

**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 Legendre 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 rotor. 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. An harmonic 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.