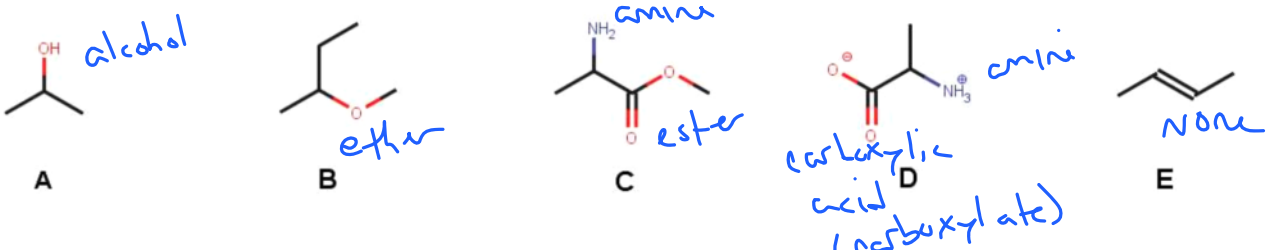
PS1key

Problem Set 1 **(Due January 18th)**

1. Examine the image to the right and answer each of the following questions:

   a. What does this image represent? How strongly two molecules of opposing charge interact as the distance between them is changed.
   b. Units are missing for the x and y axes. Based on what you know about the meaning of this image, propose units for each axis. Energy = J, kJ, kJ/mol, etc. radius = m, nm, pm, μm, etc.
   c. There is a very important physical law that is used to understand this figure. Name it and discuss how each variable influences the stabilization energy. Coulomb's law. Two charged particles – charges represented by q1 and q2. If they are opposing, it makes the stabilizing energy negative. The radius is the distance between the two molecules. Since r is in the denominator, moving the molecules apart decreases the stabilization.
   d. The law that was just mentioned fails to completely describe the image. Why? It does not account for the unfavorable interaction as the two molecules begin to occupy the same space. This, of course, cannot happen.
   e. Which intermolecular force(s) can be explained by the trend seen in this image? For any IMF that is not governed by the trend, clearly explain why. It can explain all IMF. They are all based on the attraction between opposing charges.

2. Use the image below to answer each of the following questions. A, B, E, and I are below.

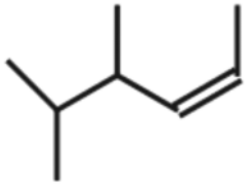


   a. Draw the complete Lewis structure for each compound.
   b. Identify all intermolecular forces that each compound can participate in.
   c. Which compound (if any) can be an H-bond acceptor but not a donor? B and C. O can accept H-bonds. There is not an O-H, N-H, or F-H present, so there is not an H-bond donor.
   d. Identify all functional groups that are present in each molecule.
   e. Is compound E a cis or trans alkene? trans
   f. Rank these compounds based on their solubility in water. Lowest solubility is 1 and the highest solubility is 5. E < B < A < C < D. This is based on the number and strength of interactions with water. D has two ions – Ion/dipole is very strong and will make D quite soluble. E is nonpolar

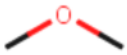
and will not interact with water. B can accept 2 H-bond, A can make 3 H-bonds (accept two and donate one) and C can make 7 H bond (3 from N and 2 from each O).

g. Which compound do you expect to have the lowest melting point? E – weakest IMF (LDF only)
h. Which compound do you expect to have the highest melting point? D – strongest IMF (ion/ion)
i. Determine the hybridization on each atom in compound C.

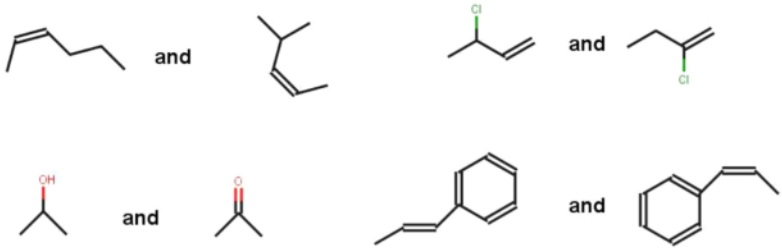
3. Draw 3 possible isomers of each of the compound shown below. Many possibilities. Here are 3



4. How many hydrogen bonds can this compound form with water? Clearly explain your answer. 2. Each lone pair on the oxygen can accept a H-bond from water



5. Determine if each pair are structural isomers, stereoisomers, or neither.



6. The effectiveness of a drug is influenced by its ability to "partition" between aqueous solutions and non-polar solutions. The equilibrium below represents this reaction where the reactant is a compound dissolved in water and the products is the same compound dissolved in octane.

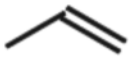
$$X\ (H_2O) \rightleftharpoons X\ (Octane)$$

Consider the two compounds below. Which would have a more negative ΔG^0 for this reaction? The second compound Which would have a smaller K? The first compound.

The first compound should be reasonably soluble in water because it is polar. The second compound, however, will not be soluble in water. It will, however, be quite soluble in a nonpolar solvent like octane. So, Compound 2 is more soluble in octane than water, so it will favor the products side of the reaction ([Prod] > [Reactants]). Consequently, K > 1. Compound 1 will be more soluble in water, so [React] > [Prod] and K < 1 (remember $K = \frac{[Products]}{[Reactants]}$). So…Compound has a smaller K.

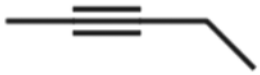
ΔG° = -RTlnK. As K gets bigger, ΔG° gets smaller. If products are favored, the reaction is spontaneous and ΔG° is negative. Since Compound 2 has a larger K, it will have a more negative ΔG°.

7. Name each compound using the common organic name.

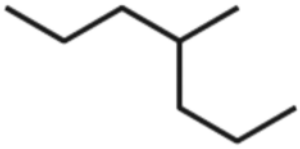


1-propene

1-fluoroethane

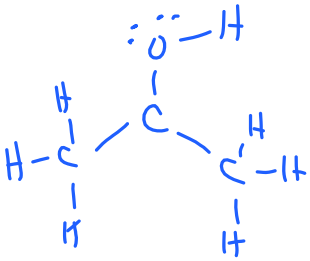


2-propyne



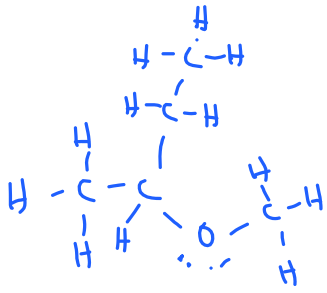
4-methylheptane

2) A



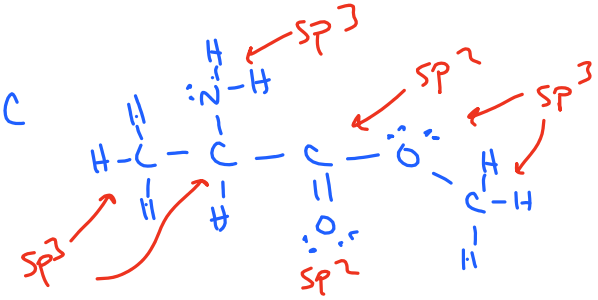
LDF / dipole-dipole
H-bond

B



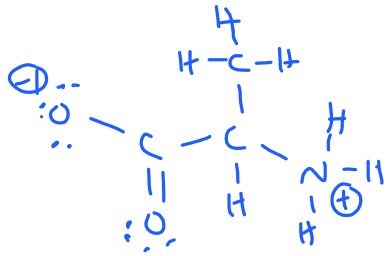
LDF / dipole-dipole

C



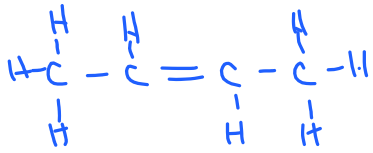
LDF / H-bond / dipole dipole

D



LDF / Ion Ion / Dipole/Dipole / H-bond

E



LDF only