Symmetry in Chemistry - Assignment 2

Due Date: May 9th, 2021

(For each solution, show your work through a set of important steps)

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1. Identify the point group of the following molecules:

   (a) 1,3-Dichlorobenzene

   (b) 1,3-Dichloroallene

   (c) Cyclo-octasulfur

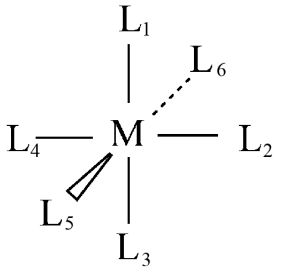
   (d) Ferrocene (staggered)

   (e) Ferrocene (eclipsed)

   For each case, discuss if the molecule has a dipole moment. (5 pts)

2. Derive the group multiplication table for C_{3v} point group.(3 pts)

3. How does the point group of an octahedral complex ML_6 change when:



   (a) the bonds $M - L_5$ and $M - L_6$ are equally stretched out?

   (b) the bond angle L_1ML_2 is reduced to 45°?

   (c) the bond angles L_1ML_2 and L_3ML_4, both are reduced to 45°? (3 pts)

4. Show that in a group $\mathbb{G}$, if g_1 is conjugate with g_2 and g_3, then g_2 and g_3 are conjugate with each other. (You can refer to the textbook by F. A. Cotton Sec. 2.4) (2 pts)

5. $\mathbb{G}$ is a group under a binary operation $*$ and $g_1, g_2, e \in \mathbb{G}$. Prove the following:

   (a) If $g_1 * g_2 = e$, then $g_2 * g_1 = e$. (In general, $\mathbb{G}$ can be non-commutative ,i.e., g_1 and g_2 may not commute. e is the identity element in the group.)

(b) $(g_1 * g_2)^{-1} = g_2^{-1} * g_1^{-1}$ (2 pts)

6. Identify the 2D plane group of graphene and h-BN layers. Also, for each case, identify the lattice points, at least two primitive unit cells, and the point group at the lattice points. (3 pts)

7. Solve Q11.3 from Cotton. In addition, for each pattern, identify the repeating unit, the type of unit cell and the asymmetric unit. (9 pts)

8. The 2D hexagonal lattice has a C_6 axis at each lattice point. Starting with a C_6 axis and translational symmetry operations, derive other unique symmetry axis within the unit cell. (3 pts)
