MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Applications of Group Theory to the Physics of Solids—6.734J & 8.510J

PROBLEM SET # 2

Issued: February 15, 2002 Due: February 22, 2002

1. (a) Explain the symmetry operations pertaining to each class of the point group D_{3h}. You may find the stereograms in Fig. 3.2 useful.

   (b) Prove that the following irreducible representations are orthonormal:
   - E_1 and E_2 in the group D_5 (see Table 3.27).
   - F_{2g} and G_u in the group I_h (see Table 3.39).

   (c) Given the group T (see Table 3.32), verify that the equality

   $$\sum_j \ell_j^2 = h$$

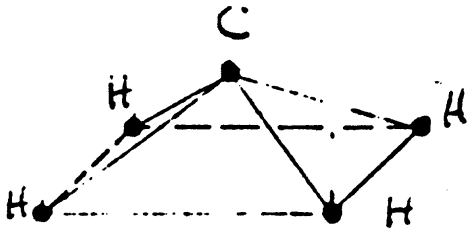
   is satisfied. What is the meaning of the two sets of characters given for the two-dimensional irreducible representation E? Are they orthogonal to each other or are they part of the same irreducible representation?

   (d) Which symmetry operation results from multiplying the operations σ_v and σ_d in group C_{4v}? Can you obtain this information from the character table? If so, how?

2. Make stereographic sketches for groups C_5, C_{5v}, D_{5h}, and D_{5d}, such as are given in Fig. 3.2.

3. (a) What are the symmetry operations of a regular hexagon?
   (b) Find the classes. Why are not all the 2-fold axes in the same class?
   (c) Find the self-conjugate subgroups, if any.
   (d) Identify the appropriate character table.
   (e) For some representative cases (two cases are sufficient), check the validity of the "Wonderful Orthogonality and Second Orthogonality Theorems" on character, using the character table in (d).

4. Consider the hypothetical molecule CH_4 where the four H atoms are at the corners of a square $(\pm a, 0, 0)$ and $(0, \pm a, 0)$ while the C atom is at $(0, 0, z)$, where $z \ll a$. What are the symmetry elements? (See problem #2 in Problem Set #1.)



   (a) Identify the appropriate character table.
   (b) Using the basis functions in the character table, write down a set of (2×2) matrices which provide a representation for the two-dimensional irreducible representation of this group.
   (c) Find the 4 linear combinations of the four H orbitals (assume identical s-functions at each H site) that transform as the irreducible representations of the group. What are their symmetry types?
   (d) What are the basis functions that generate the irreducible representations in (c)?
   (e) Check that xz forms a proper basis function for the two dimensional representation of this point group and find its partner.
   (f) What are the irreducible representations and partners of the following basis functions in the point group (the hydrogens lie in the xy plane): (i) xyz, (ii) x^2y, (iii) x^2z, (iv) $x + iy$?
   (g) What additional symmetry operations result in the limit that all H atoms are coplanar with atom C? What is now the appropriate group and character table? (The stereograms in Table 3.2 of the class notes may be useful.)