CHEM 352: Homework for chapter 4.

1. Find all the possible symmetry operations for 1,2-propadiene:



2. Derive the C_{2v} multiplication table by applying two successive symmetry operations and identifying the resulting operation. Note that C_{2v} point group is Abelian.

Note that you need to construct a multiplication table not a direct product table.

3. What are the symmetry elements and point groups for the following molecules:



4. What are the irreps for s, p and d atomic orbitals in D_{6h} point group?

5. The following are the normal vibration modes of water molecule:



Apply the C_{2v} symmetry operations for these modes and determine their irreducible representations (consider the directionality of the vectors shown). 6. Consider H₂O molecule residing in yz plane (symmetry C_{2v}). Let H₁ and H₂ denote their 1s orbitals. What are the irreps for the following linear combinations: $S_1 = H_1 + H_2$ and $S_2 = H_1 - H_2$? Which oxygen atom valence orbitals may form molecular otabitals with S_1 and S_2 ?

7. Function f_1 exhibits symmetry corresponding to irrep E_2 and function f_2 irrep A_1 in C_{6v} point group. Show that integral $\int f_1 x f_2 d\tau = 0$ (x represents multiplication by x coordinate).

8. The the ground state electronic wavefunction in H₂O has A_1 symmetry in C_{2v} point group. What the symmetries of the excited states that can absorb liearly polarized light in a) x, b) y and c) z directions?