

M.Sc. Semester I - Chemistry

PAPER: CHEM 405: QUANTUM MECHANICS AND GROUP THEORY

[CSIR- UGC - NET - TOPICS: 1(P), 2(P), 5(P)]

Total Credits – 3

Total Hours – 45

Objectives:

- To understand atomic and molecular electronic structure using high-level mathematics as a tool.
- To obtain proficiency in the study of symmetries of physical systems, and the use of groups to classify and quantify natural phenomenon.

Unit-1 Basic principle of quantum mechanics

The Schrödinger Equation, Postulates, Operators, The Particle in a Box, Harmonic Oscillator, Angular Momentum, Hydrogen Atom, Theorems of Quantum Mechanics, Many-Electron Atoms. Atomic structure and spectroscopy: many-electron systems and anti-symmetry principle.

Unit -2 Methods of quantum mechanics

The Variation Method, Perturbation Theory up to second order in energy, Applications.

Unit -3 Symmetry and group theory

Symmetry Elements and Operations, Point Groups; Groups of Low and High Symmetry, Properties and Representations of Groups; Matrices, Representation of Point Groups. Applications of Symmetry; Molecular Orbital Theory in Organic Chemistry, Inorganic and Organometallic Compounds, Ligand Field Theory, Molecular Vibrations, Crystallographic Symmetry.

References:

1. Quantum Chemistry by Ira N. Levine Published by Pearson, seventh Edition 2014.
2. Fundamentals of Quantum Chemistry Molecular Spectroscopy and Modern Electronic Structure Computations by Michael Mueller Published by Kluwer Academic Publishers 2001.
3. Inorganic Chemistry by Gary L. Miessler Donald A. Tarr Third Edition Published by Pearson Education International 2008.
4. Chemical Applications of Group Theory by F. Albert Cotton Third Edition Published by a Wiley- Interscience Publication 1990.
5. Group Theory and Symmetry in Chemistry by L. H. Hall, Published by McGraw-Hill, 1984.
6. Quantum Chemistry by R.K. Prasad Fourth Edition Published by New Age International Publishers, 1985.
7. Introductory to Quantum Chemistry by A. K. Chandra Fourth Edition Published by Tata McGraw-Hill publishing company limited, 1994.