KAT 242/3 – Spectroscopic Methods

Course Objective : To introduce the basic principles, instrumentation and applications of spectroscopic methods: Electromagnetic radiation, infrared absorption, near- infrared spectrometry, fluorometry, optical sensors, flame emission spectrometry and atomic absorption spectrophotometry.

Topic	Content	Number of lecture hours	Expected outcomes – upon completion of this course, the student should be able to:
1. Introduction to Spectroscopy	• Electromagnetic radiation • Wave properties • Interaction of electromagnetic radiation with matter • Atomic energy level diagrams • Atomic absorption • Molecular energy level diagrams • Molecular absorption • Emission of radiation • Terms in absorption spectroscopy • Beer's Law • Limitations to Beer's Law • Application of Beer's law to mixtures • Calibration techniques	4	• Recognize the regions of electromagnetic spectrum and relate it to spectroscopic methods. • Differentiate and understand the difference between atomic and molecular energy levels. • Relate energy levels with absorption and emission in various regions of electromagnetic spectrum. • Understand various terms – absorption, transmittance, absorbance, molar absorptivity. • Derive Beer's law, know and understand its limitations. • Apply Beer's law to absorbing mixtures. • Discuss and understand the following calibration techniques: o Calibration curve o Method of standard additions o Internal standard.
2. Instruments for Optical Spectrocopy	• Components of optical instruments • Sources, wavelength selectors, sample containers, detectors and signal processors	4	• Recognize and understand the components in optical instruments. • Draw the block diagrams for various types of instruments – absorption, fluorescence, emission. • Understand the functions of various components.

Topic	Content	Number of lecture hours	Expected outcomes – upon completion of this course, the student should be able to:
3. Ultraviolet /Visible Spectroscopy (UV/Vis)	• Basic principles • Absorbing species containing π, σ and *n* electrons • Organic chromophores • Absorption by inorganic ions • Charge transfer absorption • UV/Visible spectrophotometers • Qualitative and quantitative analyses	5	• Understand the basic principles of UV/Visible spectrophotometry. • Understand how UV/Vis spectra are obtained from organic molecules and inorganic molecules and ions. • Recognize the arrangement of components in UV/Vis spectrophotometers. • Understand the applications of UV/Visible spectrophotometry-photometric titrations, determination of K_a, qualitative analysis of functional groups.
4. Infrared Spectrophoto-metry (IR)	• Basic principles • Requirements for absorption of infrared radiation – dipole moment changes • Vibrational and rotational transitions • Infrared spectrum • Infrared sources and detectors • Infrared instruments - Dispersive instruments - Fourier transform spectrometers • Quantitative analyses (baseline method) • Sample handling techniques • Applications	3	• Understand the theory of infrared absorption. • Explain the types of molecular vibrations. • Discuss the vibrational modes in molecules. • Recognize the main components of infrared spectrophotometers. • Recognize the components of Fourier transform instruments. • Understand the difference between dispersive IR and Fourier transform instruments. • Understand how quantitative analyses in infrared spectrophotometry is carried out (baseline method). • Understand how various samples are handled – gases, solutions, pure liquids, solids. • Explain how to determine cell thickness. • Understand various applications of infrared spectrophotometry.

Topic	Content	Number of lecture hours	Expected outcomes – upon completion of this course, the student should be able to:
5. Fluorescence	• Basic principles • Deactivation processes • Excitation and emission spectra, fluorescence and phosphorescence • Relationship between concentration and fluorescence intensity. • Factors which affect fluorescence and phosphorescence. • Fluorometers and spectrofluorometers • Applications	3	• Understand theories of fluorescence and phosphorescence. • Understand various deactivation processes. • Write the equation for the effect of concentration on fluorescent intensity. • Recognize the factors which affect fluorescence and phosphorescence. • Recognize the components of fluorometers and spectrofluorometers. • Discuss the applications of molecular fluorescence.
6. Atomic Spectrometry	• Types of atomic spectrometry • Atomic spectra – emission, absorption, fluorescence • Line broadening • Flame atomization • Flame structures • Nebulizers and burners • Processes occurring during atomization • Types of flames • Molecular emission spectra • Background emission	3	• Describe various types of atomic spectrometry. • Understand the function of flames. • Explain the processes occurring during atomization – from ions in solution to atoms. • Explain the various types of flames. • Understand source of molecular emission spectra and background emission.

Topic	Content	Number of lecture hours	Expected outcomes – upon completion of this course, the student should be able to:
7. Flame Emission Spectrometry (FES)	• Basic principles of FES • Relationship between concentration and emission intensity • Instrumentation for FES • Applications	1	• Understand the basic principles of FES. • Recognize the components of instrument for FES and know their functions. • Understand the applications of FES – determination of metals.
8. Atomic Absorption Spectrometry (AAS)	• Basic principles of AAS • Relationship between concentration and absorbance • Instrumentation for AAS • Flameless atomization/ electrothermal atomization (ETAAS) • Hydride generation AAS • Cold vapour mercury analysis • Applications • Interferences in AAS and FES • Sensitivity and detection limits	4	• Understand the basic principles of AAS. • Recognize the main components of instrument for AAS. • Understand the basic principles and advantages of ETAAS, hydride generation and cold vapour mercury technique. • Discuss the applications of AAS. • Understand various interferences in AAS and how to overcome them. • Understand how to calculate sensitivity and detection limits.
9. Atomic Emission Spectrometry (AES)	• Basic principles of AES • Atomic emission spectra from higher energy sources	1	• Understand the basic principles of AES based on higher energy sources.
10. Inductively Coupled Plasma (ICP) Atomic Emission Spectrometry	• Basic principles of ICP AES • ICP source • Direct current argon plasma source (DCAP) • Instrumentation for plasma AES • Types of plasma emission instruments • Applications	2	• Understand the basic principles of ICP AES and DCAP. • Recognize the main components of instruments for ICP AES and DCAP. • Discuss the applications of ICP AES.

Topic	Content	Number of lecture hours	Expected outcomes – upon completion of this course, the student should be able to:
11. Arc/ Spark Emission Spectrometry	• Basic principles • Handling of samples • Instrumentation • Applications	1	• Understand the basic principles of arc/spark emission spectrometry which involves higher energy. • Understand how samples are handled for analysis. • Recognize the components of instrumentation. • Understand the applications – direct analysis of metals in steel industries etc.
12. X-Ray Spectroscopy	• Basic principles of X-ray spectroscopy • X-ray absorption spectrum • X-ray fluorescence	1	• Understand the basic principles of X-ray spectroscopy. • Understand the source of X-ray absorption and fluorescence spectra.
13. X-Ray Fluorescence	• Basic principles of X-ray fluorescence • Instrumentation • Applications	1	• Understand the basic principles of X-ray fluorescence. • Recognize the components of instrumentation. • Understand the applications of the technique.
14. Mass Spectrometry	• Basic principles of mass spectrometry • Mass to charge ratio • Instrumentation • Resolution • Mass analyzers • Mass spectrum • Applications	3	• Understand the basic principles of mass spectrometry. • Understand what is mass to charge ratio. • Recognize the components of instrumentation. • Calculate the resolution of mass spectrometers. • Understand the various mass analyzers. • Recognize and understand a mass spectrum. • Explain the applications of the technique.
TOTAL		**36**	