KU6SECCHE102: SPECTROSCOPIC TECHNIQUES IN CHEMISTRY

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
VI	SEC	100	**KU6SECCHE102**	3	60

Learning Approach (Hours/ Week)			Marks Distribution			Duration of ESE (Hours)
Lecture	Practical/ Internship	Tutorial	CE	ESE	Total	
2	2	NIL	25	50	75	1.5

Course Description: Advanced course in spectroscopic techniques for various analysis
Course Prerequisite: Preliminary understanding on basic spectroscopy is preferred.

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	Understand theory and instrumentation of UV-Vis and fluorescence spectroscopy. Also, get hands-on experience on these instruments.	E
2	Get insight into the theory and instrumentation of IR spectroscopy. Also get experience in IR spectrum analysis.	E
3	Get insight into the theory and instrumentation of NMR spectroscopy. Also get experience in NMR spectrum analysis.	E
4	To understand the scientific application of mass spectroscopy in structural analysis	E
5	Understand the scientific importance of various photoelectron spectroscopy	An

Remember (R), Understand (U), Apply (A), Analyse (An), Evaluate (E), Create (C)

Mapping of Course Outcomes to PSOs

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PSO 7
CO 1	3	1	3	1	2	2	2
CO 2	3	2	3	1	2	2	3
CO 3	3	1	3	2	2	3	2
CO 4	3	1	3	1	3	2	2
CO 5	3	1	3	1	2	2	2

Course Contents for Classroom Transaction:

MODULE	UNIT	DESCRIPTION	HOURS
1		**UV-VISIBLE AND FLUORESCENCE SPECTROSCOPY**	**7**
	1	Chromophores and effect of conjugation on the spectrum. Visible spectrum and colour in compounds	
	2	Instrumentation of UV-VIS spectroscopy	
	3	Analysis of various aromatic compounds such as coumarin, porphyrins, anthracene, Eriochrome black T, phenolphthalein etc. Calculation of molar extinction coefficient and the λ_{max}	
	4	Phenomena of Fluorescence, Jablonski Diagram, Characteristics of Fluorescence Emission, The Stokes Shift, Mirror-I mage rule,Exceptions to the Mirror-Image Rule, Fluorescence lifetime, quantum yield and quenching	
	5	Instrumentation for Fluorescence Spectroscopy	
2		**IR SPECTROSCOPY &NMR SPECTROSCOPY**	**10**
	1	The Infrared Absorption Process, Uses of the Infrared Spectrum, The Modes of Stretching and Bending, Bond Properties and Absorption Trends	
	2	Instrumentation and Preparation of Samples for Infrared Spectroscopy	

	3	Features of spectra of hydrocarbons, aromatic compounds, phenol and alcohol, carbonyl compounds and amines	

	1	Chemical environment, shielding and chemical shift. Local diamagnetic shielding and magnetic anisotropy	
	2	The Origin of Spin–Spin Splitting, Pascal's Triangle, The Coupling Constant in ^{1}H NMR. Decoupling	
	3	Instrumentation, sample preparation and various NMR solvents	
		^{13}C NMR-theory, chemical shift, proton-coupled and ^{13}C Spectra Comparison of ^{1}H and ^{13}C NMR	
	4	Prediction of ^{1}H and ^{13}C NMR spectrum of bromo-ethane, 2-bromo propane, acetyl benzoate, anthracene, o-xylene, m-xylene and p-xylene	
	5		

3	**MASS SPECTROSCOPY**		**6**
	1	Ionization Methods a) Electron Ionization (EI),b) Chemical Ionization (CI), c) Desorption Ionization Techniques (SIMS, FAB, and MALDI), d) Electrospray Ionization (ESI)	
	2	Mass Analysis a) The Magnetic Sector Mass Analyzer, b) Double-Focusing Mass Analyzers, c) Quadrupole Mass Analyzers, d) Time-of-Flight Mass Analyzers	
	3		
4	**PHOTOELECTRON AND RELATED SPECTROSCOPIES**		**7**
	1	Photoelectron spectroscopy; Experimental methods, Sources of monochromatic ionizing radiation, Electron velocity analysers, Electron detectors, Resolution. Various types of photoelectron spectroscopy (UV and X-ray PES)	
	2	Auger electron spectroscopy; Experimental method, Processes in Auger electron ejection, Examples of Auger electron spectra	
	3	X-ray fluorescence spectroscopy; Experimental method, Processes in X-ray fluorescence, Examples of X-ray fluorescence spectra	

		TEACHER SPECIFIC MODULE	30
5		Experimental analysis of red-shift, blue shift and fluorescence quenching of emission using suitable molecules. Demonstration of importance of fluorescence titration using suitable examples. Job's plot and binding ratio calculation	
		IR spectral analysis of common drug molecules such as paracetamol, amoxicillin, metformin and diclofenac -Analysis of IR spectrum of crotonaldehyde, benzaldehyde, benzoic acid, *N*-methyl acetamide and *N*-methylaniline	
		Interpretation of molecular structures of various molecules	
		Structural Analysis and Fragmentation Patterns a) Alkanes, b) Cycloalkanes, c) Alkenes, d) Alkynes, e) Aromatic Hydrocarbons, d) Alcohols and Phenols, e) Ethers, f) Aldehydes, g) Ketones, h) Esters, i) Carboxylic Acids, j) Amines	

Essential Readings:

1. J. Michael Hollas (2004), Modern Spectroscopy, John Wiley & Sons Ltd
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan (2009), Introduction to Spectroscopy, Fourth Edition.
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Third Edition, Springer.

Assessment Rubrics:

Evaluation Type		**Marks**
End Semester Evaluation (ESE)		**50 (35T+15P)**
Continuous Evaluation (CCA)		**25 (15T+10P)**
Theory		**15**
a)	Test Paper*	9
b)	Assignment	3
c)	Viva-Voce	3
Practical		**10**
a)	Record	5
b)	Viva-Voce/ skill	5
Total		**75**

*Average mark of the best two written tests may be considered for internal mark.