Objective 2

Compare 2 or more compounds and determine whether the compounds are structural isomers, the same compound, or different compounds.
Calculate formal charge and determine most likely structure.

Organic Compounds can be BIG!

There are *different* ways atoms can bond together

Isomers have the same chemical formula but different connectivity (different structure).

C_2H_6O has <u>two</u> isomers. Draw the Lewis structure and skeletal structure of each isomer.

Circle each functional group and write the name of the functional group next to your circle.

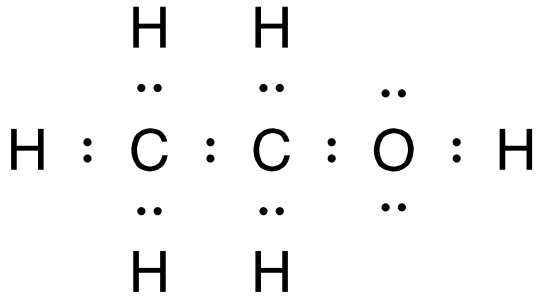
Write the **<u>expanded</u>** structure of each isomer.

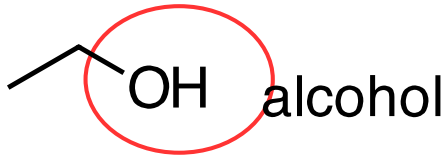
How can you distinguish between each isomer?

Organic Compounds can be BIG!

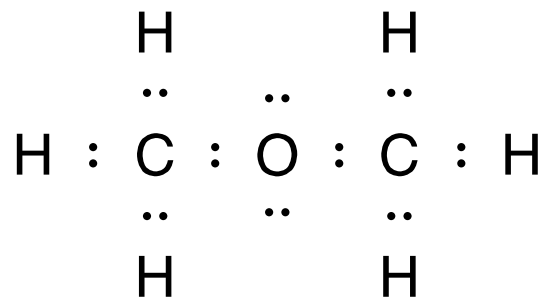
There are *different* ways atoms can bond together

C_2H_6O has <u>two</u> isomers.





CH_3CH_2OH



CH_3OCH_3

How can you distinguish between each isomer?

Molecular Structure is determined by EXPERIMENT!

Elemental analysis --> chemical formula

IR, NMR, m.p., x-ray diffraction --> Lewis structure(s)

IR Spectroscopy is used to identify bond types

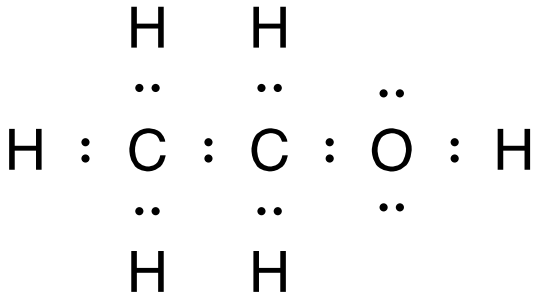
	Bond	Base Value, cm^{-1}	Strength / Shape	Comments
1	**C=O**	1715	s, "finger"	Exact position depends on type of carbonyl
2	**O-H**	3200-600	s, broad	Broad due to H bonding
3	**N-H**	3500	m	Can tell primary from secondary
4	**C-O**	1100-1300	s	Also check for OH and C=O
5	**C=C**	1650	w alkene m-s aromatic	Alkene w due to low polarity Aromatic usually in pairs
6	**C≡C**	2150	w, sharp	Most obvious in terminal alkynes
7	**C-H**	3000 (stretch) 1375 and 1450 (bend)	s m	As hybridization of C changes sp^3-sp^2-sp, the frequency increases
8	**C≡N**	2250	m, sharp	Characteristic since little else around it

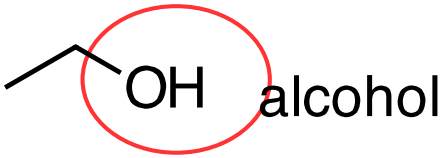
Why does C≡C bond require more energy to stretch than C=C?

How can you distinguish between each isomer?

Molecular Structure is determined by EXPERIMENT!

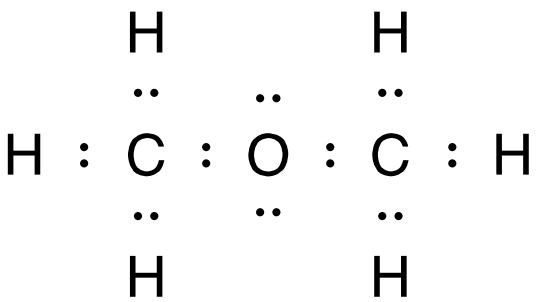
IR Spectroscopy is used to identify bond types

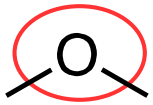




alcohol

CH_3CH_2OH





ether

CH_3OCH_3

Bond Types: C-C
C-H
C-O
O-H

C-H
C-O

IR can be used to distinguish these two compounds.

Organic Compounds can be BIG!

There are *different* ways atoms can bond together

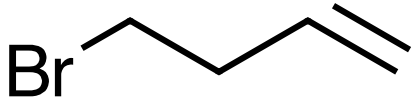
Isomers have the same chemical formula but different connectivity (different structure).

C_4H_{10} has <u>two</u> isomers. Draw the Lewis structure and skeletal structure of each isomer.

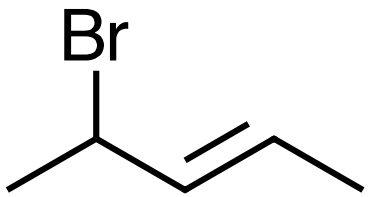
One isomer (butane) is often referred to as linear, the other (isobutane) as branched. Is butane really linear? Give reasons.

Objective: distinguish between isomers and different compounds

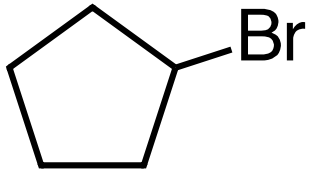
Which two structures are isomers?



A



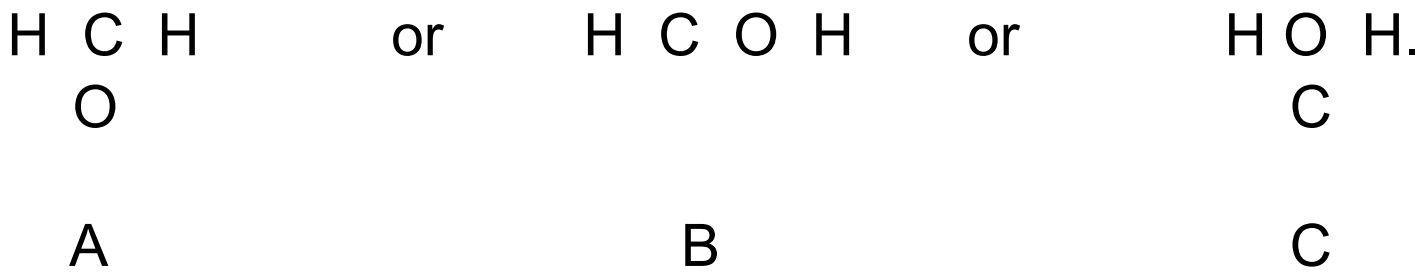
B



C

a. A and B
b. A and C
c. B and C

The Lewis structure of formaldehyde, CH_2O, can have the following connectivities (**3** possible and correct Lewis structures):



a.Complete the Lewis structure of each molecule.

b. Which structure, A, B, or C, is the most likely structure for formaldehyde?

Lewis structure rules:

Account for total # of valence electrons

Octet rule

Duet rule

Molecular Structure is determined by EXPERIMENT!

Elemental analysis --> chemical formula

IR, NMR, m.p., x-ray diffraction --> Lewis structure(s)

Sometimes structural data is hard to interpret.

If you have two or more possible structures, how can you tell which one is the ***more likely*** structure?

Use Formal Charge (FC)

FC on atom = (# of valence electrons) - 1/2(# of bonding electrons) - (# of lone pair electrons)

Or FC on atom = (# of valence electrons) - (# of lines) - (# of dots)

How To Use Formal Charge To Predict The Most Plausible Structure

Formal Charge on atom = (# of valence electrons) - (# of lines) - (# of dots)

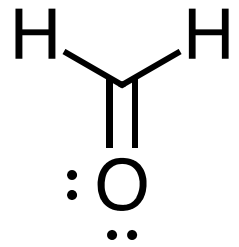
0 or Lowest Formal Charge --> most likely structure

A resonance structure in which C, N, O fits octet rule is more stable than a structure in which atom(s) lack an octet.

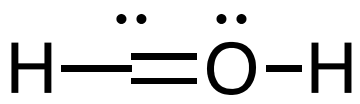
Negative FC on the more electronegative atoms is preferred.

Objective: Calculate the formal charge (FC) and use FC to determine most likely structure.

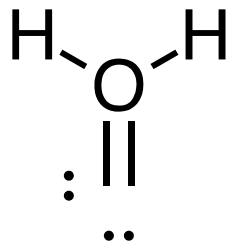
The Lewis structure of formaldehyde, CH_2O, can have the following connectivities (**3** possible and correct Lewis structures):



A



B



C

a. Complete the Lewis structure of each molecule.

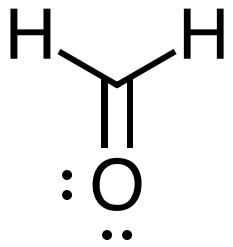
Formal Charge on each atom =

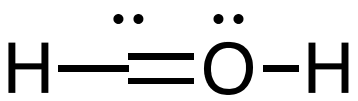
(# of valence e^-) - (# of bonds) - (# of e^- in l.p.)

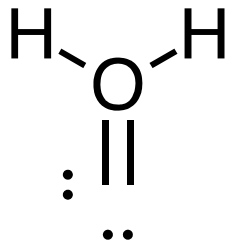
b. Which structure is the most likely structure for formaldehyde?

The General Bonding Rules usually give the **LOWEST** formal charge and most likely structure.

Atom	# of bonds	# of lone pairs	FC
C	4	0	0
N	3		
O	2		
H	1		







Klein, 2.57 Are the two compounds the same compound, constitutional isomers, or different compounds?

a.

b.