## CA S 416: MOLECULAR SPECTROSCOPY AND DIFFRACTION TECHNIQUES

### Course Outcomes

- Deals with the understanding of the spectroscopic techniques which are based on the interaction of the electromagnetic radiation in the microwave, infrared and X-ray region with the molecules.
- The techniques introduced here are major characterization techniques employed tounderstand the chemical composition of compounds and the physical characteristics.
- The paper has multidisciplinary relevance as these techniques are used in various fields namely, chemistry, physics biology and materials science.

**Unit-I** **[12 Hours]**

Introduction to spectroscopy, intensity of spectral lines, natural line width and broadening, rotational, vibrational and electronic energy levels, selection rules.

**Microwave Spectroscopy:** The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond length, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave spectrometer.

**Vibration Spectroscopy:** Vibration spectra of diatomic molecules-Linear harmonic oscillator, vibrational energies, zero point energy, force constants and bond strengths; anharmonicity of molecular vibrations-Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules-Normal modes of vibrations and nature of molecular vibrations (Ex. $CO_2$ and $H_2O$ molecules).

**UNIT-II** **[12 Hours]**

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation.

**Raman Spectroscopy**: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman spectrometer–Instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - $H_2O$, $N_2O$ & $CO_2$ molecules).

**Unit-III** **[12 Hours]**

**Diffraction Techniques**: Introduction, production of X-ray, Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments–Diffraction of X-rays by a crystalline powder (Debye-Scherrer method), powder diffractometer. Single crystal technique: Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences.

Crystalline X-ray diffractometer (4 angle), X-ray scattering by atoms and molecules, Factors affecting X-ray intensities, introduction to Crystal structure analysis.

**Electron Diffraction:** Introduction, theory of electron diffraction, Wierl equation and its significance (qualitatively). Structure of surfaces-Low and high energy electron diffraction.

**Electron microscopy (TEM & SEM):** Principle and applications.

Theory and applications of neutron diffraction. Comparison between X-ray, electron and neutron diffractions.

## References


1. Fundamentals of Molecular Spectroscopy, 4th edn., C. N. Banwell and E. M. McCash, Tata McGraw Hill (2017).
2. Spectroscopy, H. Kaur, Pragathi Prakashana (2017).
3. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampmam, G. S. Kriz and J. A. Vyvyan, Cengage Learning (2014).
4. Spectroscopy, B.K. Sharma, Goel Publishing House (2015).
5. A Basic Course in Crystallography, J. A. K. Tareen and T. R. N. Kutty, University Press (2001).
6. Essentials of Crystallography, M. A. Waheb, Narosa Publishing House (2009).
7. X-ray methods, Clive Whiston, John Wiley & Sons (1987).