Symmetry in Chemistry

A graduate course of the Chemistry Subject Board

Prerequisite:

Knowledge of:

Linear algebra: vectors and matrices and their properties

Basic quantum chemistry

Mode of evaluation: Weekly home assignments and two closed-book examinations

Course outline: **Approx. duration: 42 hours**

Part I : The Concepts

1. Introduction (3 hours)
   Concept of symmetry. Symmetry elements and symmetry operations. Symmetry in natural world. Symmetry in molecules. Symmetry in mathematical functions. Examples of:
   a. Bilateral symmetry
   b. Rotational symmetry
   c. Inversion symmetry
   d. Rotation-reflection, or improper rotation, symmetry. Why only even order improper rotations are important.
   e. Rotation-inversion symmetry
   f. Translational symmetry
2. Symmetry elements and symmetry operations on physical objects and (4 hours)
   Molecules. Hermann-Mauguin (International) and Schönflies notations of point groups: m, σ; n, C_n; $\bar{1}$, i; $n{:}m$, C_{nv}; n/m, C_{nh}; n, S_{2n}; etc. Higher order, or "special", symmetries: Linear objects, regular polygons, Platonic solids
3. Establishing the point group of an object. (2 hours)
4. Role of symmetry in physical properties of crystals and molecules (3 hours)
   a. Enantiomorphism and chirality. Asymmetry and dissymmetry
   b. Optical properties. Amino acids and proteins
   c. Pyroelectricity and Piezoelectricity
   d. Dipole moment
   e. Infrared and Raman actitivity
   f. Chirality and therapeutic activity: The case of thalidomide
5. Brief introduction to space groups (2 hours)
   a. Translational symmetry
   b. Glide plane
   c. Screw axis
   d. Symmetry notations of crystal lattices
   e. Aperiodic crystals or quasi-crystals

Part II : Mathematical treatment of symmetry groups

6. Groups (4 hours)
   a. Definition
   b. Multiplication tables of group elements
   c. Cyclic group
   d. Commutative group, or additive group

7. Rotations on an equilateral triangle, permutation and symmetric groups (2 hours)
8. Isomorphism and homomorphism
9. Subgroups
10. Cosets and coset decomposition
11. Conjugate elements, Classes (4 hours)
12. Direct product groups
13. Representation of groups (5 hours)
    a. Basis of representation
    b. Matrices as representation of point groups
    c. Reducible and Irreducible representations
    d. Characters of a representation
    e. The "Great Orthogonality Theorem" and its consequences
    f. Constructing a character table
14. Character tables and their properties. Reduction of reducible representations (1 hour)
15. Representations for cyclic groups (1 hour)
16. Direct products: Representations on direct product functions, formation of a character table by direct products (2 hours)

Part III : Applications of symmetry

17. Group Theory and Quantum mechanics: Wavefunctions as bases of irreducible representations. (1 hours)
18. Symmetry Aspects of molecular orbital theory: The Hückel approximation, Symmetry adapted linear combination of atomic orbitals. Notations for electronic states of molecules. Selection rules for electronic and vibronic transitions. (4 hours)
19. Symmetry aspects of molecular vibrations: Normal modes. Symmetry of normal modes, normal mode analysis of H_2O under C_{2v} point group. Selection rules for vibrational and Raman transitions. Polarisation of Raman spectra. (4 hours)

Recommended textbooks:

1. I. Hargittai and M. Hargittai, *Symmetry Through the Eyes of a Chemist*, VCH Publishers, 1987
2. F. A. Cotton, *Chemical Applications of Group Theory*, 2nd edition, Wiley Interscience, 1971
3. L. H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill Book Company, 1969
4. M. Ladd, *Symmetry of Crystals and Molecules*, Oxford University Press, 2014

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Course start date: January 15, 2018
Hours: 11:00 am – 12:30 pm

Days: Monday, Wednesday and Friday
Venue: Lecture Room AG-80