SEMESTER V

11.1.13. Course Code: DSC 13: ANALYTICAL CHEMISTRY-5 (AC5)
Course Title: INSTRUMENTAL METHODS OF ANALYSIS-I
Total Credits: 04 (Credits: Theory-02, Practical-02)
(Total Lectures: Theory- 30, Practical-60)

Objectives: This course is to make students understand the following concepts:

- Spectroscopic methods of analysis
- Principles of UV and Visible spectrophotometry and its applications
- Various components of UV and Visible spectrophotometry
- Single and double beam instruments
- IR spectroscopy and its applications

Learning Outcomes:
By the end of this course, students will be able to learn:

- Different types of spectroscopic methods of analysis.
- The instrumentation and the applications of the UV- Visible and IR spectrometry.

Unit 1: Basic Concepts of Spectroscopy

An introduction to spectroscopic methods of analysis: Electromagnetic radiation, frequency, wavelength, Planck's equation, Electromagnetic spectrum, mathematical description of wave, superposition of waves, optical interferences, interaction of radiation with the matter, emission of radiation, absorption of radiation, scattering, line broadening.

(Lectures: 04)

Unit 2: UV- Visible Spectrophotometry:

A. Lambert-Beer's law

B. Principles, Electronic transitions, Instrumentation, Single/double beam instrument

C. Industrial/Research Applications: Effect of solvent and conjugation on λ_{max}, Effect of cis-trans geometrical isomerism (e.g. stilbene, cinnamic acid, maleic and fumaric acid), calculation λ_{max} of different compounds (homo- and heteroannular dienes, unsaturated carbonyl compounds) (Woodward-Fieser Rule and Schott's Rule) and calculation of stoichiometric ratios of metal-ligand complex using Job's method.

(Lectures: 12)

Unit 3: IR Spectrophotometry:

A. Principle, Modes of vibrations, Bands (Fundamental, overtones, etc)

B. Instrumentation: FT-IR, sample handling, special cautions during scanning.

C. Applications: Identification of the functional groups (mention the use of fingerprint region and functional group region) and simple organic molecules, Factors affecting the absorption frequency.

(Lectures: 10)

Unit 4: Raman spectroscopy:

Introduction, basic principle, instrumentation, the difference between Raman and IR, Applications of Raman spectroscopy.

(Lectures: 04)

PRACTICALS (Credits: 02, Laboratory Periods: 60)

1. Comparison of UV spectra of $K_2Cr_2O_7$ in aqueous and acidified medium (UV range 180-250 nm).
2. Determination of the pK_a of an indicator (methyl orange) using a spectrophotometer.
3. To find the stability constant and reaction stoichiometry of the complex formed between iron and 1,10-phenanthroline.
4. Identification of the structure of organic compounds using IR- spectroscopy (IR spectra should be provided).
5. Partial reduction of m-dinitrobenze to m-nitro aniline and its characterization using IR spectroscopy.

6. Synthesis of benzoic acid from benzamide and its characterization using IR spectrum.
7. Isolation of DNA from onion and its characterization using UV spectroscopy.
8. Extraction of carotene and xanthophyl from plants and recording its IR spectra.
9. Discuss the IR spectra of alcohols, carbonyl compounds, carboxylic acids and esters. (*Provide IR spectra*).
10. Oxidation of benzaldehyde to benzoic acid and compare the IR spectra of product with starting material.
11. Visit to Central Instrument Facility Centre- Delhi University and prepare a report.

REFERENCES:

- Kemp, W. (1991), Organic Spectroscopy, Palgrave Macmillan.
- Pavia, D.L., et al. (2015) Introduction to Spectroscopy, Cengage Learning India Private Limited.
- Banwell, C.N. (2006), Fundamentals of Molecular Spectroscopy,Tata McGraw-Hill Education.
- Kalsi, P.S. (2002) Spectroscopy of Organic Compounds, New Age International Publishers.
- Smith, B.C. (1998), Infrared Spectral Interpretations: A Systematic Approach, CRC Press.
- Plummer, D.T.(2001), Introduction to Practical Biochemistry, McGraw-Hill.
- B D Khosla, et al. (2018) Senior Practical Physical Chemistry, R Chand & Co.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions

Assessment Methods:

- Class Tests at Periodic Intervals.
- Written assignment (s) / Presentation by individual students
- End semester University Theory and Practical Examination

Keywords: UV-Vis Spectroscopy, IR-Spectroscopy and Raman Spectroscopy