

2H43 THEORETICAL CHEMISTRY

Molecular symmetry and Group Theory

4 Lectures/workshops by Dr S. H. Ashworth.

Material

Groups and their properties: We will see what constitutes a group in the mathematical sense.

Symmetry elements and symmetry operations: We will look at relevant symmetry elements and the difference between symmetry elements and the associated symmetry operations.

Symmetry operations as members of a group: We will see that the symmetry operations for a molecule form a group.

Symmetry point groups: Molecules can be classified using molecular point groups and this process facilitates application of group theory in molecular problems.

Reducible and irreducible representations: There are an infinite number of ways of representing a group. The irreducible representations are, however, special in that all other representations can be expressed in terms of them.

Character tables: Character tables are a compact summary of the irreducible representations of a group and often contain additional information: a valuable labour-saving device.

Direct products: Direct product tables are often published with character tables to save duplication of effort.

Group theory and quantum mechanics: Finally we will apply what has gone before to avoid having to go through lengthy calculations in order to produce an answer of exactly zero.

Objectives

After completing this part of the course you should be able to demonstrate that you can:

- Define a group.
- Identify symmetry elements of an object (*e.g.* a molecule).
- Distinguish between a symmetry element and a symmetry operation.
- Identify the point group of a molecule.
- Use a character table to identify the symmetry species of vibrational modes of a molecule.
- Distinguish between the Raman and IR active vibrational modes of a molecule.
- Use a character table and direct product table to determine allowed and forbidden molecular transitions.