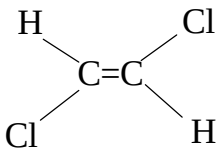
Chemistry 734b

Problem Set 3 Due: Wednesday, February 27, 2008

This problem set is designed to show how to construct character tables. Its not that long.

1.) Consider the molecule *trans*-dichloroethylene:



which has C_{2h} symmetry.

a) **Almost anything can be used to construct matrix representatives!** Use the two Cl atoms as basis set members to derive the four 2x2 matrices for the operations of the C_{2h} point group: {E, C_2, i, σ_h}. Show that the resultant character set does not correspond to an irreducible representation.

b) The character set in part a) can be reduced to two irreducible representations with character sets: {1,1,1,1} and {1,-1,-1,1}. What are the Mulliken symbols of these irreducible representations?

c) Using a unit vector **z** positioned at the origin of the molecule and pointing out of the plane of the paper as a basis vector,construct a 1x1 matrix representation for the operations corresponding to the C_{2h} point group. What is the Mulliken symbol of this irreducible representation?

d) Find the character set of the fourth and last irreducible representation for the C_{2h} point group. Construct the character table for C_{2h}.

2.) Consider a general vector **v**, whose base is at (0,0,0) and whose tip is a (x,y,z) in the point group C_{2h}

a) Derive the set of four 3x3 matrices for the operations: {E, C_2, i, σ_h} that constitute the reducible representation, Γ_m, by which **v** transforms. What is the character set for this representation?

b) Using the character table you derived in question 1 to reduce Γ_m into its component irreducible representations.

c) Show that the four matrices comprising Γ_m obey the same group multiplication table as the operations of C_{2h}.