

Semester	JAN 2022
Open to semester	4
Course code	CH2233
Course title	Fundamentals of Molecular Spectroscopy
Credits	3 /
Course Coordinator & participating faculty (if any)	Pankaj Mandal
Nature of Course	Lectures and Tutorials
Pre-requisites	Chemical Principle. This course is a pre-requisite for “Advanced Molecular Spectroscopy” and “Photochemistry and photophysics” courses.
Objectives (goals, type of students for whom useful, outcome etc)	The objective of this course is to teach the fundamentals of major branches of Spectroscopy and its applications. Spectroscopy is an important research tool in all areas of science (Chemistry, Physics and Biology). The interaction of light with matter provides a great deal of molecular-level information about a system of interest. In this course, this radiation-matter interaction and the quantitative information it can provide about molecular systems will be examined. The students will be exposed to UV/Vis, IR, Raman, and NMR spectrophotometers and able to build the basic foundation in spectroscopy which will be an asset throughout their scientific career.
Course contents (details of topics /sections with no. of lectures for each)	<p>Section 1 (2 L) Introduction to radiation-matter interaction Topics: Electromagnetic spectrum, Electromagnetic radiation, Basic elements of spectroscopy, selection rules, intensity of spectral lines.</p> <p>Section 2 (6 L) Rotational spectroscopy Topics: Rotation of molecules; Moments of inertia, Rotational spectra: Diatomic molecules; Rigid rotor approximation, Intensities of rotational spectral lines, Techniques and instrumentation.</p> <p>Section 3 (6L) Vibrational spectroscopy Topics: Vibration of diatomic molecules. Harmonic and anharmonic oscillators, Vibrational-rotational couplings,</p>

	<p>Vibration of polyatomic molecules, Techniques and instrumentation, Analysis of molecules by Infrared spectroscopy. Introduction, Quantum and classical theories of Raman effect, Pure rotational Raman spectra, Vibrational Raman spectra, techniques and instrumentation.</p> <p>Applications of vibrational spectroscopy.</p> <p>Section 4 (2L)</p> <p>Electronic spectroscopy of Atoms</p> <p>Topics: Energy levels in atoms, Coupling of angular momenta, Term symbol and selection rules, Spectra of hydrogen atom and others.</p> <p>Section 5 (5 L)</p> <p>Electronic spectroscopy of molecules</p> <p>Topics: Electronic energy levels and selection rules, Term symbols, electronic spectra of diatomic molecules, Franck-Condon principle, Electronic spectra of polyatomic molecules, Fluorescence and Phosphorescence, Spectrophotometer and the Beer-Lambert law.</p> <p>Section 6 (7 L)</p> <p>Magnetic resonance spectroscopy</p> <p>Topics: Nuclear magnetic resonance (NMR): The magnetic field; The energies of nucleus in a magnetic field; Nuclear spins and magnetic moments; The origin of Nuclear magnetic Resonance Spectra; The NMR spectrometer; The chemical shift; Spin-spin coupling and the fine structure in NMR; Fourier Transform NMR spectroscopy; Examples of NMR spectra.</p> <p>Determination of structure of unknown compounds using NMR spectroscopy</p>
Evaluation /assessment	<p>End-Sem Examination-50%</p> <p>Mid-Sem Examination-50%</p> <p>Others-%</p>
Suggested readings (with full list of authors, publisher, year, edn etc.)	<ol style="list-style-type: none"> 1) Fundamentals of molecular spectroscopy: C. N. Banwell and E. M. McCash, 4th edition, Tata McGraw Hill. 2) Modern Spectroscopy, J. Michael Hollas, 4th Edition, Wiley. 3) Physical Chemistry, P. W. Atkins, Oxford University Press. 4) Introduction to spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, India Edition, Brooks/Cole Cengage Learning.