

Course Code	Course Name	Credits
26PH508	MOLECULAR SPECTROSCOPY	04

Course Objectives

- To understand the fundamental principles of molecular spectroscopy and the interaction of electromagnetic radiation with matter.
- To study rotational and vibrational spectra of molecules using microwave and infrared spectroscopy.
- To analyze Raman spectra and understand the quantum and classical theories underlying the Raman effect.
- To explore electronic spectroscopy of molecules including vibrational structure and photoelectron spectroscopy.
- To understand spin resonance techniques such as NMR, ESR, and Mössbauer spectroscopy and their applications.

Learning Outcomes

After completion of the course, students will be able to:

- Recognize spectroscopy in microwave, Rotational spectra of rigid diatomic molecules, selection rules, interaction of spectral lines
- Study of Vibrating diatomic molecule, energy levels of a diatomic molecule, simple harmonic oscillator, Scattering of light, Raman Spectrum. rotational & vibrational Raman Spectra
- Learn Electronic spectra of diatomic molecules.
- Make Students aware of the fine structure of ESR absorption, Hyperfine structure, Double resonance in ESR, Techniques of ESR spectroscopy.

Unit 1 - Microwave Spectroscopy (12 Hrs.)

Characterization of Electromagnetic Radiation - Quantization of energy - Regions of the Electromagnetic spectrum, width and Intensity of spectral lines - Rotation of Molecules, Rotational Spectra - A Diatomic Rigid Rotator - Non rigid rotator- Intensity of Spectral lines- Effect of isotopic substitution.

Unit 2 – Infra-Red Spectroscopy (12 Hrs.)

Vibrating diatomic molecule - Simple Harmonic Oscillator - anharmonic oscillator, diatomic vibrating rotator, vibrations of polyatomic molecules - fundamental vibrations and their symmetry - overtones and combination frequencies.

Unit 3 - Raman Spectroscopy (12 Hrs.)

Introduction - Quantum theory of Raman effect - Classical theory of Raman effect - Pure rotational Raman spectra- Linear molecules, symmetry top molecules, asymmetric top molecules- vibrational Raman spectra – Raman activity of vibrations - rule of Mutual Exclusion – rotational fine structure.

Unit 4 – Electronic Spectroscopy of Molecules (12 Hrs.)

Born Oppenheimer approximation - vibrational coarse structure, Frank-Condon Principle - Intensity of vibrational - electronic spectra - dissociation energy and dissociation products - Molecular photo-electron spectroscopy - X-ray photoelectron spectroscopy.

Unit 5 - Spin Resonance Spectroscopy (12 Hrs.)

Spin and an applied field - nature of spinning particles - interaction between spin and a magnetic field - population of energy levels - the Larmor Precession - Fourier Transform Nuclear Magnetic Resonance spectroscopy - Electron-spin Resonance Spectroscopy - g factor - hyperfine structure due to electron – nucleus coupling - double resonance - techniques in ESR spectroscopy- Introduction to Mossbauer spectroscopy.

Reference Books:

1. Aruldas, G. (2014). Molecular Structure and Spectroscopy, (2nd Ed.). PHI Learning Private Ltd.
2. Svanberg, S. (2004). Atomic and Molecular Spectroscopy, (4th Ed.). Springer.
3. McHale, J. L. (2017). Molecular Spectroscopy, (2nd Ed.). CRC Press.
4. Straughan, B. P., & Walker, S. (1976). Spectroscopy Volume 1-3, Chapman & Hall Publishers.
5. Chatwal, G. R., & Anand, S. K. (2009). Spectroscopy. Himalaya Publishing House.

Websites and eLearning Sources:

1. <https://nptel.ac.in/courses/104101099>
2. <https://youtu.be/eU6VqGIc-2Q?si=iRtfTDN8Zb8jqNxx>
3. <https://youtu.be/Xau9cP699yE?si=5kgKSM9MPUUIcIds>

COs and Bloom's Taxonomy Mapping – 26PH508

Course Outcomes	On successful completion of this course, students will be able to	BTL
CO1	Recall fundamental principles of molecular spectroscopy and energy transitions.	K1, K2
CO2	Apply spectroscopic techniques to analyze molecular structure and spectra.	K3
CO3	Analyze rotational, vibrational, Raman, and electronic spectra.	K4
CO4	Evaluate spectroscopic methods for identifying molecular properties.	K5
CO5	Develop interpretations and applications of spectroscopy in research.	K6

BTL (Bloom's Taxonomy Level) - K1 – Remembering, K2 – Understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6 - Create

Relationship Matrix – 26PH508

Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)						Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	3	2	1	1	1	1	3	2	1	1	1	1	1.58
CO2	3	3	2	1	1	1	2	3	2	2	2	1	1.92
CO3	3	3	3	2	1	1	2	3	3	2	2	2	2.25
CO4	3	3	3	2	2	1	2	3	3	3	2	2	2.42
CO5	3	3	3	3	2	2	3	3	3	3	3	2	2.75
Total												2.18	

Mean Score: 3- High, 2- Medium/Moderate, 1-Low

