SEMESTER VI

11.1.16. Course Code: DSC 16: ANALYTICAL CHEMISTRY-6 (AC6)

Course Title: INSTRUMENTAL METHODS OF ANALYSIS-II

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

Objectives: The Objective of this course is to make students aware of the following concepts:

•Atomic spectroscopy
• NMR spectroscopy and its applications
• ESR spectroscopy

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

- What are the different types of spectroscopic methods of analysis that can be used to analyze the samples.
- The instrumentation and the applications of the NMR and ESR spectroscopy.

Unit 1: Atomic Spectroscopy

A. Basic principle and Bohr theory of hydrogen atom
B. Types
C. Atomizer
D. Atomic absorption and photoelectron spectroscopy
E. Applications of absorption and photoelectron spectroscopy

(Lectures:06)

Unit 2: ^{1}H NMR Spectroscopy

A. Principle
B. Instrumentation and sample handling
C. Spin-spin and spin-lattice relaxation
D. Chemical shift
E. Solvents, Internal and external reference compounds

F. Factors affecting chemical shift (Electronegativity, diamagnetic anisotropy, *etc.*)
G. Spin-spin coupling
H. Coupling constants and its applications in characterization of organic molecules including *cis*- and *trans*-isomers
I. Discussion on Chemical shift equivalent nuclei and Magnetic equivalent nuclei with suitable examples
J. Deuterium exchange, Effect of restricted rotation (*e.g.* DMF) and low temperature NMR.
K. Identification of simple organic compounds including tautomer's using ^{1}H NMR spectral data.

(Lectures:18)

Unit 3: ESR spectroscopy:

Basic principles, Relaxation and line width, zero-field splitting and Kramer's degeneracy, g-factor and factor affecting g-factor, Hyperfine coupling constants splitting in triplet spectra, ESR of simple radicals.

(Lectures:06)

PRACTICALS (Credits: 02, Laboratory Periods: 60)

1. Determination of sodium in ORS using atomic absorption spectroscopy.
2. Determination of copper in drinking water using atomic absorption spectroscopy.
3. Multi-step organic synthesis and characterization of compounds using ^{1}H NMR spectral data (^{1}H NMR spectra of the compounds will be provided to students)
   (a) Aniline to *p*-bromoacetanilde
   (b) Nitration of bromobenzene
   (c) Substitution (S_N2) reaction of 1-iodobutane and 2-naphthol
   (d) Synthesis of chalcones, coumarins and xanthenes
4. Separation and identification of organic mixtures containing up to ***two components*** (Use functional group test only).
5. ESR spectra of simple radicals should be discussed in detail with students.

REFERENCES:

- Skoog, D.A. et al (2018) Principles of Instrumental Analysis, Cengage Learning India Private Limited.
- Kemp, W. (1991), Organic Spectroscopy, Palgrave Macmillan.
- Pavia, D.L., et al. (2015) Introduction to Spectroscopy, Cengage Learning India Private Limited.
- Silverstein, R.M. (2014) Spectrometric Identification of Organic Compounds. John Wiley & Sons.
- Kalsi, P.S. (2002) Spectroscopy of Organic Compounds, New Age International Publishers.
- Chang, R. (1971) Basic Principles of Spectroscopy, McGraw-Hill, New York.
- Ahluwalia, V.K.; Dhingra, S. (2000), Comprehensive Practical Organic Chemistry: Qualitative Analysis, Universities Press.
- Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989),Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons.

- Mann F.G, and Saunders, B.C. (2009) Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
- Vogel A.I. (2010) Elementary Practical Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

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: AAS, AES, ^{1}H NMR Spectroscopy and ESR Spectroscopy.

11.1.17. Course Code: DSC17: CHEMISTRY6 (C6)

Course Title: QUANTUM CHEMISTRY AND SPECTROSCOPY

Total Credits: 04 (Credits: Theory-02, Practical-02)

(Total Lectures: Theory- 30, Practical-60)

Objectives: The objective of this course is to introduce the students to the concepts and methodology of quantum mechanics, its applications to spectroscopy and establish the relation between structure determination and spectra.

Learning Outcomes:

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

- Understand basic principles of quantum mechanics: operators, eigen values, averages, probability distributions.
- Understand and use basic concepts of microwave, IR and UV-VIS spectroscopy for interpretation of spectra.
- Explain Lambert-Beer's law, quantum efficiency and photochemical processes.

Unit 1: Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Schrodinger equation and its application to free particle and particle in a 1D box

Qualitative treatment of H and H like atoms. Setting up of Schrodinger equation for many electron atoms.

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels.

(Lectures: 12)

Unit 2: Spectroscopy

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter.

Types of spectroscopy. Difference between atomic and molecular spectra. Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

IR Spectroscopy: Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

(Lectures: 12)

Unit 3: Photochemistry

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells.

(Lectures: 6)

PRACTICALS (Credits:02, Laboratory Periods: 60)

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and K_2Cr2O_7 (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J $molecule^{-1}$, kJ mol^{-1}, cm^{-1}, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$ (*Use solutions of different pH*)

3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Verify Lambert-Beer's law and determine the concentration of $K_2Cr_2O_7$ in a solution of unknown concentration.
5. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
6. Study the kinetics of iodination of propanone in acidic medium.
7. Determine the dissociation constant of an indicator (phenolphthalein).
8. Study the kinetics of interaction of phenolphthalein with sodium hydroxide.
9. Study the kinetics of interaction of crystal violet with sodium hydroxide.

REFERENCES:

Theory

- Banwell, C.N.; McCash, E.M.(2006), Fundamentals of Molecular Spectroscopy, Tata McGraw- Hill.
- Kapoor, K.L.(2015),A Textbook of Physical Chemistry, McGraw Hill Education, ,Vol 4, 5th Edition, McGraw Hill Education.
- McQuarrie, D.A.(2016),Quantum Chemistry, Viva Books.
- Chandra, A. K.(2001),Introductory Quantum Chemistry, Tata McGraw-Hill.

Practical:

- Khosla, B.D.; Garg, V.C.; Gulati, A. (2015),Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
- Kapoor, K.L. (2019),A Textbook of Physical Chemistry, Vol.7, 1st Edition, McGraw Hill Education.
- Garland, C. W.; Nibler, J. W.; Shoemaker, D. P.(2003),Experiments in Physical Chemistry, 8th Edition, McGraw-Hill, New York.

Additional Resources:

- Castellan, G. W .(2004),Physical Chemistry, Narosa.
- Petrucci, R. H.(1989),General Chemistry: Principles and Applications, Macmillan Publishing

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: Quantisation, Selection rules, Schrodinger equation, Operator, Spectrum, Quantum efficiency.