

Applications of Group Theory

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Lectures

H33, Mondays, 14:15

H34, Thursdays, 14:15

Exercises

5.0.21, Wednesdays, 13:15

Sheet 6

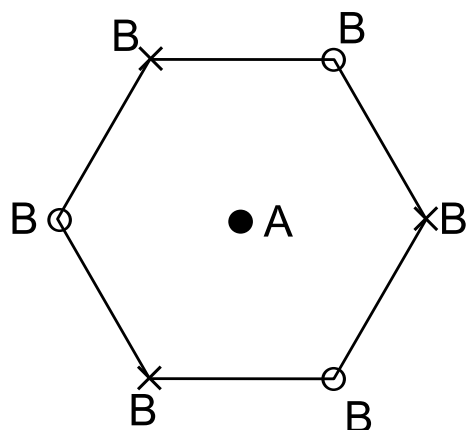
1. Basis functions and representations of D_3 and D_{3h}

Consider the point group D_3 and the basis functions partners to its irreducible representations:

1. What are the matrix representations for the bases $(x^2 - y^2, 2xy)$ and (R_x, R_y) in the point group D_3 ?
2. Using the results in 1), find the unitary transformation which transforms the matrices for the representation corresponding to the basis functions $(x^2 - y^2, 2xy)$ into the representation corresponding to the basis functions (x, y)
3. Using projection operators, check that xy is a proper basis function of the two dimensional irreducible representation E in the point group D_3 . Using the matrix representation found in 1) and the projection operators find the other partner of the representation.
4. Using the basis functions in the character table for D_{3h} , write a set of (2×2) matrices for the two two-dimensional representations E' and E'' .

2. The molecule AB_6

Consider a molecule AB_6 (see Figure) where the atom A lies in the xy plane ($z = 0$), the three B atoms indicated by a circle lie in the plane $z = c > 0$ and the B atoms indicated by a cross lie in the plane $z = c' < 0$. When projected onto the xy plane, all B atoms occupy the corners of a hexagon.



1. Find the symmetry elements and classes.
2. Construct the character table. To which point group does the molecule correspond? How many irreducible representations are there? How many are one-dimensional and how many are of higher dimensionality?
3. Using the basis functions in the character table of this point group, find a set of matrices for each irreducible representation of the group.
4. Find the linear combination of the six s-orbitals of the B atoms that transform as each of the irreducible representations of the group.
5. What additional symmetry operations result in the limit $c = c' \neq 0$? and in the limit $c = c' = 0$? Indicate the associated point groups and draw the corresponding stereograms.

Frohes Schaffen!