

Course Handout

Date: 02.08.2010

Course No. : CHM201
Course Title : Spectroscopic and other physical methods
Instructor : Angshuman Roy Choudhury

1. **Course Description:** The course will cover basic principles of different spectroscopic methods, which would include physical concepts of microwave spectroscopy, IR and UV-VIS spectroscopy, Raman spectroscopy, NMR, EPR and basic techniques involving X-ray diffraction.

2. **Scope & Objective of the Course:** The course would build up through introduction to various terms, techniques and concepts in spectroscopy in general. Detail understanding of rotational (microwave) spectroscopy, vibrational (IR) spectroscopy, electronic (UV-VIS) spectroscopy, Raman scattering and rotational Raman spectroscopy, photoelectron and Auger spectroscopy, magnetic resonance (NMR and EPR)

3. **Text Book(T):** (1) Colin N. Banwell and Elaine M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed, Tata McGraw-Hill Publishing Company, New Delhi, (2) F. A. Cotton, Chemical Applications of Group Theory, Indian Edition, 3rd Ed, Wiley-India, Noida, 2003

4. **Reference Book(R):** (1) W. Kemp, Organic Spectroscopy, 3rd Ed, Palgrave, New York, 1991; (2) Ira N. Levine, Physical Chemistry, 5th Ed, Tata McGraw-Hill Publishing Company, New Delhi, 2007.

3. **Course Plan:**

Lec. Nos.	Learning Objectives	Topics to be Covered	Book/Chapter Number
1-2	Introduction to the course and spectroscopic terms and techniques	Electromagnetic radiation, quantization of energy, spectral regions, representation of a spectra, practical spectroscopy, instruments, signal-to-noise ratio, resolution, Fourier transformation, sources for different spectral regions, Lasers and synchrotron, X-ray	T1, 1.1-2.10
3-7	Microwave spectroscopy	Rotation of simple molecules, diatomic and polyatomic molecules, linear and non-linear molecules, isotopic substitution, techniques and instrumentation.	T1, 2.1-2.7
8-11	Infra-red spectroscopy	Vibration of diatomic molecule, vibrating rotor, rotation-vibration spectra of CO ₂ , vibration of polyatomic molecules, instrumentation and physical applications	T1/3.1-3.3, 3.5-3.8
12-15	Raman Spectroscopy	Pure rotational Raman spectroscopy, vibrational Raman spectra, polarization of light and the Raman effect, structure determination from Raman and IR spectroscopy, techniques and instrumentation.	T1/4.1-4.6
16-19	Electronic spectroscopy	Structure of atoms, electronic angular momentum, many electron atoms, angular momentum of many electron atoms, spectroscopic term symbols, photoelectron spectroscopy, Auger spectroscopy, the Zeeman effect, influence of nuclear spin.	T1/5.1-5.8
20-24	Nuclear magnetic resonance spectroscopy	Concept of nuclear spin, interaction between nuclear spin and magnetic field, population of energy levels, Larmor precession, relaxation, theory of NMR, chemical shift, coupling constant, multiplicity, practical examples, instrumentation and technique.	T1/7.1.1-7.1.5, 7.2.1-7.2.5, 7.4.

25-26	Electron spin resonance spectroscopy	Introduction, ESR absorption and g factor, hyperfine structure in ESR, e-n and e-e coupling, technique	T1/7.5
27-31	X-ray diffraction	Introduction, concept of lattice and symmetry in 2D and 3D, crystal symmetry and crystallographic point groups, point group representations, inter-relation between lattice symmetry, crystal symmetry and diffraction symmetry, additional symmetry elements-screw axis, glide plane, standard symbols for symmetry elements, 230 space groups and their representation in 2D, Miller indices, hexagonal systems & Miller-Bravies indices, Bragg's law, concept of reciprocal lattice, powder X-ray diffraction and its application, single crystal X-ray diffraction and its application.	T2/11.1-11.8, class note

4. Evaluation Scheme:

EC NO.	Evaluation Component	Duration	Marks	Date Time Venue	Nature of Component
1.	Mid-sem I	1 hr.	40		Closed Book
2.	Mid-sem II	1 hr.	40		Closed Book
3.	Surprise tests (4) in tutorials	-	10 x 4		Closed Book
4	Surprise quiz (4) in regular class	-	5 x 4		Closed Book
4.	Final Exam.	3 hrs	100		Closed Book

5. **Chamber Consultation hours:** To be announced in the class.

6. **Make-up Policy:** Make-up will be granted following institute rules.

7. **Notices:** Relevant notices regarding the course will be displayed on Notice Board.

Instructor
CHM201