

Due, March 2, 1999

1. Sketch the π and π^* MO's of ethylene and label them according to symmetry.
2. Sketch the π and π^* orbitals of trans butadiene and label them according to symmetry. (Note that relevant group is in C_{2h} , given below)
3. Consider the CH_3F molecule.
 - a) Now consider a basis set with an atomic s orbital centered on each the three H atoms. Conduct the symmetry adapted MO's comprised of these s basis functions.
 - b) Now consider the $2p_x$, $2p_y$, $2p_z$, and $2s$ orbitals on F. Indicate which of these atomic orbitals mix with the various symmetry-adapted H_{1s} orbitals derived in part a).
4. Consider the $\begin{matrix} F \\ \diagdown \\ C=S \\ \diagup \\ F \end{matrix}$ molecule. Assume that it has C_{2v} symmetry. Determine the number of vibrations of each symmetry type and sketch these (using arrows).

| C_{2h} | E | C_2 | I | σ_h | | |
|----------|---|-------|----|------------|------------|---------------------|
| A_g | 1 | 1 | 1 | 1 | R_z | z^2, y^2, z^2, xy |
| B_g | 1 | -1 | 1 | -1 | R_x, R_y | xz, yz |
| A_u | 1 | 1 | -1 | -1 | z | |
| B_u | 1 | -1 | -1 | 1 | x, y | |