OC S 415: MOLECULAR SPECTROSCOPY AND DIFFRACTION TECHNIQUES

Course Outcome

- 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 to understand 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 & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO_2 and H_2O).

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 **[12Hours]**

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 & 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 & J. A. Vyvyan, Cengage learning (2014).
4. Spectroscopy, B.K. Sharma, Goel Prakashan (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).