

Course Title: Quantum Chemistry

<u>Semester:</u>	VII
<u>Course Code:</u>	CH-481
<u>Credit Hours:</u>	3-0
<u>Pre-requisite:</u>	Nil

1. Course Objectives Students will acquire knowledge about quantum chemistry including Schrödinger wave equation and its applications to define the behavior and properties of different systems. In addition they will learn about different molecular spectroscopic techniques.

Contents

2. Quantum Chemistry: Operators and their properties. Angular momentum. Central field problem. Approximate methods. Perturbation methods and variation principle. Many electron systems. Treatment of simple harmonic oscillator, diatomic rigid rotor. Valence bond and molecular orbital theories. pi-electron calculations.

3. Molecular Spectroscopy. Interaction of electromagnetic radiation with matter. Symmetry properties of molecules. Microwave and infrared spectroscopy. Rotational, vibrational and rotational-vibrational spectra of diatomic and polyatomic molecules. Electronic spectra of simple molecules. Nuclear magnetic resonance spectroscopy.

Text Book

4. Griffiths, David J., Introduction to Quantum Mechanics 2nd ed., Prentice Hall (2004). Hayward, David O., Quantum Mechanics for Chemists 1st ed., John Wiley (2003). Gray J.D. Molecular Spectroscopy, New York, McGraw-Hill (1988).

5. Recommended Books

- Micheal D.F. Elements of Quantum Mechanics Oxford University Press (2005).
- Whiffen D. H. Spectroscopy Longmans Green and Co.: London, (1966).
- Barrow G. Molecular Spectroscopy McGraw Hill (1962).
- Becker E. D. High Resolution NMR; Theory & Chemical Application, New York, Academic Press (1980).
- House, James E., Fundamentals of Quantum Mechanics 2<sup>nd</sup> ed., Elsevier-Academic Press (2003).

Course Outcomes

6. Upon completion of this course, students will have knowledge about quantum chemistry including Schrödinger wave equation and its applications to define the behavior and properties of different systems. In addition they will have learnt about different molecular spectroscopic techniques.