MCYE105 Molecular Spectroscopy (3-0-0) (3 credits)

Module I (8 hours)

Basic elements of spectroscopy, Interaction of Radiation with matter, Time dependent perturbation. Einstein coefficients. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legandre polynomials). Spectra of complex atoms. Zeeman and Stark effects.

Module II (8 hours)

Introduction to molecular spectroscopy: Rotational spectroscopy of diatomic molecules. Rigid rotor approximation. Determination of bond lengths and/ or atomic masses from microwave spectral data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules.

Vibrational spectroscopy: Homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands.

Dissociation energies from vibrational spectral data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation.

Module III (8 hours)

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability of molecules. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem.

Module IV (10 hours)

NMR: General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift, Karplus curve, variation of coupling constant with dihedral angle.

Electron Spin Resonance: Electron spin and Magnetic moment , Resonance condition in ESR and significance of 'g' value . ESR spectra of organic free radicals , McConnel relation , applications of ESR.

Principles of Mossbauer spectroscopy: basic principles, achirality of nucleus, Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Text Books (Molecular Spectroscopy)

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, Springer, 4th edn, 2004.
2. J. M. Hollas, Modern Spectroscopy, Wiley, 4th edn, 2003.

Reference Books

1. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Interscience, New York, (1994).
2. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991.
3. Bunker & Jensen, Molecular Symmetry & Spectroscopy, 1998.
4. Bernath, Spectra of Atoms and Molecules, 1995.