MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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

PROBLEM SET # 3

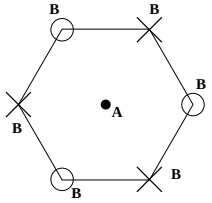
Issued: February 22, 2002 Due: March 1, 2002

1. (a) Find the unitary transformation which transforms the matrices for the Γ_2 irreducible representation of group D_3 corresponding to the basis functions $(xy, x^2 - y^2)$ into the representation corresponding to the basis functions (x, y).

   (b) Using projection operators, check that xy forms a proper basis function of the two-dimensional irreducible representation Γ_2 in point group D_3. Using the matrix representation found in (a) and projection operators, find the partner of xy.

   (c) Using the basis functions in the character table for D_{3h}, write a set of (2×2) matrices for the two 2-dimensional representations E' and E''.

2. Consider a molecule AB_6 where the A atom lies in the central plane and three B atoms indicated by "o" lie in a plane at a distance c above the central plane and the B atoms indicated by "×" lie in a plane below the central plane at a distance $-c$. When projected onto the central plane, all B atoms occupy the corners of a hexagon (see p.61–62 of class notes).



   (a) Find the symmetry elements and identify the appropriate point group.

   (b) How many irreducible representations are there? How many are one-dimensional and how many are of higher dimensionality?

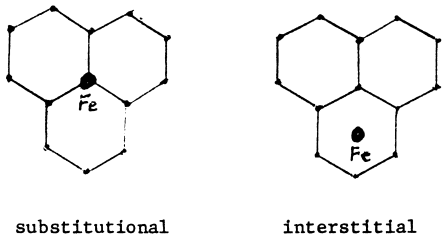
   (c) Find the linear combinations of the six (hydrogenic) 1s-orbitals of the B atoms that transform as the irreducible representations of the group.

   (d) What additional symmetry operations result in the limit that all B atoms are coplanar with A? What is now the appropriate group and character table for this more symmetric molecule?

   (e) Indicate which stereogram in Fig. 3.2 is appropriate for the case where the B atoms are not coplanar with A, and the case where they are coplanar.

3. Suppose that an iron (Fe) impurity is introduced into a two-dimensional honeycomb lattice of an insulating host material. A honeycomb lattice is a hexagonal lattice with atoms at the hexagon corners but not at

the center. Suppose that the Fe impurity is placed first in a substitutional location and second in an interstitial location at the center of the hexagon.



(a) What is the difference in crystal potential (include only nearest neighbors) between the substitutional and interstitial locations?

(b) For the interstitial case, express your result in part (a) in terms of spherical harmonics for the lowest order terms with angular dependencies.

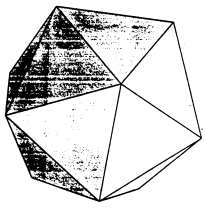
(c) What is the proper point group symmetry and character table in each case?

(d) Give the crystal field splitting of the 5-fold d-levels of the Fe impurity in the crystal fields in part (a).

(e) Identify the basis functions associated with each of the levels in part (d).

(f) Since the bonding orbitals lie lower in energy than the antibonding orbitals, indicate how the ordering of the levels might indicate whether the Fe impurity is located substitutionally or interstitially in the honeycomb lattice.

4. Consider the hypothetical XH_{12} molecule which has I_h icosahedral symmetry, and the X atom is at the center. The lines connecting the X and H atoms are 5-fold axes.



(a) Suppose that we stretch the XH_{12} molecule along one of the 5-fold axes. What are the resulting symmetry elements of the stretched molecule?

(b) What is the appropriate point group?

(c) Consider the G_u and H_g irreducible representations of group I_h as a reducible representation of the lower symmetry group. Find the symmetries of the lower symmetry group that were contained in a 4-fold energy level that transforms as G_u and in a 5-fold level that transforms as H_g in the I_h group. Assuming the basis functions given in the character table for the I_h point group, give the corresponding basis functions for each of the levels in the multiplets for the stretched molecule.

(d) Show (by finding the characters of the rotation group) that the d-level for a transition metal impurity in a metal cluster with I_h point symmetry is not split by the icosahedral crystal field.