CH_2-CH_3$

condensed structure



skeletal structure

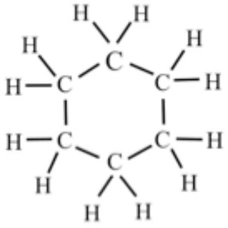
Understanding Check: Draw the ***condensed and skeletal*** structure for 6-isopropyl-2,3-dimethylnonane.

Cycloalkanes

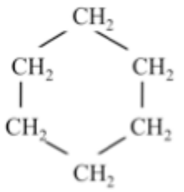
Some alkanes contain carbon atoms bonded, not in a linear sequence, but in a "**ring**" pattern.

These alkanes are called ____________________.

- **Example** of a cycloalkane: *cyclohexane* (shown below).



Line Bond Structure



Condensed Structure

Skeletal Structure

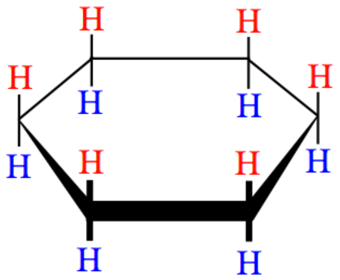
It is very common to see five- and six-carbon rings that occur in nature. The reason for this is that the bond angles in 5- and 6-carbon rings is fairly close to the 110° bond angles expected in molecules with AB_4 geometry.

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



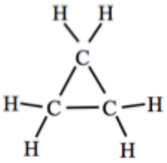
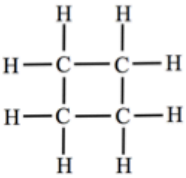
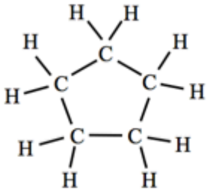
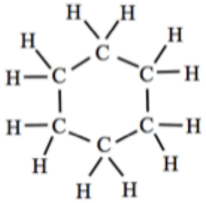
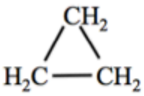
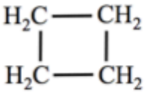
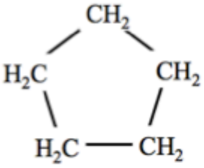
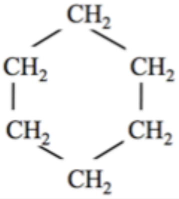
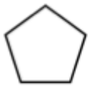
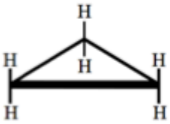
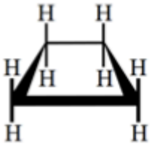
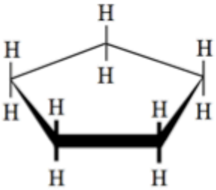
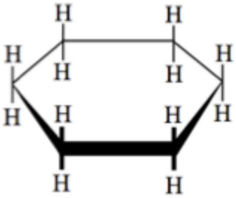
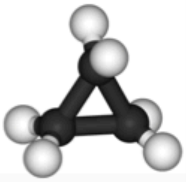
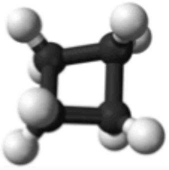
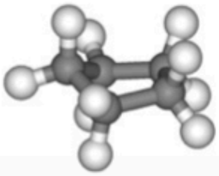
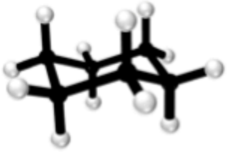
side-view structure

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.

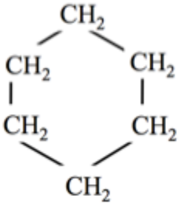
Note that these names are based on the names used for the parent chains of branched alkanes, ***however*** **the term "** __________ **" is used as a prefix.**

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

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

Step 2. Name any alkyl groups substituents.

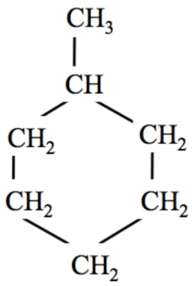
The alkyl groups are named in the *same way* as we did for branched alkanes (methyl, ethyl, propyl, isopropyl, etc.).

Step 3. Determine the *point of attachment* of alkyl group(s) to the parent chain.

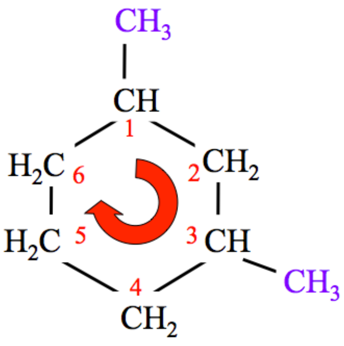
We use the following rules for assigning position numbers to the ring-carbons.

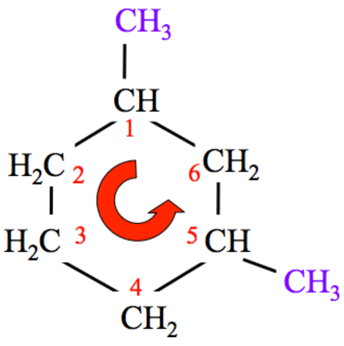
- If there is ***only*** ________ ***substituent***, a position number is not used.
    - Name the molecule by placing the alkyl group substituent name in front of the parent chain name; ***no further steps are needed***.
    - For example, consider the molecule drawn ***to the right*** with a single, 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:**





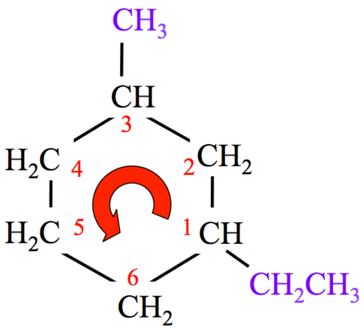
1,3-dimethylcyclohexane vs. 1,5-dimethylcyclohexane

(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.

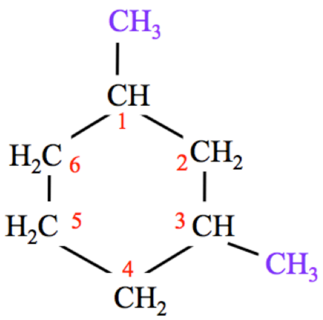
We number the ring-carbons in the **counter-clockwise direction** in order to result in the *smallest sum of position numbers.*



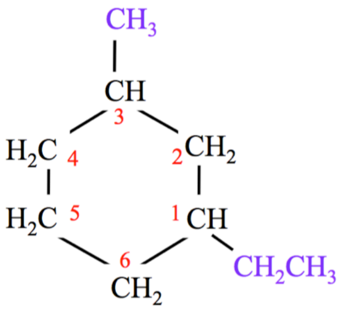
1-ethyl-3-methyl

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.



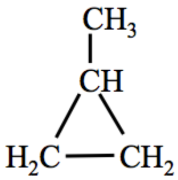
1,3-dimethylcyclohexane



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:

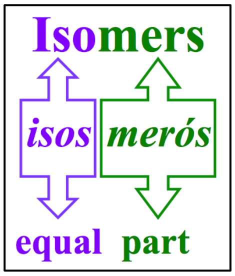
Draw the line bond, condensed, **and** skeletal structures of the following cycloalkanes:

a. 1,1-dimethylcyclobutane

b. 1-methyl-3-propylcyclopentane

c. 1,4-diethylcyclohexane

Isomers



Isomers 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

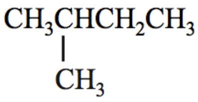
______________ ____________.

Example: Consider the *three* constitutional isomers that have the molecular formula of C_5H_{12}.

$CH_3CH_2CH_2CH_2CH_3$

pentane

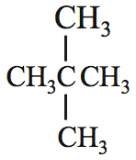
boiling point = 36°C



$CH_3CH(CH_3)CH_2CH_3$

2-methylbutane

boiling point = 28°C



$CH_3C(CH_3)_2CH_3$

2,2-dimethylpropane

boiling point = 10°C

Understanding Check: Draw the constitutional isomers for C_4H_{10}

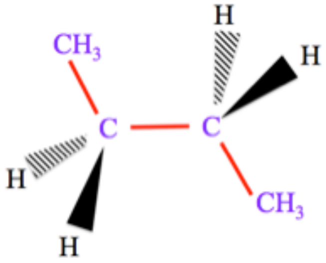
Understanding Check: Draw and **name** the ***five*** constitutional isomers of C_6H_{14}

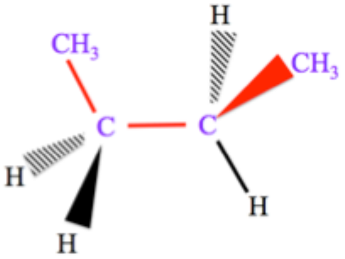
Conformations

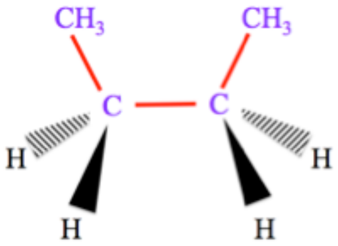
The infinite number of shapes that a molecule can take, because of the rotation around bonds, are called

__________________.

Example: A *few* of the infinite conformations of *butane* resulting from rotation about the single bond between carbon number 2 and carbon number 3.







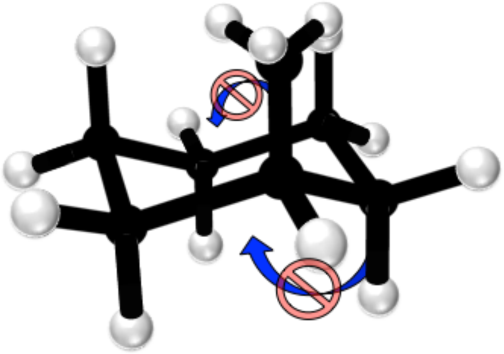
Common Error Warning: Do not confuse ***conformations*** with ***constitutional isomers***!

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

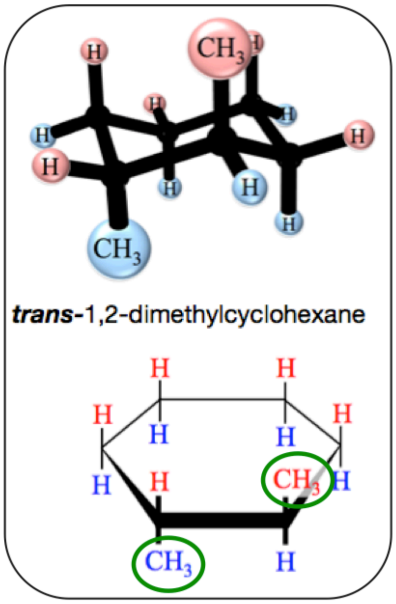
  So far the definition of stereoisomers is the same as conformations - but the next item makes them quite different.
- **cannot** be converted from one to another without ***breaking and reforming bonds***

It is ***not*** possible for one stereoisomer to take the shape of another stereoisomer by rotation around a bond.

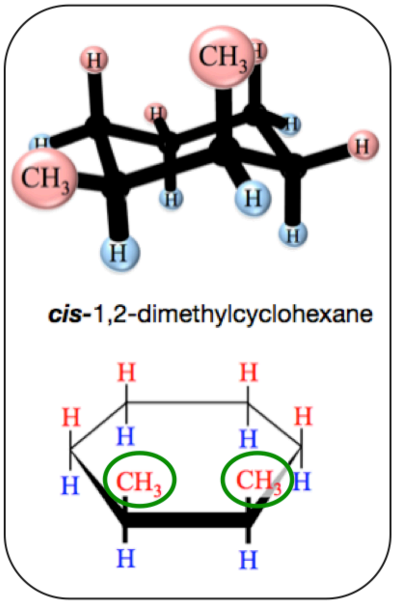
Geometric Isomers

When *stereoisomers* exist because of ***restricted bond rotation***, the stereoisomers are called ____________________ ***isomers***.

Examples:



trans-1,2-dimethylcyclohexane



cis-1,2-dimethylcyclohexane

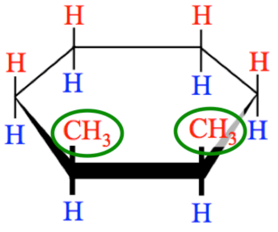
Geometric isomers come in ***pairs*** – one is the "______**-**" and one is the "_________**-**" isomer.

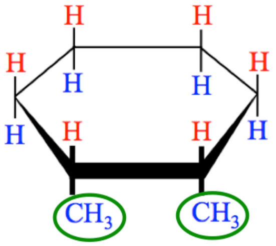
When cycloalkanes have ______ ***substituents***, ***each on a different ring-carbon***, then there are two geometric isomers.

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).

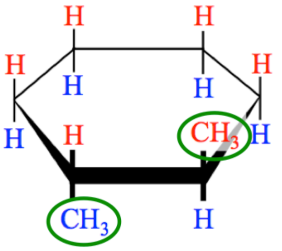
Conversely, a ***trans*** geometric isomer has the two ***substituents*** oriented in opposite directions (**one** *pointing* ***above*** the ring structure and the **other** *pointing* ***below*** the ring structure).

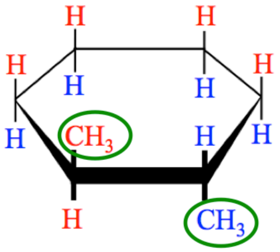
two ways to draw *cis* cyclic compounds:





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.

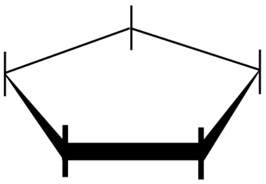
Because alkyl group substituents cannot rotate through the center of the ring, the ***trans*** and ***cis*** isomers of cycloalkanes are ***two different molecules***; they have slightly different physical properties (density, melting points, vapor pressure, etc.) and different chemical properties.

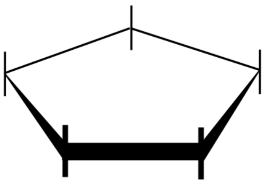
There are only slight differences in many properties because the isomers are very similar (but not identical).

- 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

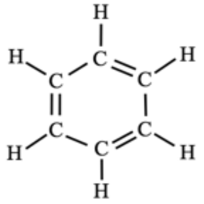
b) 1-ethyl-2-propylcyclobutane

c) 1-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***.

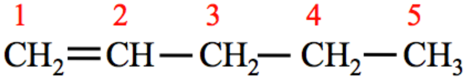
The parent chain is named by combining a *numbering prefix* that specifies the number of carbon atoms in the parent chain, with the "**-**_________" suffix, which identifies the molecule as an **alkene**.

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***.

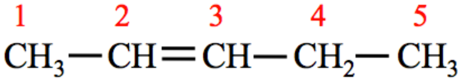
For alkenes with ***more than three carbons***, the position of the double bond must be indicated by adding a *position number* to the parent chain name.

- Position number **1** is assigned to the carbon at the end of the parent chain that is **closest to the double bond.**



$$\overset{1}{\mathrm{CH_2}}=\overset{2}{\mathrm{CH}}-\overset{3}{\mathrm{CH_2}}-\overset{4}{\mathrm{CH_2}}-\overset{5}{\mathrm{CH_3}}$$

- 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.



$$\overset{1}{\mathrm{CH_3}}-\overset{2}{\mathrm{CH}}=\overset{3}{\mathrm{CH}}-\overset{4}{\mathrm{CH_2}}-\overset{5}{\mathrm{CH_3}}$$

- 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*.

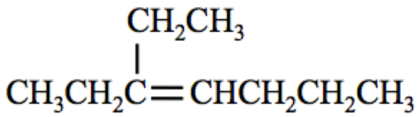
Step 2. Name any alkyl group substituents.

- **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:

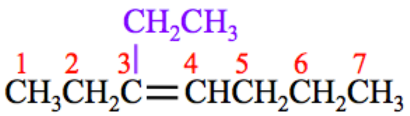


$$CH_3CH_2\overset{CH_2CH_3}{\overset{|}{C}}=CHCH_2CH_2CH_3$$

Step 1. Find and name the *parent chain.*

The *parent chain is the longest, continuous chain of carbon atoms that* ***contains the double bond****.*

- There are seven carbons in the parent chain.



$$\overset{1}{C}H_3\overset{2}{C}H_2\overset{CH_2CH_3}{\overset{3|}{C}}=\overset{4}{C}H\overset{5}{C}H_2\overset{6}{C}H_2\overset{7}{C}H_3$$

Position number **1** is assigned to the carbon *at the end* of the parent chain that is **closest to the double bond.**

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.

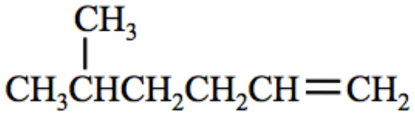
There is one substituent in this example: **ethyl**

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:

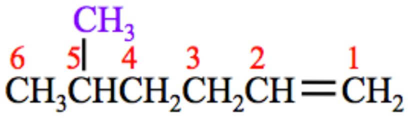


$$CH_3\overset{CH_3}{\overset{|}{C}}HCH_2CH_2CH=CH_2$$

Step 1. Find and name the *parent chain.*

The *parent chain is the longest, continuous chain of carbon atoms that* ***contains the double bond****.*

- There are six carbons in the parent chain.



$$\overset{6}{C}H_3\overset{CH_3}{\overset{5|}{C}}H\overset{4}{C}H_2\overset{3}{C}H_2\overset{2}{C}H=\overset{1}{C}H_2$$

Position number **1** is assigned to the carbon *at the end* of the parent chain that is **closest to the double bond.**

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.

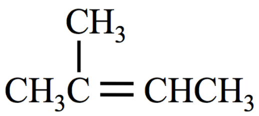
There is one substituent in this example: **methyl**

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.**

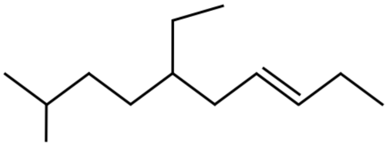
The name of this molecule is: **5-methyl-1-hexene**

Understanding Check: Write the name of this alkene.



$$CH_3C(CH_3){=}CHCH_3$$

Understanding Check: Write the name of this alkene.



Understanding Check

Draw the **line bond**, **condensed**, ***and*** **skeletal structure** for each of these alkenes.

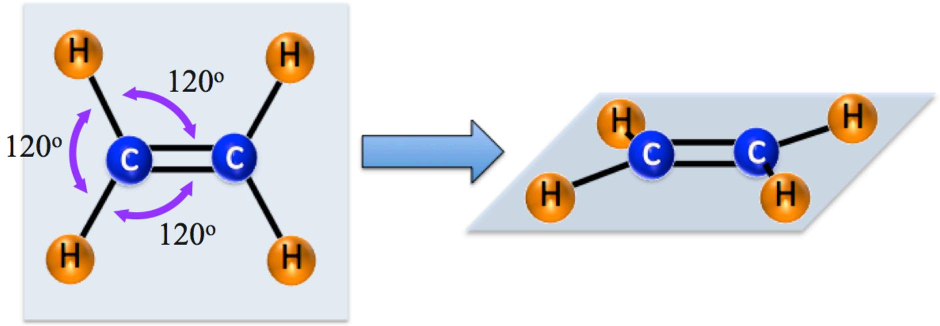
a) 2-methyl-1-butene
b) 3-ethyl-4-methyl-3-hexene

Geometric Isomers of Alkenes

Unlike the case for single bonds, ***there is no rotation around double bonds***.

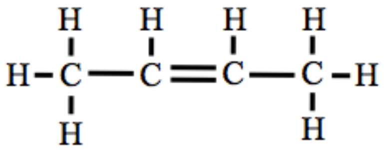
All other bonds to both double-bonded carbon atoms in alkenes are at 120º angles and ***are on the same*** _______________ ***as the double bond***.

- **Example:** Ethene



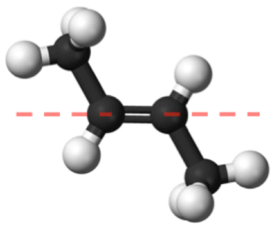
Because of the *geometry and lack of rotation around double bonded carbons*, **some alkenes can exist as ____________________ ____________ (*cis* and *trans*).**

- **Example:** 2-butene

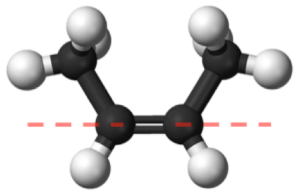


$H_3C-CH=CH-CH_3$

There are two possible geometric arrangements of the two methyl groups attached to the double bonded carbons.



***trans*-2-butene**



***cis*-2-butene**

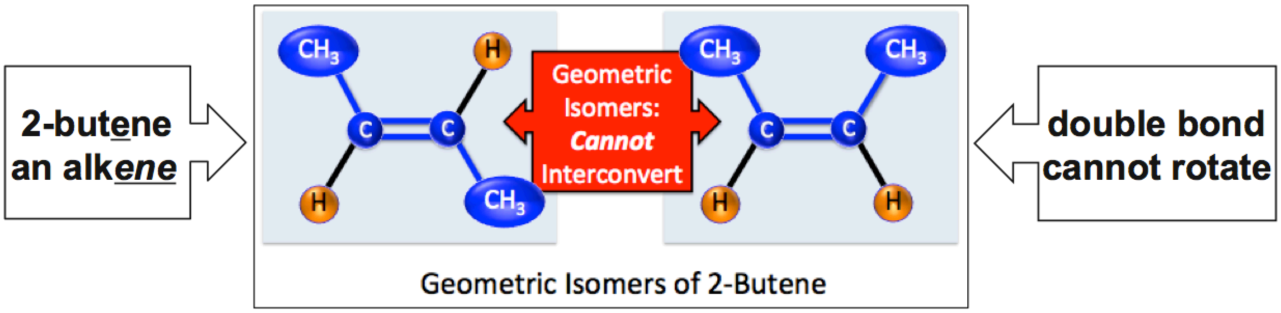
We identify the ***cis*** and ***trans*** isomers by noting the positions of alkyl groups on each of the double-bonded carbons relative to an imaginary line passing *along the double bond.*

When the alkyl groups are on ________________ ***sides*** of the imaginary line, we have the ***trans*** geometric isomer.

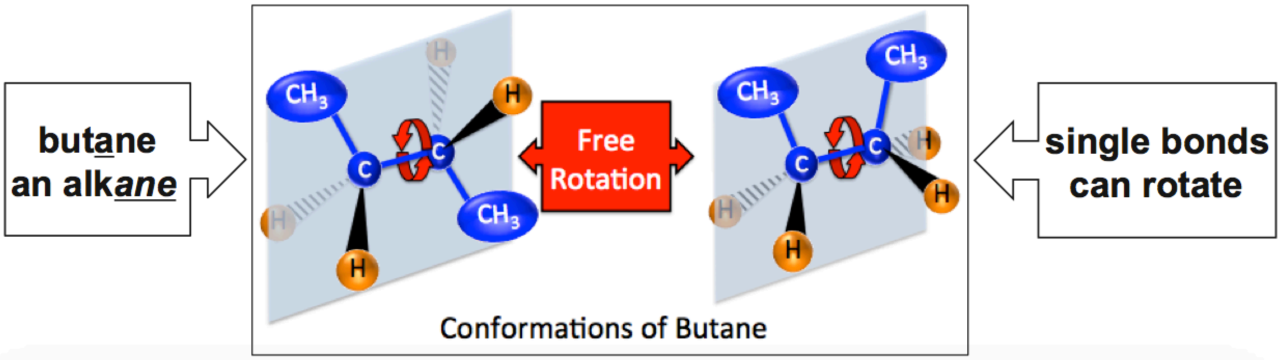
When ***both*** of the alkyl groups are on the ________________ ***side*** of the imaginary line, we have the ***cis*** geometric isomer.

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.

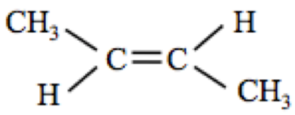


Geometric Isomers of 2-Butene

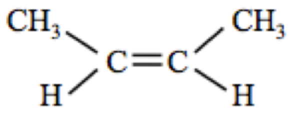


Conformations of Butane

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.

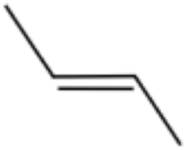


***trans*-2-butene**

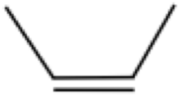


***cis*-2-butene**

In ***skeletal structures***, the bonds to the alkyl groups that emanate from the double-bonded carbons are oriented as shown below.



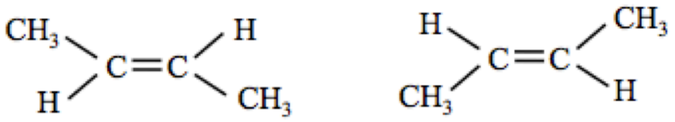
***trans*-2-butene**



***cis*-2-butene**

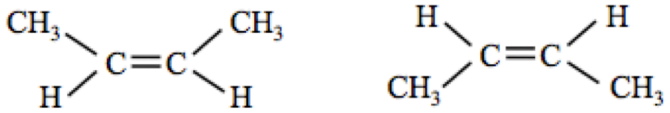
There will be *two correct ways* to draw **each *cis*** and **each *trans*** isomer.

- 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**

Understanding Check

Draw the ***condensed*** **and** ***skeletal structures*** for each of the following molecules.

a) *trans*-2-pentene
b) *cis*-2-pentene
c) *trans*-3-hexene
d) *cis*-3-hexene

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.

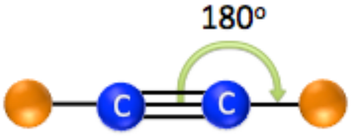
- Example:

$$CH_3-C\equiv C-CH_2-CH_3$$

2-pentyne

Alkyne Molecular Geometry

Alkynes involve a triple bond and the bond angles around the triple-bonded carbons are 180° as illustrated below.



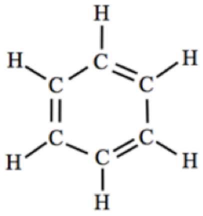
Each of the triple-bonded carbons can have only one other group single bonded to it (octet rule) and **this AB_2 geometry cannot result in geometric (*cis/trans*) isomers.**

Aromatic Hydrocarbons

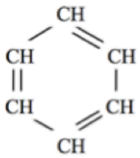
Aromatic hydrocarbons have alternating single and double bonds between the carbons that form the ring.

The smallest and simplest aromatic hydrocarbon that occurs is called ______________.

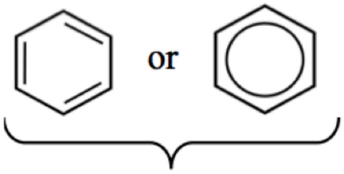
- The line bond, condensed, and skeletal structures of ***benzene*** are shown below.



line bond structure



condensed structure



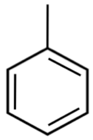
skeletal structures

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***.

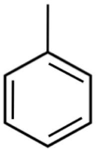


methylbenzene

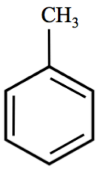
As was the case for cycloalkanes, we do not need to use a position number when there is only one substituent bonded to a ring structure.

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*:



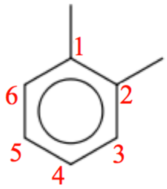
skeletal



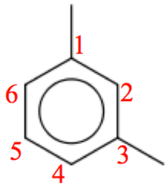
condensed/skeletal hybrid

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.

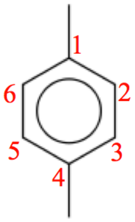
When cyclic compounds have *more than one substituent,* position numbers are included (you did so for cycloalkanes). **Examples:**



1,2-dimethylbenzene
(*ortho*-xylene)



1,3-dimethylbenzene
(*meta*-xylene)



1,4-dimethylbenzene
(*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***.

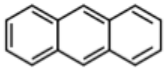
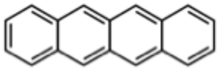
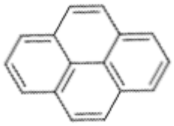
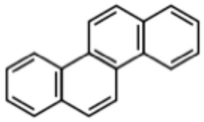
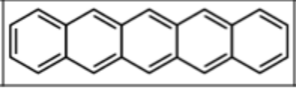
Fused rings occur when neighboring rings *share carbon atoms*.

- 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.

A specific example of an alcohol is ethanol. The condensed structural formula for ethanol is shown below.

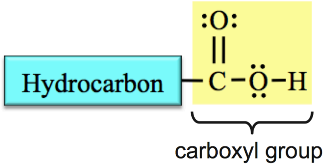
$$CH_3CH_2{-}OH$$

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.

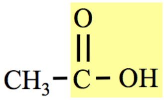
The Carboxylic Acid Family

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.



A specific example of a carboxylic acid is *acetic acid*. The condensed structural formula for *acetic acid* is shown below.



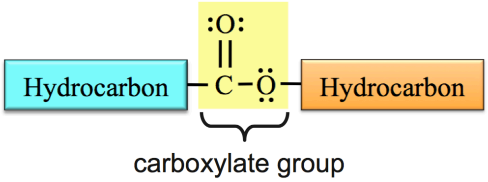
$$CH_3{-}\overset{\overset{\displaystyle O}{\|}}{C}{-}OH$$

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.

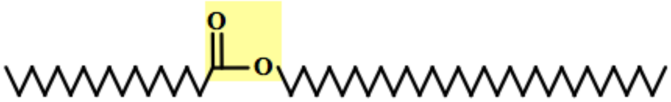
Carboxylate groups contain both a ***carbonyl group*** (**C=O**), ***and*** an ***oxygen atom.***



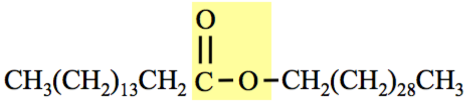
The boxes that represent hydrocarbons (alkyl groups) are shaded with different colors because the two hydrocarbon parts *are not always identical*.

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.

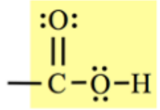
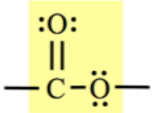


When drawing *condensed structures* of large molecules, such as the ester shown above, neighboring - CH_2 - groups can be further condensed in parenthesis as shown below:



$$CH_3(CH_2)_{13}CH_2\,\overset{\overset{\displaystyle O}{\|}}{C}{-}O{-}CH_2(CH_2)_{28}CH_3$$

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	 $-\overset{\overset{:O:}{\Vert}}{C}-\ddot{\underset{\cdot\cdot}{O}}-H$ carboxyl group	Carboxyl group bonded to a hydrocarbon
Ester	 $-\overset{\overset{:O:}{\Vert}}{C}-\ddot{\underset{\cdot\cdot}{O}}-$ carboxylate group	Carboxylate group bonded ***between*** two hydrocarbons