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:

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- 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.