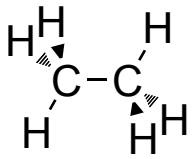
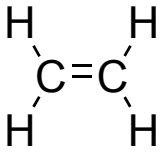
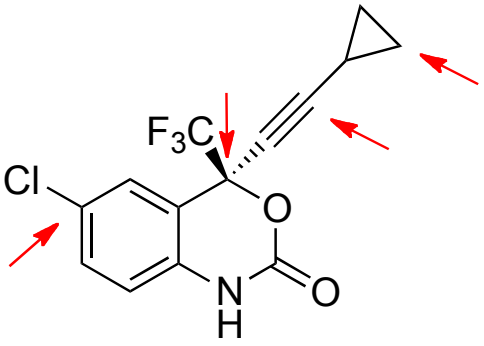
Problem Set 1 *due MONDAY March 18th* ***IN CLASS*** Chem 132
Dr. Fantini March 4, 2013

Name: _____ SB#: _____

1. Please complete the following table:

property of molecule:			
name of shape at central atom			
hybrid orbital set			
# of left-over *p* orbitals			
typical bond angles			
% *s*-character			
C–H bond length (write "longest" and "shortest" at the correct ends of the arrow)			
C–H acidity (write "most acidic" and "least acidic" at the correct ends of the arrow)			

Questions 2—11 refer to the following compound, which is efavirenz, a non-nucleoside reverse transcriptase inhibitor (antiviral used for the treatment of HIV).



2. What is the molecular formula of this drug?

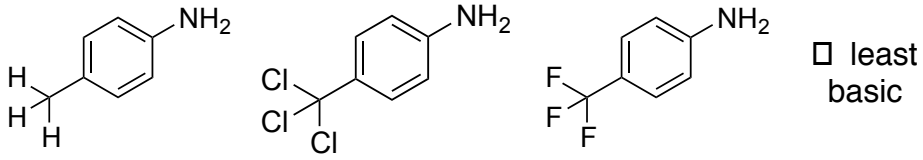
3. Draw a “regular” Lewis structure for this molecule (make it big). A “regular” Lewis structure is one that has all element symbols explicitly shown.

4. Mark up the large drawing of the molecule with δ+ and δ- as appropriate to show polar bonds. Also draw the bond dipole symbol in the proper manner at each polar bond.
5. Identify the hybridization at each carbon atom.
6. Write the bond angles around the atoms marked with red arrows.
7. Identify the carbon atom (or atoms) where there is the greatest *s*-character in the hybrid orbital.
8. Which bond do you expect to be the shortest in the molecule? (It is from H to another atom.) Why?

9. Which bond from a carbon atom to a halogen is longer? Why? (The halogens are the elements of group 17.)

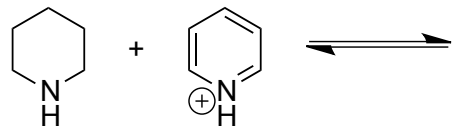
10. Which is the longest C—O single-bond in the molecule? Why?

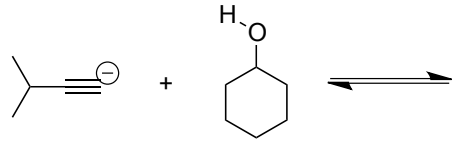
11. The following amines are ordered according to base strength:

most basic  least basic

Explain, using resonance and inductive effects, the trend in base strength for these three compounds.

12. Draw products, label conjugate acid-base pairs, and predict which side of the reaction is favored. Under each reaction, briefly explain if you used element, inductive, resonance, or hybridization trends in your reasoning.

(a) 

(b) 

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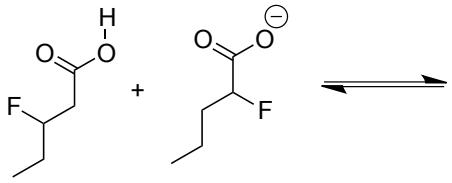
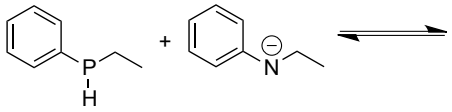
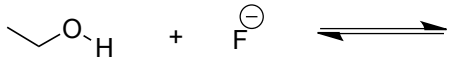
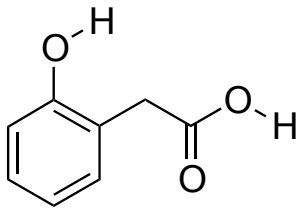
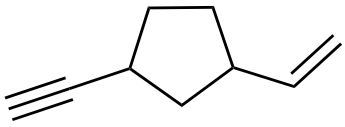
(c) 

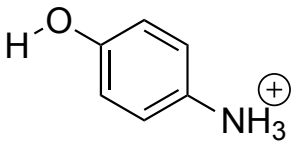
(d) 

(e) 

13. Circle the most acidic H in each molecule or ion. (Draw in the H if necessary.)



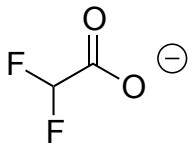
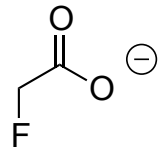
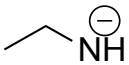
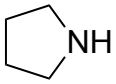




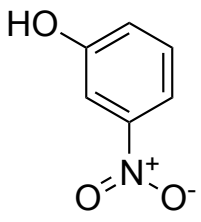
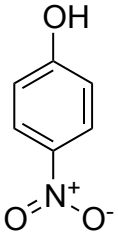
14. Arrange these compounds in order of increasing acidity.

CH_3SH CH_3OH HI NH_3

15. Arrange the bases in order of increasing basicity. (Redraw in order in the box.)

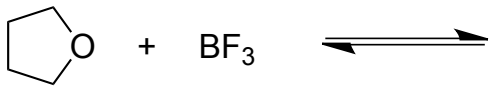





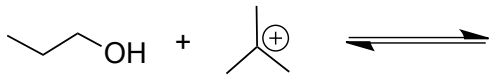
16. Explain and justify that 4-nitrophenol is a stronger acid than 3-nitrophenol. (Invoke resonance effects in your answer.) The H on the oxygen is the acidic H.

3-nitrophenol 4-nitrophenol

17. Identify the Lewis acid and Lewis base in each reaction. Draw the Lewis acid–base adduct as the product. (For (c), there are two bonds to Br in the product.)

(a) 

(b) 

(c)