

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-CO₂& H₂O).

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 - H₂O, N₂O & CO₂ 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 (5th Ed), G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.