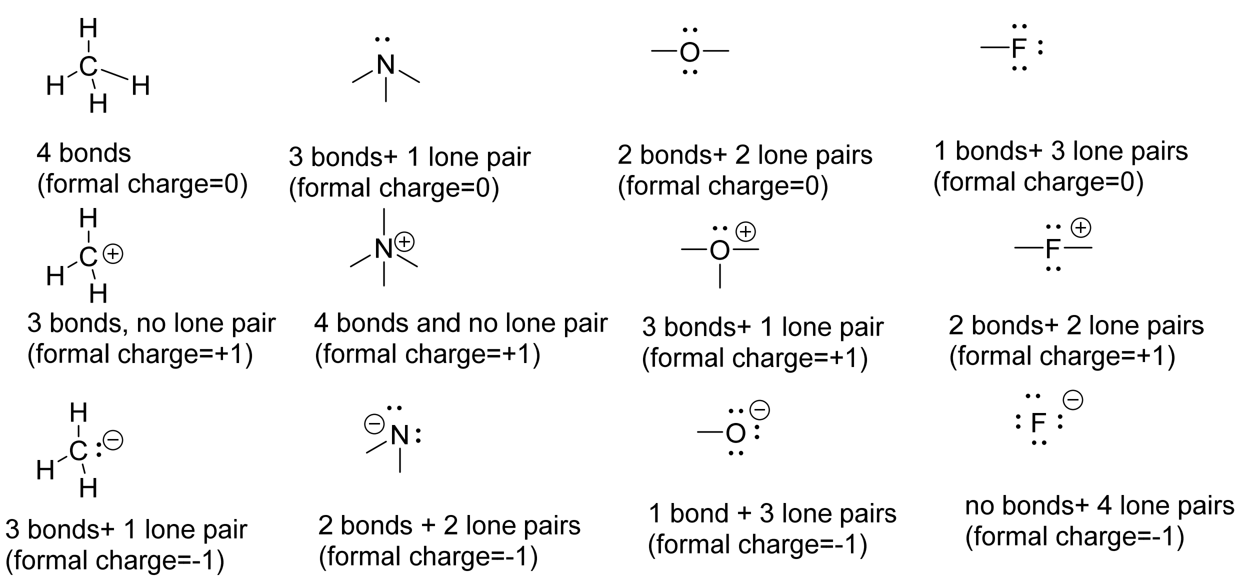
Organic Chemistry Boot Camp Fall 2020 Instructor: Mihaela C. Stefan

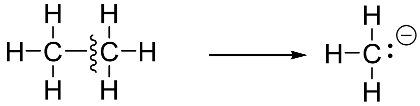
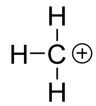
1) Octet rule

Hydrogen has only a first shell and thus only one 1 orbital➔ **hydrogen forms one bond!**
Covalent bond➔ two electrons shared between two atoms.
Carbon is a second shell atom➔ there are four orbitals in the second shell (one s and three p orbitals)➔ **a maximum of 8 electrons is allowed**
All second shell atoms can form a maximum of four bonds attached to that atom➔ 2 electrons involved in each bond to give a total of 8 electrons.
The observation of a maximum of four bonds to second-row atoms was demonstrated by G.N. Lewis in 1916.
SECOND ROW ATOMS WILL BE MOST STABLE WITH EIGHT ELECTRONS IN THE OUTER SHELL.

Formal Charges

4 valence electrons	5 valence electrons	6 valence electrons	7 valence electrons
IV	V	VI	VII
C	N	O	F
Si	P	S	Cl
Ge	As	Se	Br
Sn	Sb	Te	I
Pb	Bi	Po	



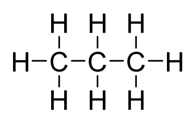
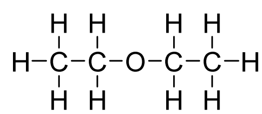
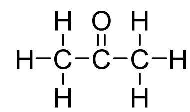
carbanion (8 electrons) carbocation (6 electrons)

Bond breaks in such a way that one carbon takes both electrons from the bond and the other carbon takes no eletrons

2) Representation of Bonds in Organic Compounds

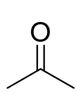
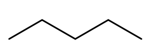
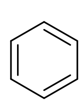
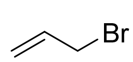
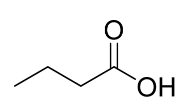
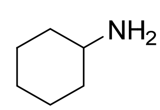
Condensed structural formulas➔ all atoms are indicated in this representation with bonding shown by the placement of atoms in formula➔ read this from left to the right

Examples:

Condensed Structural Formula	$CH_3CH_2CH_3$	$CH_3CH_2OCH_2CH_3$	$CH_3C(O)CH_3$
Flat Representation			
	propane	diethyl ether	acetone

For some compounds, an atom is only bonded to one other atom and not two atoms➔ oxygen atom in diethyl ether.
If an atom is only bonded to the heavy atom to the left, but not the one following in the formula➔ the atom is placed in closed parenthesis➔ see the molecule of acetone

Line angle drawings ➔ bonded atoms are drawn with a line indicating each bond between two atoms. Two atoms that are double bonds between each other they will have two bonds between the two atoms. To make the drawings easier, all carbons are assumed. Any end point or angle change in a structure is a carbon position. All other non-hydrogen atoms have to be explicitly drawn; only carbon is assumed. Each carbon is assumed to have filled the outer shell, and the hydrogens are not drawn. A given carbon has enough hydrogens attached to have the octet rule obeyed. If a given carbon is singly bonded to two other atoms, it also has two bonds to hydrogen.

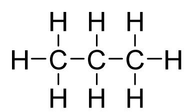
     

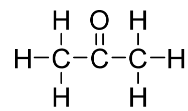
3) Lewis dot structures

All valence electrons are indicated as dots. Carbon has 6 electrons, but only 4 electrons are valence electrons. These 4 electrons can be used to form bonds with other atoms to allow the carbon to have 8 electrons on its outer shell. The electrons in a covalent bond are shared between both atoms which means that atoms use electrons on time average to fill its own outer shell. In a simplified Lewis dot structure, the two electrons shared can be drawn as a line.

Condensed Structural Formula — $CH_3CH_2CH_3$ — $CH_3C(O)CH_3$

Flat Representation

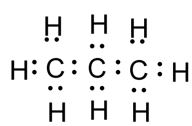


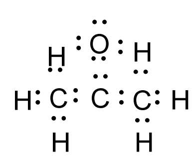


propane

acetone

Lewis Dot Representation





4) Electronegativity and Bond Polarity

Electrons are shared in covalent bonds. By sharing electrons, each atom can have filled outer shell to satisfy the octet rule. However, two electrons may not be shared equally in a bond. The electrons can be closer to one atom than the other on time average. When a bond is between identical atoms, the electrons will be shared equally. When the bond is between two different atoms, the electrons will not be shared equally. The property of atoms attracting electrons is called ELECTRONEGATIVITY. When two different atoms are bonds, the more electronegative of the two atoms will attract more the electrons on time average.

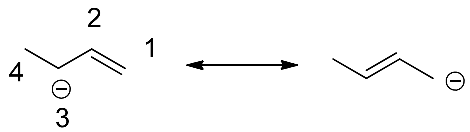
Electronegativity →

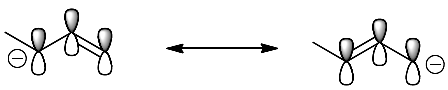
4 valence electrons	5 valence electrons	6 valence electrons	7 valence electrons
IV	V	VI	VII
C	N	O	**F**
Si	P	S	Cl
Ge	As	Se	Br
Sn	Sb	Te	I
Pb	Bi	Po	

↑ Electronegativity

Fluorine is the most electronegative atom!

5) Hybridization = number of sigma bonds + number of lone pairs





Exception: Carbon 3 hybridization is sp2 and not sp3. The definition above applied as would give you sp3 hybridization for carbon 3. If you write a resonance structure, you will get the correct answer which is sp2 hybridization for carbon 3. The following statement can help you to easily determine the hybridization of carbon 3. "If an atom (X) has one or more lone pairs of electrons and it is bonded to an sp2 hybridized atom then the hybridization of the atom (X) is also sp2. This is not a rule, and it is only given to you to help you to determine hybridization without writing the resonance structure. However, the correct answer comes from the resonance structure.

Atomic Orbitals:	**s**	**p**	**d**	**f**
	1	**3**	**5**	**7**

no of atomic orbitals = no of hybrid orbitals (if we combine 4 atomic orbitals we generate 4 hybrid orbitals)

sp3 hybridization ➔ 1s atomic orbital + 3 p atomic orbitals ➔ 4 sp3 hybrid orbitals
sp2 hybridization➔ 1s atomic orbital + 2 p atomic orbitals ➔ 3 sp2 hybrid orbitals + 1 unhybridized p orbital
sp hybridization ➔ 1s atomic orbital + 1p atomic orbital ➔ 2 sp hybrid orbitals + 2 unhybridized p orbitals

<u>Sigma (σ) bond</u> ➔ single bond ➔ forms from sp3, sp2, sp, and p orbitals
<u>Pi (π) bond</u> ➔ multiple bond➔ forms by side to side overlap of p orbitals (cannot form from sp3, sp2, or sp orbitals)
Double bond = one sigma bond + one pi bond
Triple bond = one sigma bond + 2 pi bonds

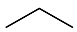
6) Key Points for Writing Resonance Structures

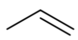
1) **Write the Lewis structure of the analyzed compound**
2) **Only electrons move.** Atoms do not move.
3) **Only π (pi) electrons and lone pairs move.** Pi electrons are electrons in pi bonds. Pi bonds are formed by the side-to-side overlap of unhybridized p orbitals.
4) **Sigma bonds (single bonds) never move.**
5) **The total number of electrons in the overall structure does not change.**

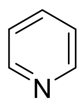
ONLY ELECTRONS IN P ORBITALS RESONATE!!!!!!

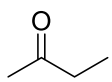
Problems

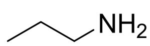
1) Indicate the hybridization of carbons and heteroatoms in the listed structures. Determine the hybridizations of carbons and heteroatoms in each structure. Determine what orbitals are used to make bonds between the atoms in each structure.

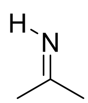
a) 

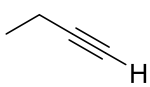
b) 

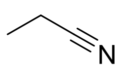
c) 

d) 

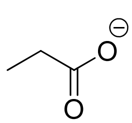
e) 

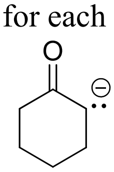
f) 

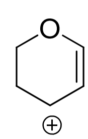
g) 

h) 

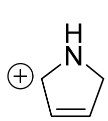
2) Draw a second resonance structure for each ion.



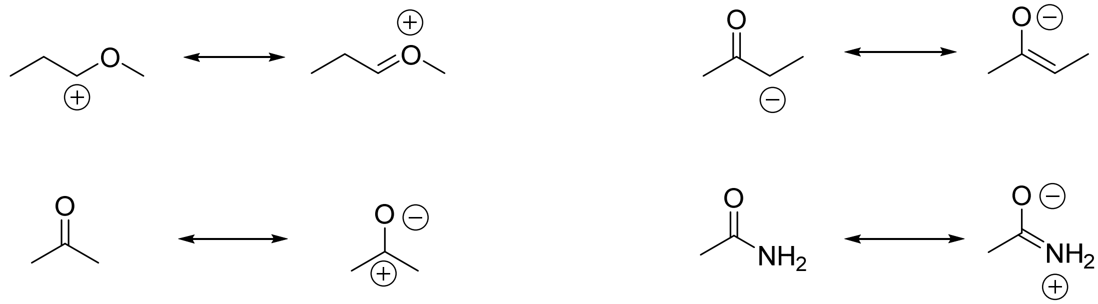




3) Draw all resonance forms of the following compound. Circle the resonance form that is lowest in energy.



4) For the following four pairs of resonance structures, circle the one that is the most stable.

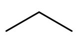


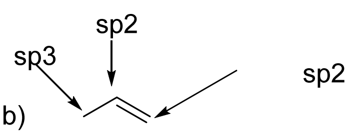
Keys

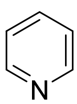
1) Indicate the hybridization of carbons and heteroatoms in the listed structures.

Hybridization = number of sigma bonds + number of lone pairs

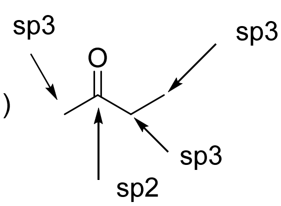
Exception; if an atom (A) has one or more lone pairs of electrons and it is attached to an sp2 hybridized atom =➔ hybridization of the atom (A) is also sp2

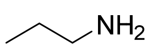
a)  all carbons sp3

b) 

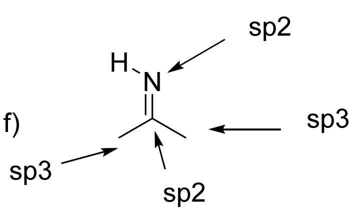
c) 

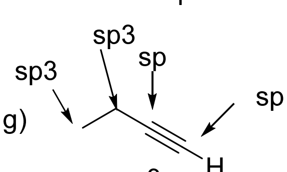
all carbons sp2, nitrogen sp2

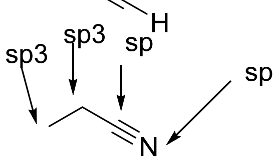
d) 

e) 

all carbons sp3, nitrogen sp3

f) 

g) 

h) 

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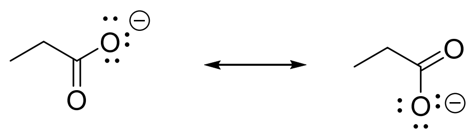

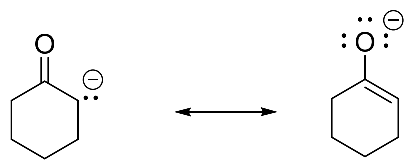

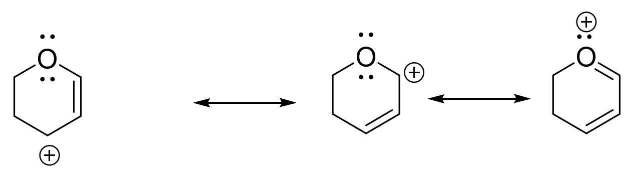

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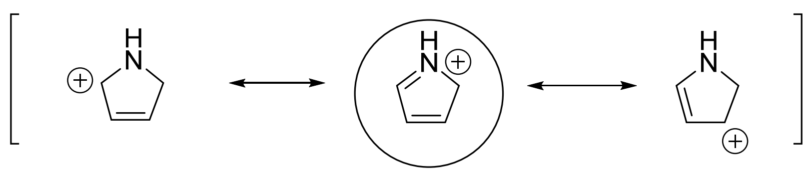

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