Additional Problems for Bonding and Molecular Orbital Theory

1. The calculated H-C-H bond angle in methyl radical is 120°, the calculated H-C-F angle in H_2F radical is 115°, and the F-C-F angle in CHF_2 is 112°. Rationalize why the structures become more pyramidal with increasing fluorine substitution.

2. Predict the hybridization state, sp^i, for the carbon hybrid orbitals used for the C-H bonds of CH_3Cl (H-C-H angle of 110.5°) and the C-H bonds of ethylene (H-C-H angle of 117.3°)

3. Draw mixing diagrams using σ(out) orbitals that compare the formation of the C-C σ-bond in ethane, created by the approach of two pyramidal groups, to the formation of the C-F bond in CH_3F. Use the same energy axis for both plots. Highlight the differences, and explain how this diagram would rationalize the reactivity differences in alkanes and alkyl fluorides with nucleophiles.

4. Formaldehyde has a fairly large dipole moment of 2.33 D, but CO has a small dipole moment of 0.11D. Use resonance and electronegativity arguments to explain these results.

5. Sketch the sigma and pi group orbitals for a Fischer carbene, shown below. Use orbital mixing diagrams to show the interaction of the appropriate orbitals on the metal and the carbene.