

Course Title: Molecular Spectroscopy

Course Code: CH-818

Credit Hours: 3-0

Prerequisite: Nil

Course Objectives

The course introduces the three key spectroscopic methods used by chemists and biochemists to analyse the molecular and electronic structure of atoms and molecules. These are UV/Visible, Infra-red (IR) and Rotational spectroscopies. The course teaches application and theory, with descriptions of applied spectroscopic techniques. Alongside the coverage of modern spectroscopy, the course provides an accessible treatment of the science behind vision, flames, solar cells and photochemical smog as well as some aspects of their industrial applications.

Course Outcomes

After having completed the course, the candidates would be able to:

- a. Have knowledge about the fundamental principles of the spectroscopy of molecules.
- b. Give quantitative/qualitative information of molecular structure and description of optical properties of the molecules.
- c. Account for how optical phenomena are correlated/influenced by the physical and electronic properties with respect to their structure.
- d. Account for the physical and/or chemical phenomena behind important techniques for their characterization.
- e. Determines rates of the reactions using some specific optical properties.

Course Contents

Rotational Spectroscopy: Moments of Inertia for differently shaped molecules, Rotational IR, Millimetre Wave and Microwave Spectra, Diatomic & Linear

Polyatomic Molecules, Symmetric Rotors, Stark Effect, Asymmetric Rotors and Spherical Molecules, Structure Determination and Applications of Rotational Spectroscopy. **Vibrational Spectroscopy:** Molecular Vibrations, Diatomic molecules, IR Spectra, Raman Spectra, Anharmonicity Vibration-Rotation, (Rovibrational) Spectroscopy, Polyatomic molecules, Vibrational Selection Rules, Vibration-Rotation (Ro-vibrational) Spectroscopy, Raman Spectra, Anharmonicity, Applications of vibrational spectroscopy. **Electronic Spectroscopy:** Atomic Spectroscopy; Energy Levels in Atoms, Coupling of Angular Momenta, Term Symbols and Selection Rules, Russell-Saunders Coupling, Alkali Metal Atoms, Hydrogen Atom and Others, Magnetic fields: Zeeman effect. **Diatomic Molecules:** Molecular Orbital Theory, Classification of Electronic States, Vibrational Course Structure, Franck-Condon Principle, Transitions, Fluorescence and Phosphorescence, Applications of electronic spectroscopy.

Recommended Books

1. C.N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd Edition, Mc-GRAW Hill, 1983.
2. Ira. N. Levine, Molecular Spectroscopy, [A Wiley-Interscience publication](#), 1975.
3. Rita Kakkar, Atomic and Molecular Spectroscopy, Cambridge University Press, 2015.