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

11.1.14. Course Code: DSC14: CHEMISTRY-5 (C5)
Course Title: COORDINATION CHEMISTRY AND ORGANOMETALLICS

Total Credits: 04 (Credits: Theory-02, Practical-02)
(Total Lectures: Theory- 30, Practical-60)

Objectives: The course introduces the students to basics of coordination chemistry and organometallics which are of immense importance to biological systems, qualitative and quantitative analysis, catalysis, medicines, paints and pigments etc. Nomenclature, isomerism,

bonding in coordination compounds has been dealt with in sufficient detail along with special emphasis on important coordination compounds in the biological system. In organometallic chemistry, the students are introduced to classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species with special emphasis on metal carbonyls.

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

- Understand terms: ligand, denticity of ligands, chelate, coordination number.
- Systematically name coordination compounds.
- Discuss the various types of isomerism possible in Octahedral and Tetrahedral coordination compounds.
- Use Valence Bond Theory to predict the structure and magnetic behaviour of metal complexes and understand the terms inner and outer orbital complexes.
- Explain the meaning of the terms Δ_o., Δ_t, pairing energy, CFSE, high spin and low spin and how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy.
- Explain magnetic properties and colour of complexes on basis of Crystal Field Theory
- Apply 18-electron rule to rationalize the stability of metal carbonyls and related species.
- Learn how IR data can be used to understand extent of back bonding in metal carbonyls

Unit I: Introduction to Coordination compounds

Brief discussion with examples of types of ligands, denticity and concept of chelate. IUPAC system of nomenclature of coordination compounds (mononuclear and binuclear) involving simple monodentate and bidentate ligands. Structural and stereoisomerism in complexes with coordination numbers 4 and 6.

(Lectures: 06)

UNIT II: Bonding in coordination compounds

Valence Bond Theory (VBT): Salient features of theory, concept of inner and outer orbital complexes, Drawbacks of VBT.

Crystal Field Theory: Splitting of d orbitals in octahedral symmetry. Crystal field effects for weak and strong fields, Crystal field stabilization energy (CFSE), concept of pairing energy, Factors affecting the magnitude of Δ, Spectrochemical series, Splitting of d orbitals in tetrahedral symmetry, Comparison of CFSE for octahedral and tetrahedral fields, tetragonal distortion of octahedral geometry, Jahn-Teller distortion

(Lectures: 14)

UNIT III: Organometallic chemistry

Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, sigma, pi and multicentre bonds), Structure and bonding of methyl lithium and Zeise's salt, Structure and bonding of ferrocene, mononuclear and polynuclear carbonyls of 3d metals, 18-electron rule as applied to carbonyls, π-acceptor behaviour of carbon monoxide (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

(Lectures: 10)

PRACTICALS: (Credits: 02; Laboratory Periods: 60)

1. Estimation of Mg^{2+} by direct complexometric titrations using EDTA.
2. Estimation of Zn^{2+} by direct complexometric titrations using EDTA.
3. Estimation of Ca^{2+} by direct complexometric titrations using EDTA.
4. Preparation of the following inorganic compounds and their characterization using appropriate analytical techniques:
   (i) Tetraamminecopper(II) sulphate
   (ii) Potassium trioxalatoferrate(III) trihydrate
   (iii) Chrome alum
   (iv) Cuprous chloride
   (v) Manganese(III)phosphate ($MnPO_4.H_2O$)
   (vi) Potash alum
   (vii) Acetylacetonate complex of Cu^{2+} and Fe^{3+}
   (viii) Tetraamminecarbonatocobalt(III)nitrate

REFERENCES:

Theory:

- Huheey, J.E.; Keiter, E.A., Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry-Principles of Structure and Reactivity, Pearson Education
- Shriver, D.D.; Atkins, P.; Langford, C.H. (1994), Inorganic Chemistry 2nd Ed., Oxford University Press.
- Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Inorganic Chemistry, 5th Edition, W. H. Freeman and Company.
- Cotton, F.A.; Wilkinson, G.; Gaus, P.L. Basic Inorganic Chemistry, 3rd Edition, Wiley India.
- Douglas, B.E.; McDaniel, D.H.; Alexander, J.J. (1994), Concepts and Models of Inorganic Chemistry, John Wiley & Sons.
- Greenwood, N.N.; Earnshaw, A. (1997), Chemistry of the Elements, 2nd Edition, Elsevier.

Practical:

- Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989),Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons.
- Marr, G.; Rockett, B.W. (1972), Practical Inorganic Chemistry, Van Nostrand Reinhold.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Power point presentation on important topics.

Assessment Methods:

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

Keywords: Coordination Compounds, Organometallic Chemistry.