OC S 406-Molecular Spectroscopy & 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.
- Student will be able to learn instrument like x-ray, TEM, SEM and their applications

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& 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 and flat plate camera), powder diffractometer. Interpretation of power patterns (analytical technique). Single crystal technique - :Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences. Crystalline X-ray diffractometer (4 angle), Intensities of diffracted X-rays and structural analysis, X-ray scattering atoms and molecules, Factors affecting X-ray intensities, introduction to Crystal structure analysis. 9hrs.

Electron Diffraction: Introduction, Theory of electron diffraction, Wierl equation and its significance (qualitatively), Elucidation of structure of simple gas molecules. Structure of surfaces - (Low and high Energy Electron Diffraction, Transmission electron microscopy (TEM), SEM. Theory and applications of Neutron diffraction. Comparison between X-ray, electron and Neutron diffractions. 3hrs .

REFERENCES:

1.Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill, New Delhi) 2007.
2. Spectroscopy, H. Kaur (Pragathi Prakashana,Meerut), 2012.
3.Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.
4.Spectroscopy, B.K.Sharma (Goel prakashan, Meerut), 2013.
5. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).
6. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),
7. X-ray methods, Clive Whiston, (John Wiley & Sons, New York) 1987.

OC P 407: INORGANIC CHEMISTRY PRACTICALS – I

COURSE OUTCOME:

- Students will have hands on experience on the analysis of Hematite Dolomite, Pyrolusite, Solder,
- Analysis of Halide Mixture, Colorimetric Determination, Gravimetric determinations and Statistical Analysis of Data.
- To understand Complexometric determination and hardness of water
- It enables the students to learn Statistical Analysis of Data.

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using $Ce^{4+.}$
2. Analysis of Dolomite - insoluble residue by gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Statistical Analysis of Data.

Reference :

1. Vogel's Text Book of Quantitative Chemical Analysis (5^{th} Ed), G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.