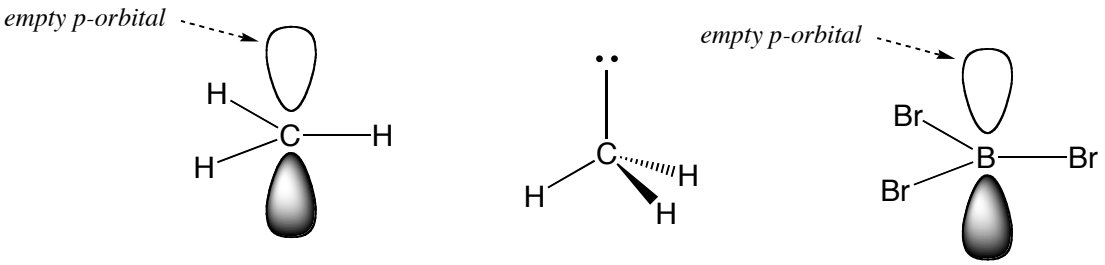
Answers to Problem Set #2

Question 1. For each of the following molecules or ions, provide the hybridization state of the carbon or boron atom and draw a three-dimensional structure that clearly defines the molecular shape.

a) $\overset{\oplus}{C}H_3$ b) $:\overset{\ominus}{C}H_3$ c) BBr_3



Carbon is sp^2-hybridized
Molecule is planar

Carbon is sp^3-hybridized
Molecule is pyramidal

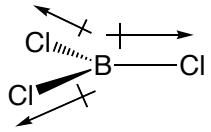
Boron is sp^2-hybridized
Molecule is planar

Question 2. You are an electron, and you have the choice of occupying either an sp, sp^2 or sp^3 orbital. Which do you pick (i.e., which orbital is lowest in energy)? Which orbital is highest in energy? Make sure to justify your answer.

Electrons are lower in energy if they are closer to a positive charge (the nucleus). An s-orbital is closer to the nucleus (has greater orbital penetration) than a p-orbital, which has a node at the nucleus. The sp-orbital is 50% s, so it is lowest in energy. The sp^3-orbital is only 25% s, and highest in energy.

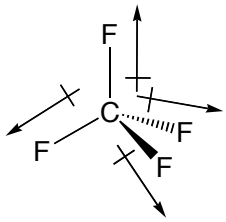
Question 3. Determine which of the following molecules has a molecular dipole. *Hint: the molecular dipole is the sum of all bond dipoles – even if a bond is polar, that does not necessarily mean the molecule is.*

a) BCl_3



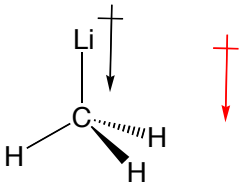
all the dipoles cancel - no molecular dipole

c) CF_4



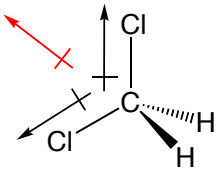
all the dipoles cancel - no molecular dipole

b) CH_3Li



C–H bonds have almost no dipole, so the molecule has a strong dipole in the direction indicated in red.

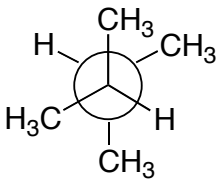
d) CH_2Cl_2

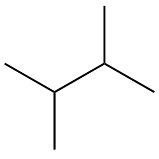


The molecule has a strong dipole in the direction indicated in red.

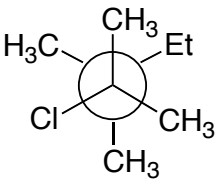
Question 4. Translate the following Newman projections into Lewis structures (line structures are OK).

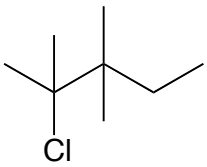
a)



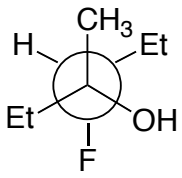


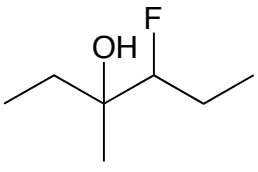
b)





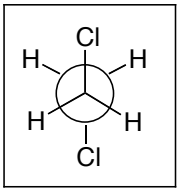
c)



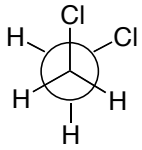


Question 5. Translate the following compounds into staggered Newman projections.

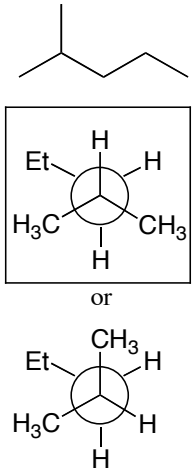
a) 1,2-dichloroethane



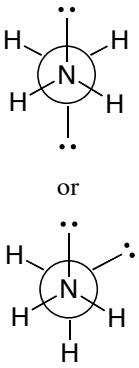
or



b)



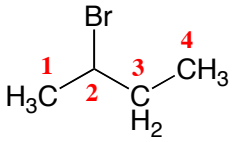
c) H_2NNH_2



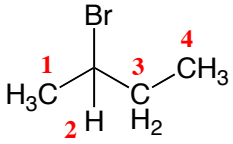
The conforational isomers in boxes for parts a and b above are the lowest energy conformations. Why might this be? (Part c is much more complicated)

Question 6. How many "different" carbons do the following compounds contain? How many "different" hydrogens? *Note: part b is tricky!*

a) 2-bromobutane

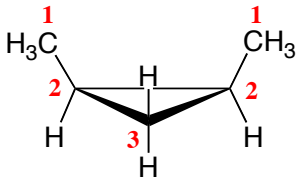


4 different carbons

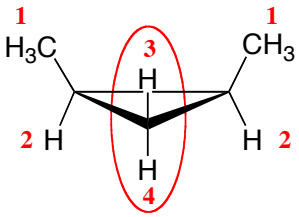


4 different hydrogens as well

b) *cis*-1,2-dimethylcyclopropane



3 different carbons



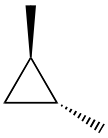
4 different hydrogens

*The circled hydrogens are **not** the in the same environment - even though the connectivity is the same! Hydrogen **3** is on the same side of the ring as the two methyl groups, while hydrogen **4** is on the opposite ring face. These hydrogens are therefore "different" and will be seen as different by methods such as NMR spectroscopy.*

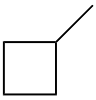
Question 7. Draw structures for all <u>alkanes</u> with the molecular formula C_5H_{10}. Can you name them?

cyclopentane

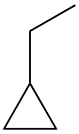
1,1-dimethylcyclopropane



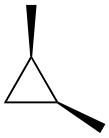
trans-1,2-dimethylcyclopropane



methylcyclobutane



ethylcyclopropane



cis-1,2-dimethylcyclopropane