## COURSE–4 CHEMICAL SPECTROSCOPY

**Block-1**

Properties of electromagnetic radiation: Wave property-interference, diffraction. Particle property- Photoelectric effect. Regions of the electromagnetic spectrum, energies corresponding to various kinds of radiation. Interaction of electromagnetic radiation with matter (absorption, emission, transmission, reflection, dispersion, polarisation and scattering.). Electron Paramagnetic Resonance (EPR) Spectroscopy: Basic principles, Selection rules, intensity, width, position of spectral line, multiplet structure of EPR spectra, hyperfine interaction, spin-orbit coupling. Affecting the magnitude of values. Instrumentation. Applications to the study of free radicals, Coordination compounds, biological studies, rate of electron exchange reactions

**Block-2**

Introduction – Interaction of radiation with matter, transition moment integral, selection rules. Classification of polyatomic molecules. Rotation spectra of diatomic molecules –rigid and non rigid rotators. Rotational quantum number and selection rules. Effect of isotopic substitution on rotation spectra. Relative intensities of spectral lines. Applications to determination of bond length and moment of inertia of diatomic molecule. Electronic spectroscopy- Absorption – Beer's law. Theory of molecular absorption. Frank-Condon principle. Vibration-rotation, fine structure of absorption bands: $\sigma \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$, $n \rightarrow \sigma^*$, $n \rightarrow \pi^*$. Solvent effect on the spectral lines. Empirical rules for predicting the wave length of maximum, - olefins, conjugated dienes, ketones and substituted benzene.

**Block-3**

Vibration of diatomic molecules, vibrational energy curves of simple harmonic oscillator. Effect of anharmonic oscillator. Vibration-rotation spectra of carbon monoxide. Fundamental and overtone frequencies. Vibration of polyatomic molecules- degree of freedom of vibrations. Parallel and perpendicular vibrations ($CO_2$ and $H_2O$). Intensity of absorption band and types of absorptions. Important spectral regions – hydrogen stretching region, double and triple bands region, fingerprint region. Applications for $XY_2$ - linear, $XY_3$ – planar. Factors affecting the group frequency – electrical effect, hydrogen bonding, sterric and ring strain. Raman spectroscopy – Introduction, Raman and Rayleigh scattering, Stokes and antistokes lines, polarization of Raman lines, depolarization factor, polarizability ellipsoid.

Theories of Raman spectra – classical and quantum theory. Rotation-Raman and vib-Raman spectra. Comparison of Raman and IR spectra, rule of mutual exclusion princilple. Advantages of Raman spectra.

**Block-4**

Introduction, nuclear spin, energy absorption & relaxation. Basic ideas about instrument, chemical shift & factors affecting it, magnetic anisotropy, spin-spin coupling, coupling constant. First order & non first order splitting for two, three & four interacting nuclei. Mass Spectrometry: Principle & theory, Instrumentation, different ionization techniques, (EI, CI, FAB, FD) General modes of fragmentation. Nuclear Quadra pole Resonance (NQR) Spectroscopy-Quadrupole nuclei, Quadrapole movement, electric field gradient, The NQR experiment, structural information from NQR spectra.

**Reference books**


1. Banwell, C. N. Fundamentals of molecular Spectroscopy, 4th Ed. *Tata Mc Graw hill* **1994**.
2. Raymand Chang, Basic principles of Spectroscopy, *Mc Graw Hill*, **1970**.
3. J. M. Holla. Modern spectroscopy, 4th Ed., *John Wiley*, **2004**.
4. Drago, R .S. Physical Methods in Chemistry- Thomson Learning, **1977**.
5. Nakamoto, K. Infrared Spectra of Inorganic and Coordination Compounds, 6th Ed, *Wiley-Blackwell*, **2009**.
6. Rao, C.N.R. Infrared Spectroscopy-*Academic Press Inc*, **1963**.