

## Applications of Group Theory

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Lectures

Exercises

9.2.01, Mondays, 14:15

H34, Wednesdays, 14:00

## Sheet 6

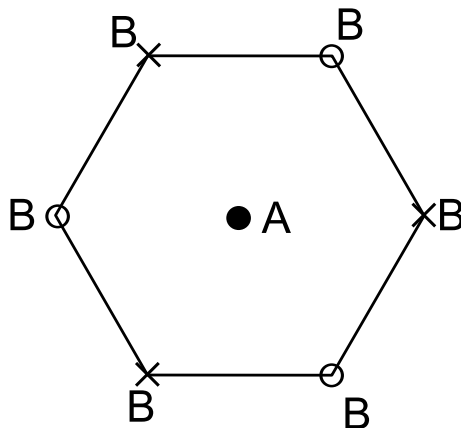
**1. Basis functions and representations of  $D_3$  and  $D_{3h}$** 

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

1. What are the matrix representations for the bases  $(2xy, x^2 - y^2)$  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  $(2xy, x^2 - y^2)$  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  $(2 \times 2)$  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 central plane and three B atoms indicated by a circle lie in a plane at distance  $c$  above the central plane and the B atoms indicated by a cross 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.



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!**