BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI – Hyderabad Campus
AUGSD
First Semester 2021-2022
Course Handout

Date: 18.08.2021

In addition to part I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No.	CHEM G554
Course Title	Physical Methods in Chemistry
Instructor-in-charge	Nilanjan Dey
Team of Instructors	Anupam Bhattacharya, Arijit Mukherjee

Course Description:
This course describes the principles and practice of modern instrumental methods of chemical analysis. Emphasis will be given on spectroscopic techniques such as UV-Visible, Infrared, XPS, XRF, NMR (^{1}H, ^{13}C and other elements, NOE, correlation spectroscopies), ESR, Mass spectroscopy, atomic absorption and emission spectroscopies, fluorescence spectroscopy and microscopy and chromatographic techniques such as GC/HPLC. Other topics will include electroanalytical methods, thermal analysis and diffraction methods like XRD.

Scope and Objective of the Course:
Chemists extensively use modern sophisticated electronic and optical instruments in various areas such as chemical analysis, structure elucidation, identification of reaction pathways, reaction rates etc. This course aims to introduce the basic theory and experimental details of such instrumentations. Some of the popular absorption spectroscopic techniques such as UV-Visible, IR, NMR, etc. will be discussed in detail; other techniques such as XPS, XRD, mass spectrometry, thermal analysis, chromatographic techniques – GC, HPLC, etc. will also be covered.

Text Books:
T1. Kemp W, "Organic Spectroscopy", 3rd ed., Palgrave, New York (1991).
T2. Lampman G.M., Pavia D.L., Kriz G.S., and Vyvyan J.R., "Spectroscopy", 4th Edition, Cengage Learning (2010).
T3. W. Massa, Crystal Structure Determination], 2nd English Edition, Springer-Verlag Berlin Heidelberg (2004)

Reference Books:
R1. Silverstein R. M., and Webster F. X., "Spectrometric Identification of Organic Compounds",6th Edition, John Wiley & Sons, New York (1998).

R2. Willard H. H., Merritt L. L., Dean J. A., and Settle F. A. Jr., "Instrumental Methods of Analysis", 7th Edition. Wadsworth, New York (1989).
R3. Kalsi P. S., "Spectroscopy of Organic Compounds", 6th Edition, New Age International Publishers, New Delhi (2005).

Course Plan :

A. Lecture Sessions :

Lec. No.	Topics to be covered	Learning Objectives	Learning outcomes	Reference: Chap./Sec. #(Book)
1	Energy and Electromagnetic spectrum	Regions of Electromagnetic Spectrum; units.	1) Explain the interaction between light and matter 2) Contrast various regions of the electromagnetic spectrum Estimate the energy of transition and relate to the units	Ch.1 (T2)
2	Ultraviolet (UV) and visible spectroscopy: Light Absorption, theory, instrumentation	Chromophore concept; electronic energy levels.	1)Relate the basic principle of UV-Vis spectroscopy and explain relevant terms 2) Outline the working principle, analyzing the spectra and extend the construction of device	4.1-4.3 (T2)
3-4	UV-Visible: Solvents, applications	Solvent effects; Absorption wavelength calculations based on empirical rules	1)Recall the basic concepts of electronic transitions and organize the study of solvent effect on UV-Spectra 2)Calculate the wavelength of absorption in conjuagted systems using Woodward rule	4.4-4.10 (T2)
5	Circular Dichroism Spectroscopy	Principle of Circular Dichroism, details and applications	1) Principle and basics of CD and ORD spectrosocpy 2) Analyzing an CD spectrum, information about the chirality 3) Application of CD spectroscopy in biomolecular analysis (DNA and protein)	Lecture Notes
6-7	Fluorescence and phosphorescence	Principles of fluorescence and phosphorescence and applications	1) Define fluorescence and phosphorescence 2) Elaborate Jablonskii diagram 3) Interpret fluorescence property of the molecules 4) Decide quenching phenomenon 5) Fluorescence lifetime and its applications 6) Fluorescence microscopy	4S.2 (T1) & 16.15 (T2)
8	Infrared spectroscopy: Molecular vibrations; related factors	IR absorption due to molecular vibrations; influence of factors such as hydrogen bonding.	1) Understanding the basis of IR spectroscopy and how Hooke's law is used in IR spectroscopy. 2) Identify bonds which are IR active. 3) Relate IR absorption to factors such as hydrogen bonding, dipole moment, hybridization etc.	2.1-2.3 (T2)
9	Infrared spectroscopy: Instrumentation, Applications	IR instrumentation details; FT-IR; sample preparations recording details	1) What are the key components/parts in an IR spectrometer? 2) What is FT-IR? 3) How to do sample recording? Solid/Liquid/Gas Basis of using a particular compound for sample preparation.	2.4-2.7 (T1) & 2.1-2.9 (R1)

10-11	Infrared spectroscopy: Correlation charts; Supplementary materials	Obtaining structural information from IR spectrum; Reflectance mode IR spectra	1) Analysis of an IR spectrum, to obtain information about presence of functional groups and also examine the possibility of getting some structural insights. 4) IR in the reflectance mode; key aspects.	2.8-2S.3 (T1) & 2.10-2.21 (R1)
12-13	Raman Spectroscopy	Principles of Raman spectroscopy and applications	1) Understanding the basics of Raman spectroscopy 2) Key differences with IR 3) Analysis of an Raman spectrum, to obtain information about the functional groups and structural insights.	Lecture Notes
14-15	Atomic absorption, emission spectroscopy	Specific atomic energy levels for different elements; instrumentation; quantitative estimations; interferences etc.	1)Will be able to interpret atomic absorption spectra 2) Explain the basic principles of AAS. 3)Can Illustrate the working principle and outline of AAS 4) Recall Maxwell's distribution law 5) Discuss the above similarities with Flame emission spectrophotometry	Ch 17 (T2)
16-17	Thermo analytical methods	Differential Thermal Analysis; Thermo Gravimetric Analysis; Differential Scanning Calorimetry etc.	1)Define and demonstrate the thermoanalytical methods: DTA, TGA and DSC 2)Conclude the changes in the sample, exothermic or endothermic can be detected relative to the inert reference 3) Develop knowledge pertaining to the appropriate use of the instrument for thermal analysis.	Ch. 20 (R3)
18-19	Characterization of materials by XPS and XRF	Basic theory and applications in characterizing various materials	Understanding the basis X-ray based absorption and emission techniques	Lecture notes
20-24	Characterization of materials by XRD	Basic theory of XRD and its application in characterizing different inorganic material	1. Define lattice, crystal systems 2. Explain the mechanism of X-ray Generation 3. Explain diffraction with Laue and Bragg equations 4. Define Ewald Construction to depict reciprocal space 5. Define and use of symmetry elements 6. Analysis of powder diffractograms in a qualitative manner	Lecture notes
25-26	Chromatographic Techniques: GC, HPLC, Electrophoresis	Theories of separation techniques; stationary and mobile phases etc.	1)Infer the theoretical aspects of techniques used for separation 2) Make use of mobile and stationary phases and estimate certain physical parameters dealing with the above-mentioned techniques	Ch. 19 20.1, 21.1(T2)
27-28	Nuclear Magnetic Resonance (NMR) spectroscopy Proton NMR Theory, chemical shift, related factors	Understanding Magnetic Resonance phenomena and the concept of chemical shift	1) Identifying magnetically active nuclei. 2) Understanding the importance of nuclear spin. Basis of NMR spectroscopy. Showing the importance of the chemical shift.	3.1-3.4 (T1)

29-31	NMR- Correlation Data, Solvents, Integrals, spin-spin coupling, related factors	Extracting chemical shift related structural information from simple NMR spectrum; spin-spin coupling and its effect on the spectrum	1) Solving the structure of a molecule by using NMR data. 2) Type of solvents to be used in NMR. 3) What is spin-spin coupling and its role?	3.5-3.9 (T1)
32-33	NMR- Non first order spectra, simplification of spectra, tables, ^{13}C NMR applications	What is meant by non-first order NMR spectrum; different methods of extracting information from such spectra; ^{13}C NMR how to interpret.	1) Meaning of non-first order spectra and extracting structural information from such spectra. 2) What is ^{13}C NMR and how to interpret ^{13}C NMR spectrum?	3.10-3.16 (T1)
34-35	NMR-double irradiation, multi pulses, NMR for other isotopes ^{19}F, ^{31}P, ^{15}N, ^{17}O etc.	Understanding a few of the advanced methods in NMR; Interpreting NMR spectra of nuclei other than ^{1}H and ^{13}C	1) What are the various advanced methods in NMR and how to obtain molecular structure-related information from them? 2) How to interpret the NMR data for other magnetically active nuclei like ^{19}F, ^{31}P, ^{15}N, ^{17}O etc.?	3S.1-3S.6 (T1)
36-37	Mass spectrometry: Basics, Instrumentation, Isotopic abundance, and Molecular ion.	Principles of mass spectrometry; the effect of isotopic abundance in the mass spectrum	1) The basic principle of mass spectroscopy. 1) Understanding the effect of isotopic abundance in the mass spectrum.	5.1-5.4 (T1) & 8.3-8.5 (R1)
38-39	Mass spectrometry: Metastable ions, fragmentation processes	Understanding the molecular fragmentations at the time of ionization and during flight; stabilities of fragments.	1) Understanding the molecular fragmentations and stabilities of the fragments generated at the time of ionization and during flight. 2) How to interpret mass spectrum?	5.5-5.6 (T1)

Evaluation Scheme: Total 200 marks

Components	Duration	Weightage	Date & Time	Remarks
Mid-Sem	---	26 %	---	Open Book
Seminar	---	39 %	Continuous	Open Book
Comprehensive Examination**	---	35 %	---	Open Book

* There will be 3 seminars, each carrying 13 % weightage

** The mid-semester and comprehensive examination will have objective and descriptive portions.

Makeup Policy: See Part I for details. However, it may be noted that it is difficult to arrange to make up of practical sessions.

Notices: All the notices pertaining to this course will be displayed on the **CMS**.

Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester, and no type of academic dishonesty is acceptable.

Course Policies:

Absences: Students are responsible for all materials presented in the course as well as for acquiring missed information.

Nilanjan Dey
Instructor-in-charge

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