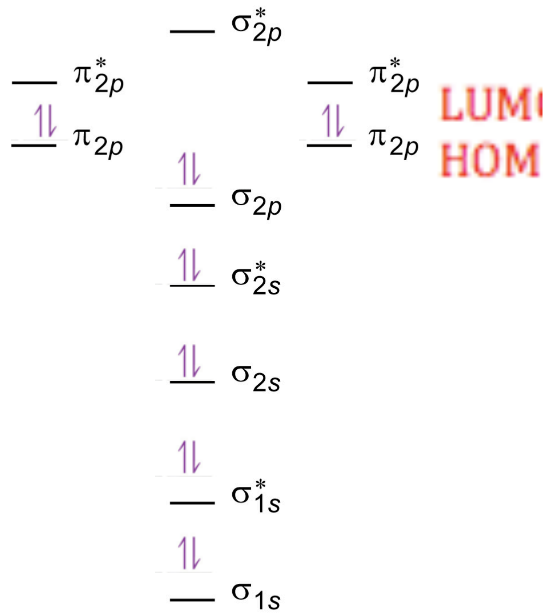
Department of Chemistry
University of Texas at Austin

Name:____________________

IMF Unit - RAQ

1. Fill in the Molecular Orbital diagram for CO.
Please state the bond order.
Please state whether this compound is expected to be paramagnetic or diamagnetic.
Please identify on the drawing the location of the HOMO and the LUMO.



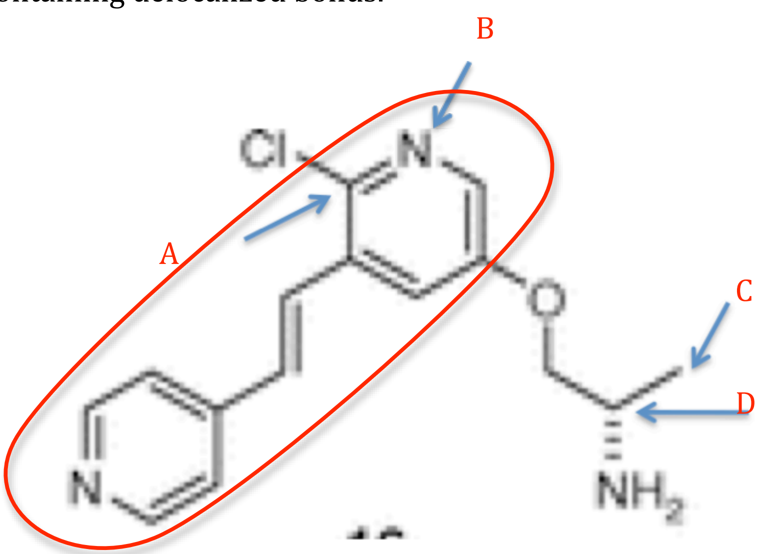
Carbon has 6 total electrons
Oxygen has 8 total electrons

BO = ½ (Bonding – Antibonding)
BO = ½ (10 – 4) = 3

Diamagnetic

Outcomes: 9,10,11,12

2. From the line drawing write the correct molecular formula.
State the valence bond hybridization around the "central" atoms where indicated with an arrow. In addition state the electronic geometry and molecular geometry around each of these "central atoms". State the number of pi bonds. Circle the regions containing delocalized bonds.



Correct Molecular Formula: $C_{15}H_{16}N_3OCl$
A – sp^2, trigonal planar (electronic), trigonal planar (molecular)
B – sp^2, trigonal planar (electronic), bent (molecular)
C – sp^3, tetrahedral (electronic), tetrahedral (molecular)
D – sp^3, tetrahedral (electronic), tetrahedral (molecular)

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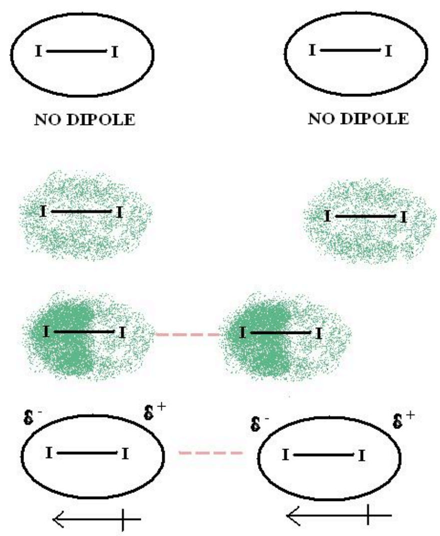
pi bonds: 7 according the valence bond theory
The circled region is ONE large delocalized pi system according the MO theory

Outcomes: 1,2,3,4,5,6

3. Fully describe (macroscopic and "molecular" view with words and pictures) the two solids I_2 (mp = 386 K) and KI (mp = 959 K).

I_2 – Molecular Solid

- Only non-metals
- Non-polar molecules
- Held together by dispersion forces only
- Solid at room temp because the large iodine atoms have a lot of electrons making the I_2 molecules highly polarizable!



KI – Ionic Solid

- Metal and non-metal
- Columbic attractions (ionic interactions) hold the solid together
- Crystal lattice structure of alternating K^+ cations and I^- anions
- Solid is not a good conductor but in liquid form or when dissolved KI is a good conductor

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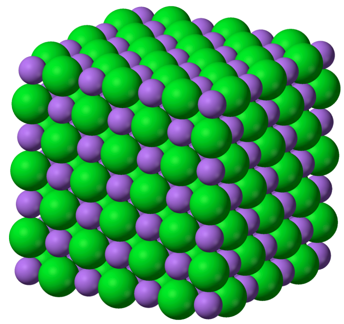
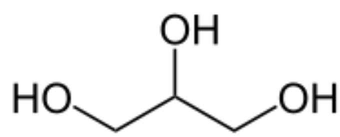


Purple: K^+ cations
Green: I^- anions

Outcomes: 13,17,18

4. Propanol ($CH_3CH_2CH_2OH$) and Glycerol ($CH_2OHCH_2OHCH_2OH$) are both considered to be alcohols. While they both exist as liquids at room temperature, their liquid properties are different. Explain how you expect the properties to be different. Support your answer with a full molecular explanation.

Propanol: 

Glycerol: 

Surface Tension: Glycerol **greater** than propanol
Viscosity: Glycerol **greater** than propanol
Vapor Pressure: Glycerol **less** than propanol
Boiling Point: Glycerol **greater** than propanol

Glycerol and propanol contain the same number of carbons, but glycerol has three times the amount of -OH groups and therefore MUCH more hydrogen bonding interactions between molecules. This stronger IMF influence holds the glycerol molecules together better.

Outcomes: 8,13,14,15

5. Given the following data provide a "molecular view" description of the trend in boiling points based on all intermolecular forces for the given molecules. In your answer include whether or not each compound exists as a solid, liquid or gas at room temperature.

Compound	*Boiling Point, Melting Point*
CHF_3	191 K, 26 K – Gas at RT
$CHCl_3$	334 K, 210 K – Liquid at RT
$CHBr_3$	415 K, 319 K – Solid at RT
CHI_3	490 K, 396 K – Solid at RT

As we look down the table, halides increase in size and therefore in polarizability. The more polarizable, the greater the dispersion forces are between molecules. The compounds lower in the table have stronger dispersion IMFs. All of the compounds also have dipole-dipole IMFs, but the IMF that is most influential in the differences observed here is the dispersion forces.

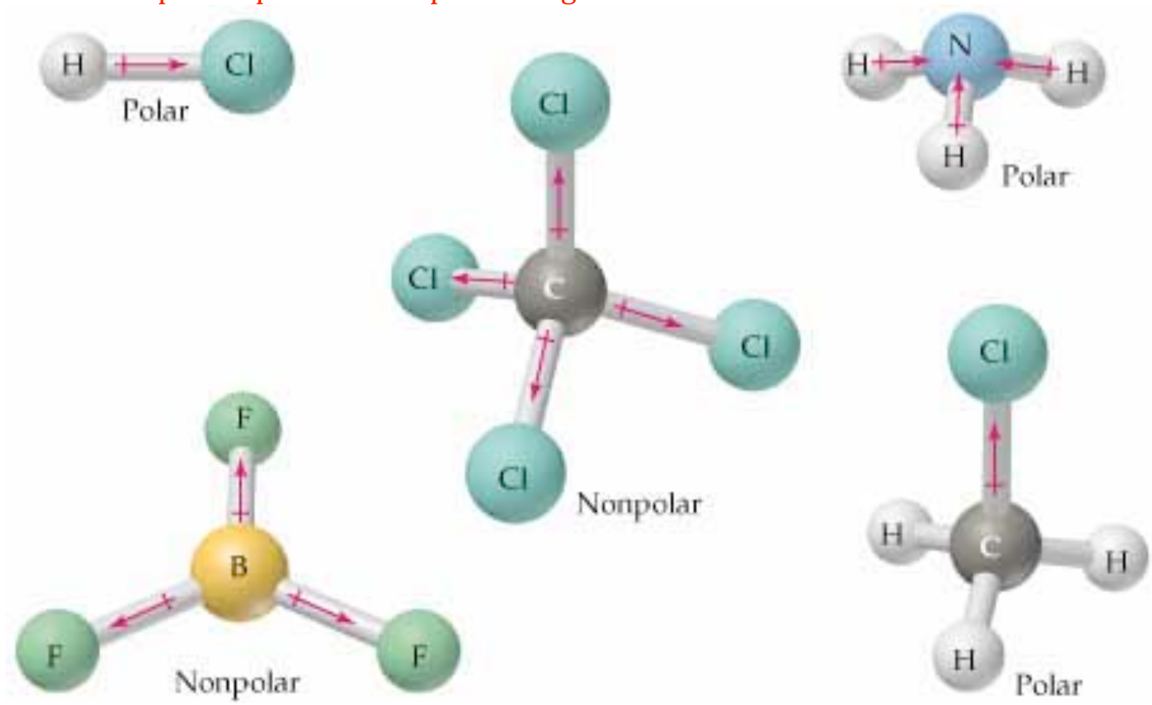
NONE of the compounds have hydrogen bonding – The hydrogens are always bonded to the carbon in these molecules and for hydrogen bonding to exist the hydrogen must be bonded directly to F, O or N.

Outcomes: 8,13,15,16,17,18

6. To fully prepare for this test you should be able to explain the following:

I. Describe the difference/similarities between a polar bond and a polar molecule.

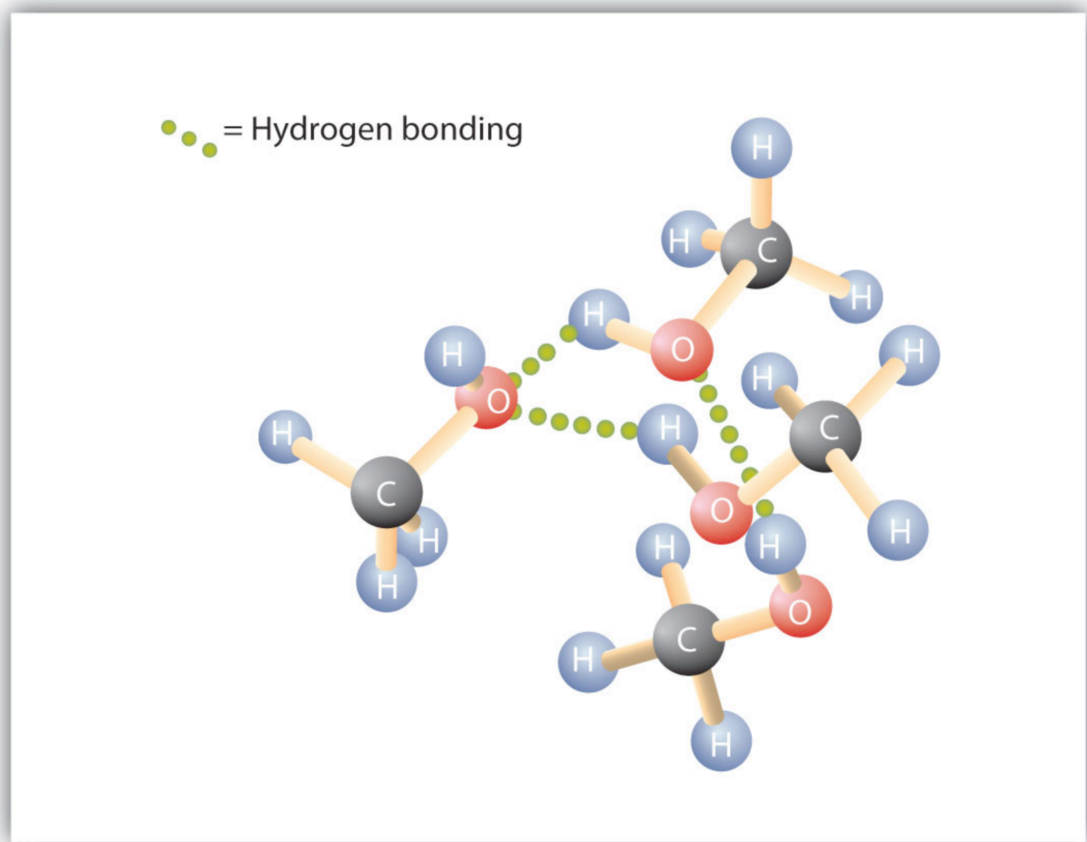
Polar Bond: Electronegativity difference between two atoms
Polar Molecule: A permanent, net dipole moment
Both: Have partial positive and partial negative areas.



Outcomes: 7,8

II. Describe the differences/similarities between a bond and an intermolecular force. Include in your description the term "hydrogen bond" in the context of IMFs.

Bond: Within a molecule. Covalent bonds are shared electrons, Ionic bonds are electrostatic interactions between charged species.
IMF: Between molecules. IMFs are electrostatic interactions too, but weaker. Hydrogen bonding is an IMF because it occurs between molecules. (See picture below of methanol molecules H-bonding)



Outcomes: 13

III. Describe the differences/similarities between polar and polarizable.

Polar: Fixed dipole moment. Molecular geometry can be important.
Polarizable: The ability to have induced dipole moments. Increases with size.
Outcomes: 16

IV. Describe the differences/similarities between molecule and molecular solid and covalent solid.

Molecule:

- A single, discrete unit of atoms
- Example: One water molecule H_2O

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Molecular Solid:

- Comprised of non-metals
- Many individual, discrete molecules held together by IMFs
- Usually a low MP and BP
- Example: An ice cube (lots of water molecules!)

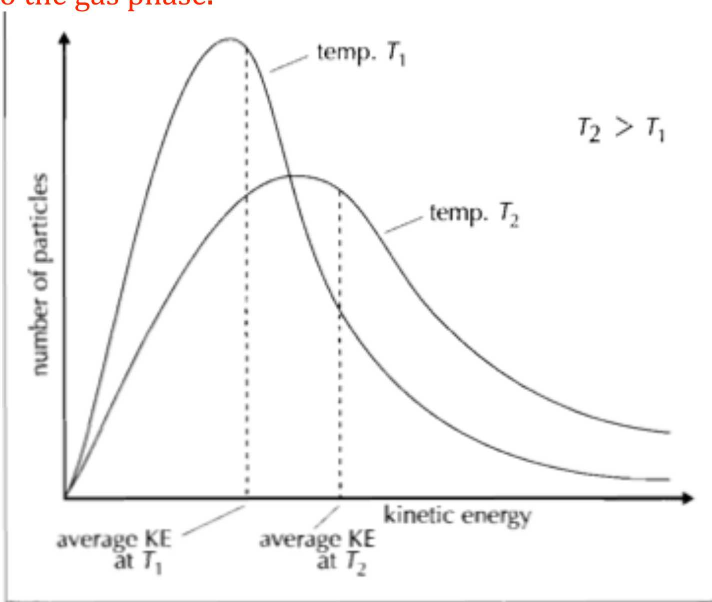
Covalent Solid:

- Comprised of non-metals
- **Covalently** bound network of nonmetals
- Usually high MP and BP
- Example: Quartz is a network of SiO_2

Outcomes: 17,18

V. Explain the relationship between boiling point, vapor pressure and the Boltzmann distribution of KE's for a liquid at given temperature in the context of IMFs.

For any liquid, the molecules have a distribution of Kinetic Energies. If a molecule has enough kinetic energy if can escape from the IMFs it experiences in liquid phase. If it is at the surface, it will escape into the gas phase. The weaker the IMFs, the more molecules (a higher percentage) at any given temperature can escape into the gas phase.



For example, propanol has a higher vapor pressure than glycerol because it experiences fewer hydrogen bonding interactions (see #4). A greater percentage of propanol molecules will be found in the gas phase compared to glycerol at any given temperature, because its IMFs are weaker.

Higher vapor pressure, lower boiling point.
Lower vapor pressure, higher boiling point.
Outcomes: 15

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Place the following outcomes next to the problems on this sheet.

Students will be able to…..

1. apply the VSEPR model to determine a molecule's electronic geometry and molecular geometry from its Lewis dot structure.
2. apply the VB model to give the atomic hybridization of any atom in a given molecule.
3. use the VB model to describe any bond in a molecule.
4. interpret line drawing of chemical compounds with implicit hydrogens, carbons, and lone pairs.
5. identify sigma and pi bonds.
6. recognize localized vs delocalized electrons within a structure.
7. identify polar bonds (we will assume C-H bonds are non-polar)
8. determine if a molecule is polar based on polar bonds and it molecular geometry.
9. recognize that MO theory is a quantum mechanical method used by chemists to determine the energy of the electron in a molecule as well as its geometry.
10. recognize that MO theory can be used to determine the energy of light absorbed by a compound by exciting electrons between MOs (from the HOMO to the LUMO).
11. should be able to interpret a given MO diagram as well as fill in electrons into an MO diagram to predict bond order for a compound and predict whether it is paramagnetic or diamagnetic.
12. recognize that constructive interference of atomic orbitals yields lower energy MO (bonding) while destructive interference leads to higher energy MO (anti-bonding)
13. be able to define the three major intermolecular forces (IMF) discussed in class: dipole-dipole, h-bonding, and dispersion (London, van der Waals, induced dipole- induced dipole, instantaneous dipole- instantaneous dipole)
14. use a compound's molecular structure to identify the types of IMFs that exists in the condensed phase.
15. relate the IMFs to liquid properties such as boiling point, vapor pressure, viscosity, and surface tension.
16. explain how size and shape affect the magnitude of the dispersion forces.
17. recognize the four types of solids: network (covalent), metallic, ionic, and molecular.
18. recognize how the macroscopic properties of solids (melting point, hardness, conductivity, ...) can be explained by the microscopic model of solids.