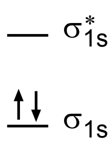
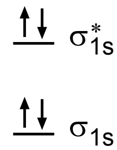
MOLECULAR ORBITAL DIAGRAM KEY

Draw molecular orbital diagrams for each of the following molecules or ions. Determine the bond order of each and use this to predict the stability of the bond. Determine whether each is paramagnetic or diamagnetic.

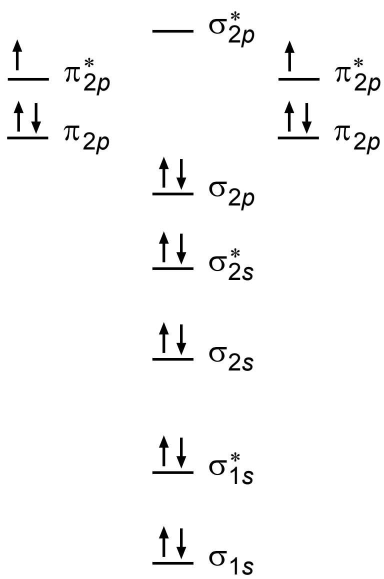
a. H_2 **B.O. = 1** **stable** **diamagnetic**



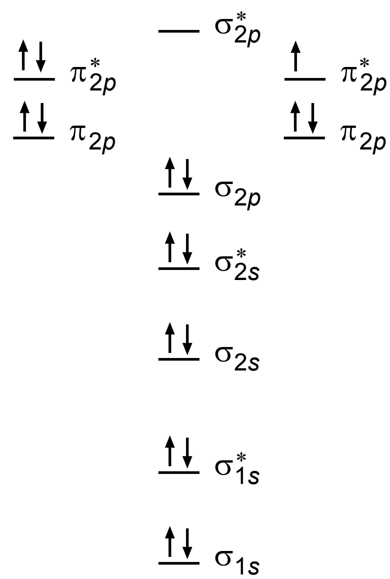
b. He_2 **B.O. = 0** **unstable** **diamagnetic**



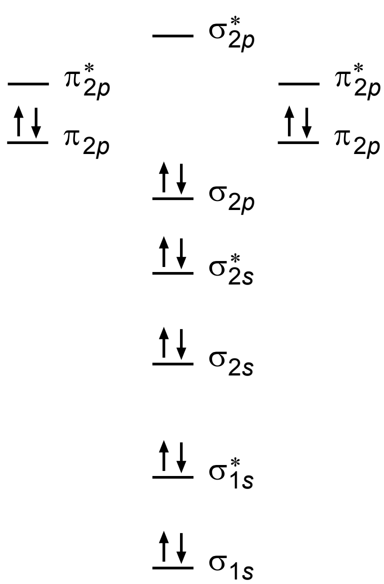
c. O_2 **B.O. = 2** **stable** **paramagnetic**



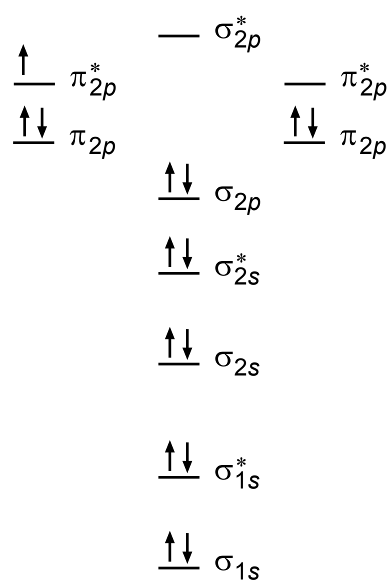
d. O_2^- **B.O. = 1.5** **stable** **paramagnetic**



e. CO **B.O. = 3** **stable** **diamagnetic**



f. NO **B.O. = 2.5** **stable** **paramagnetic**

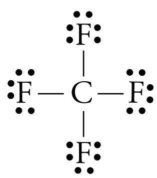


MOLECULAR GEOMETRY AND HYBRID ORBITALS KEY

For each of the following molecular formulas;

- draw a reasonable Lewis Structure,
- predict the hybridization for each atom in the structure,
- describe each bond as either sigma, pi, or delocalized pi system,
- describe how each bond is formed from the overlap of atomic orbitals,
- describe the electron group geometry,
- sketch the molecule, including bonds angles,
- and describe the molecular geometry.

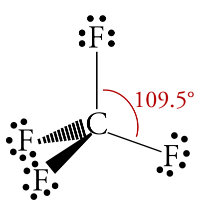
a. CF_4



hybridization for the C **sp^3** hybridization for each F **sp^3**

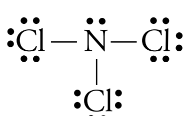
There are four sigma bonds due to sp^3–sp^3 overlap.

electron group geometry around the C **tetrahedral**



molecular geometry around the C **tetrahedral**

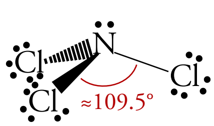
b. NCl_3



hybridization for the N **sp^3** hybridization for each Cl **sp^3**

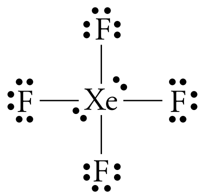
There are three sigma bonds due to sp^3–sp^3 overlap.

electron group geometry around the N **tetrahedral**



molecular geometry around the N **trigonal pyramid**

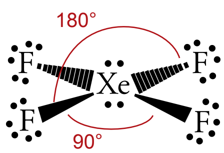
c. XeF_4



hybridization for the Xe **sp^3d^2** hybridization for each F **sp^3**

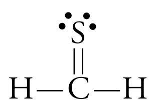
There are four sigma bonds due to sp^3d^2–sp^3 overlap.

electron group geometry around the Xe **octahedral**



molecular geometry around the Xe **square planar**

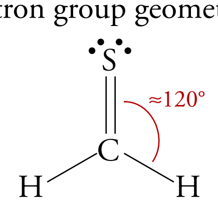
d. H_2CS



hybridization for the C **sp^2** hybridization for the S **sp^2**

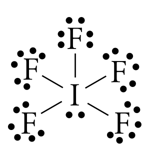
There are two C–H sigma bonds due to sp^2–1s overlap.
There is one C–S sigma bond due to sp^2–sp^2 overlap.
There is one C–S pi bond due to p–p overlap.

electron group geometry around the C **trigonal planar**



molecular geometry around the C **trigonal planar**

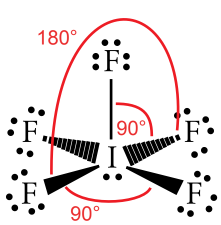
e. IF_5



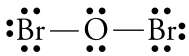
hybridization for the I **sp^3d^2** hybridization for each F **sp^3**

There are five sigma bonds due to sp^3d^2–sp^3 overlap.

electron group geometry around the I **octahedral**



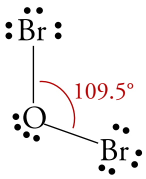
molecular geometry around the I **square pyramid**

f. OBr_2 

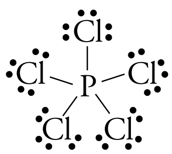
hybridization for the O **sp^3** hybridization for each Br **sp^3**

There are two sigma bonds due to sp^3–sp^3 overlap.

electron group geometry around the O **tetrahedral**



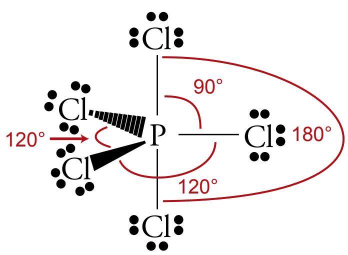
molecular geometry around the O **bent**

g. PCl_5 

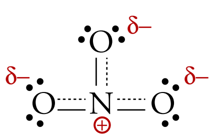
hybridization for the P **sp^3d** hybridization for each Cl **sp^3**

There are five sigma bonds due to sp^3d–sp^3 overlap.

electron group geometry around the As **trigonal bipyramid**



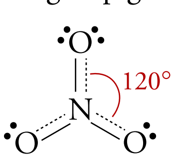
molecular geometry around the P **trigonal bipyramid**

h. NO_3^- 

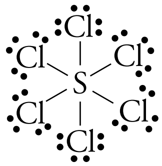
hybridization for the N **sp^2** hybridization for each O **sp^2**

There are three sigma bonds due to sp^2–sp^2 overlap.
One delocalized pi system due to the overlap of a p orbital on nitrogen with a p orbital on each of the three oxygens.

electron group geometry around the N **trigonal planar**



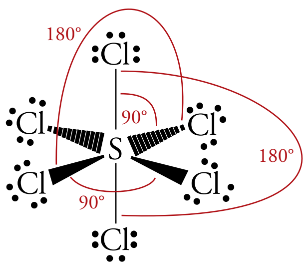
molecular geometry around the N **trigonal planar**

k. SCl_6 

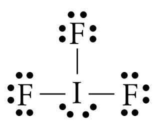
hybridization for the S **sp^3d^2** hybridization for each Cl **sp^3**

There are six sigma bonds due to sp^3d^2–sp^3 overlap.

electron group geometry around the S **octahedral**



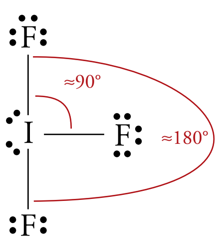
molecular geometry around the S **octahedral**

l. IF_3 

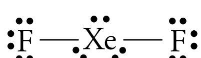
hybridization for the Ir **sp^3d** hybridization for each F **sp^3**

There are three sigma bonds due to sp^3d–sp^3 overlap.

electron group geometry around the I **trigonal bipyramid**



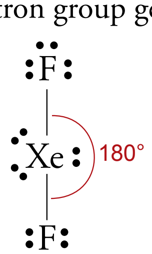
molecular geometry around the I **T–shaped**

m. XeF_2 

hybridization for the Xe **sp^3d** hybridization for each F **sp^3**

There are two sigma bonds due to sp^3d–sp^3 overlap.

electron group geometry around the Xe **trigonal bipyramid**



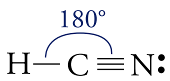
molecular geometry around the Xe **linear**

n. HCN H—C≡N:

hybridization for the C **sp** hybridization for the N **sp**

There is one C–H sigma bond due to sp–1s overlap.
There is one C–N sigma bond due to sp–sp overlap.
There are two C–N pi bonds due to p–p overlap.

electron group geometry around the C **linear**



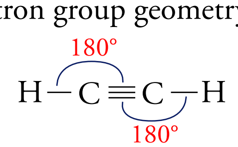
molecular geometry around the C **linear**

o. C_2H_2 H—C≡C—H

hybridization for each C **sp**

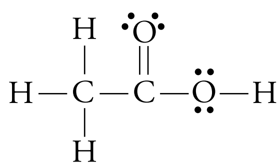
There are two C–H sigma bond due to sp–1s overlap.
There is one C–C sigma bond due to sp–sp overlap.
There are two C–C pi bonds due to p–p overlap.

electron group geometry around each C **linear**



molecular geometry around each C **linear**

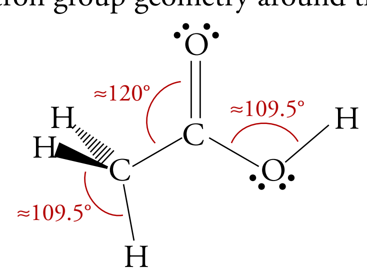
p. CH_3CO_2H



hybridization for the left C **sp^3** hybridization for the right C **sp^2**
hybridization for the top O **sp^2** hybridization for the right O **sp^3**

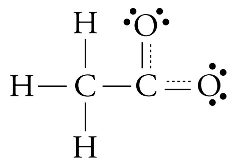
There are three C–H sigma bonds due to sp^3–1s overlap. There is one C–C sigma bond due to sp^3–sp^2 overlap. There is one C–O sigma bond due to sp^2–sp^2 overlap. There is one C–O pi bond due to p–p overlap. There is one C–O sigma bond due to sp^2–sp^3 overlap. There is one O–H sigma bond due to sp^3–1s overlap.

electron group geometry around the left C **tetrahedral**
electron group geometry around the right C **trigonal planar**
electron group geometry around the right O **tetrahedral**



molecular geometry around the left C **tetrahedral**
molecular geometry around the right C **trigonal planar**
molecular geometry around the right O **bent**

q. $CH_3CO_2^-$



hybridization for the left C **sp^3** hybridization for the right C **sp^2**

hybridization for each O **sp^2**

There are three C–H sigma bonds due to sp^3–1s overlap.

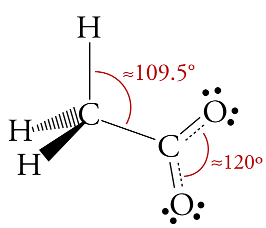
There is one C–C sigma bond due to sp^3–sp^2 overlap.

There are two C–O sigma bonds due to sp^2–sp^2 overlap.

There is one delocalized pi system due to the overlap of a p orbital one the right carbon and a p orbitals on each of the oxygen atoms.

electron group geometry around the left C **tetrahedral**

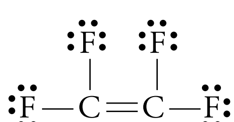
electron group geometry around the right C **trigonal planar**



molecular geometry around the left C **tetrahedral**

molecular geometry around the right C **trigonal planar**

r. CF_2CF_2



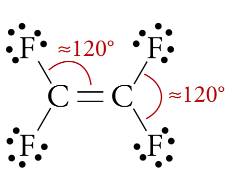
hybridization for the each C **sp^2** hybribization for each F **sp^3**

There are four C–F sigma bonds due to sp^2–sp^3 overlap.

There is one C–C sigma bond due to sp^2–sp^2 overlap.

There is one C–C pi bond due to p–p overlap.

electron group geometry around the each C **trigonal planar**



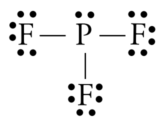
molecular geometry around the each C **trigonal planar**

CHEMISTRY 151
MOLECULAR GEOMETRY AND HYBRID ORBITALS KEY

For each of the following molecular formulas;

- draw a reasonable Lewis Structure,
- predict the hybridization for each atom in the structure,
- describe each bond as either sigma, pi, or delocalized pi system,
- describe how each bond is formed from the overlap of atomic orbitals,
- describe the electron group geometry,
- sketch the molecule, indicating the approximate bond angles in your sketch,
- and describe the molecular geometry.

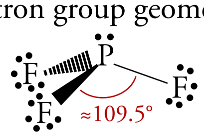
a. PF_3



hybridization for the P **sp^3** hybridization for each F **sp^3**

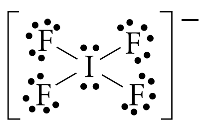
There are three sigma bonds due to sp^3–sp^3 overlap.

electron group geometry around the P **tetrahedral**



molecular geometry around the P **trigonal pyramid**

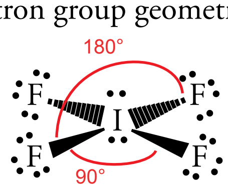
b. IF_4^-



hybridization for the I **sp^3d^2** hybridization for each F **sp^3**

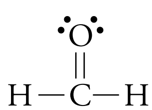
There are four sigma bonds due to sp^3d^2–sp^3 overlap.

electron group geometry around the I **octahedral**



molecular geometry around the I **square planar**

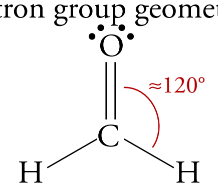
b. H_2CO



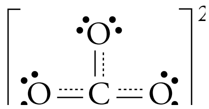
hybridization for the C **sp^2** hybridization for the O **sp^2**

There are two C–H sigma bonds due to sp^2–1s overlap.
There is one C–O sigma bond due to sp^2–sp^2 overlap.
There is one C–O pi bond due to p–p overlap.

electron group geometry around the C **trigonal planar**



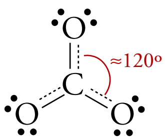
molecular geometry around the C **trigonal planar**

d. CO_3^{2-} 

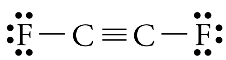
hybridization for the C **sp²**   hybridization for each O **sp²**

There are three sigma bonds due to sp²–sp² overlap.
One delocalized pi system due to the overlap of a p orbital on the carbon atom with a *p* orbital on each of the three oxygen atoms.

electron group geometry around the C **trigonal planar**



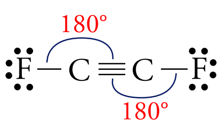
molecular geometry around the C **trigonal planar**

d. C_2F_2 

hybridization for each C **sp**   hybridization for each F **sp³**

There are two C–F sigma bonds due to sp–sp³ overlap.
There is one C–C sigma bond due to sp–sp overlap.
There are two C–C pi bonds due to *p–p* overlap.

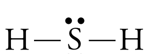
electron group geometry around each C **linear**

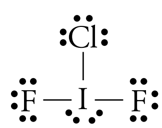


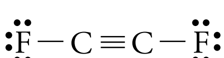
molecular geometry around each C **linear**

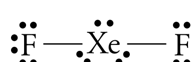
LEWIS STRUCTURES WORKSHEET KEY

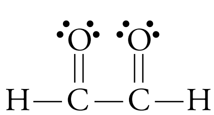
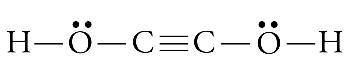
Draw reasonable Lewis structures for the following.

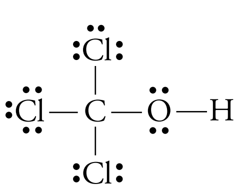
a. H_2S 

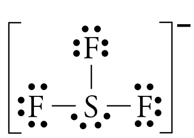
b. $IClF_2$ 

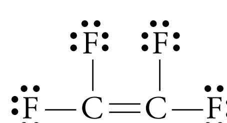
c. C_2F_2 

d. XeF_2 

e. $C_2H_2O_2$  or 

f. CCl_3OH 

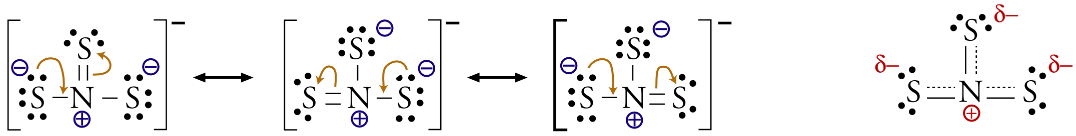
g. SF_3^- 

h. CF_2CF_2 

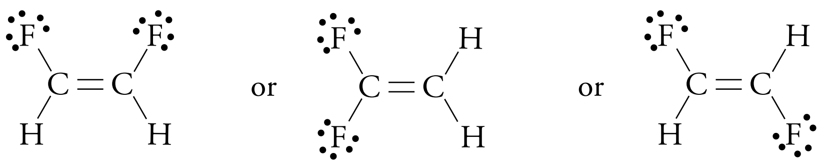
LEWIS STRUCTURES – RESONANCE KEY

For each of the following, predict whether they can be described with resonance or not. If they can, draw Lewis structures including formal charges for all of the reasonable resonance forms and sketch the resonance hybrid. If the resonance forms have different stability, indicate which is more stable.

1. NS_3^-

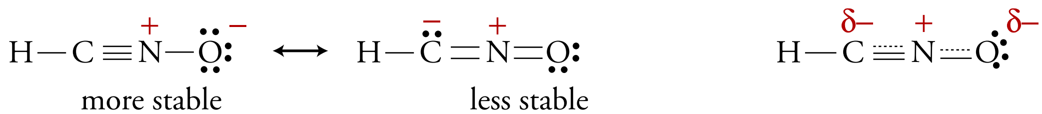


2. CH_2CF_2

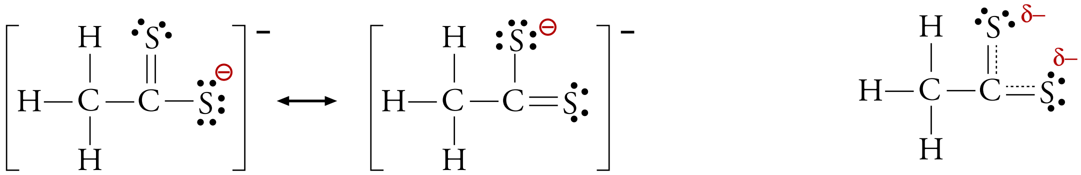


no resonance

3. HCNO

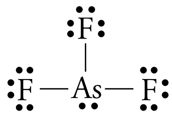


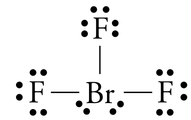
4. $CH_3CS_2^-$

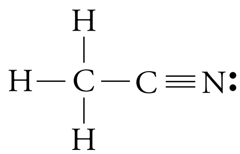


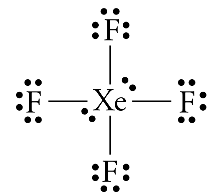
CHEMISTRY 151 – LEWIS STRUCTURES KEY

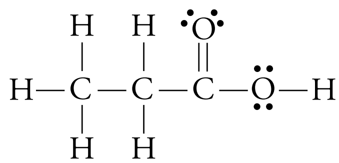
Sketch reasonable Lewis structures for each of the following. Indicate the formal charges on each atom that has them.

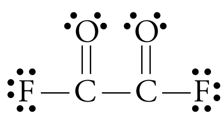
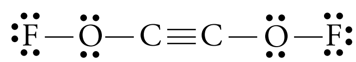
a. AsF_3 

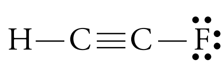
b. BrF_3 

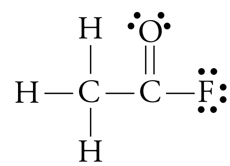
c. CH_3CN 

d. XeF_4 

e. $CH_3CH_2CO_2H$ 

f. $C_2F_2O_2$  or 

g. HCCF 

h. CH_3COF 

TYPES OF INTERACTIONS KEY

For each of the following pairs of chemical formulas,

- identify whether each substance represents a metal, an ionic compound, a network crystal, a polar molecular substance, or a nonpolar molecular substance.
- identify the primary type of interaction that holds the particles of each in the liquid and solid form: metallic bond, ionic bond, covalent bond, hydrogen bond, dipole–dipole interaction, or London force.
- identify which would have the stronger interactions between the particles in the liquid or solid.
- indicate which would have the higher boiling point.

The highlighted formulas represent the substances with the strongest attractions thus the higher boiling point.

a. **$BaCl_2$** & CH_2Br_2	Ionic stronger than dipole–dipole
b. **SiO_2** & HF	Covalent bonds stronger than hydrogen bonds
c. **CH_3NH_2** & CH_3F	Hydrogen bonds stronger than dipole–dipole
d. BF_3 & **ClF_3**	Dipole–dipole stronger than London forces
e. PCl_5 & **ICl_5**	Dipole–dipole stronger than London forces
f. CS_2 & **OBr_2**	Dipole–dipole stronger than London forces

CHEMISTRY 151 – PROPERTIES RELATED TO STRENGTHS OF ATTRACTIONS IN LIQUIDS AND SOLIDS WORKSHEET KEY

Circle the formula in each pair that you would expect to have the higher melting point and boiling point.

a. $\mathbf{C_3H_7OH}$ or CH_3COCH_3 — Hydrogen bonds stronger than dipole–diplole
b. $(C_2H_5)_2NH$ or $\mathbf{(C_3H_7)_2NH}$ — The larger molecule has the stronger London forces.
c. $\mathbf{NH_3}$ or PH_3 — Hydrogen bonds stronger than dipole–diplole
d. **C(dia)** or $C_{12}H_{25}OH$ — Covalent bonds stronger than hydrogen bonds
e. $\mathbf{Li_2CO_3}$ or CH_3OH — Ionic bonds stronger than hydrogen bonds
f. SO_2 or $\mathbf{SiO_2}$ — Covalent bonds stronger than dipole–dipole
g. $\mathbf{C_8H_{18}}$ or CH_4 — The larger molecule has the stronger London forces.
h. CF_4 or $\mathbf{PF_3}$ — Dipole–dipole stonger than London forces