Course Code: CHEMISTRY –DSE-4
Course Title: Analytical Methods in Chemistry
Total Credits: 06   **(Credits: Theory-04, Practical-02)**
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The objective of this course is to make student aware of the concept of sampling, Accuracy, Precision, Statistical test data-F, Q and t test. The course exposes students to the laws of spectroscopy and selection rules governing the possible transitions in the different regions of the electromagnetic spectra. Thermal and electroanalytical methods of analysis are also dealt with. Students are exposed to important separation methods like solvent extraction and chromatography. The practicals expose students to latest instrumentation and they learn to detect analytes in a mixture.

Learning Outcomes:

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

- Perform experiment with accuracy and precision.
- Develop methods of analysis for different samples independently.
- Test contaminated water samples.
- Understand basic principle of instrument like Flame Photometer, UV-vis spectrophotometer.
- Learn separation of analytes by chromatography.
- Apply knowledge of geometrical isomers and keto-enol tautomers to analysis.
- Determine composition of soil.
- Estimate macronutrients using Flame photometry.

Unit 1:

Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression.

Normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

(Lectures: 5)

Unit 2:

Optical methods of analysis

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules

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UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument; Transmittance. Absorbance and Beer-Lambert law

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs). Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal, Techniques for the quantitative estimation of trace level of metal ions from water samples.

(Lectures: 25)

Unit 3:

Thermal methods of analysis:

Theory of thermogravimetry (TG) and basic principle of instrumentation of thermal analyser. Techniques for quantitative estimation of Ca and Mg from their mixture.

(Lectures: 5)

Unit 4:

Electroanalytical methods

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations.Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

(Lectures:10)

Unit 5:

Separation techniques

Solvent extraction: Classification, principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media.

Chromatography: Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition & ion-exchange, Development of chromatograms: frontal, elution and displacement methods.

(Lectures:15)

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Practical:

(Credits: 2, Laboratory periods: 60)

1. Separation of mixtures by paper chromatography and reporting the R_f values:

    (i) Co^{2+} and Ni^{2+}.
    (ii)   Amino acids present in the given mixture.
2. Solvent Extractions

    (i)   To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform, and determine its concentration by spectrophotometry.

3. Analysis of soil:

    (i)   Determination of pH of soil.
    (ii)   Total soluble salt
    (iii) Estimation of calcium and magnesium
    (iv)   Qualitative detection of nitrate and phosphate
4. Ion exchange:

    (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
    (ii) Separation of amino acids from organic acids by ion exchange chromatography.

5. Spectrophotometry

    (i) Verification of Lambert-Beer's law and determination of concentration of a coloured species ($CuSO_4$, $KMnO_4$, $CoCl_2$, $CoSO_4$)
    (ii) Determination of concentration of coloured species via following methods;
         (a) Graphical method, (b) Epsilon method, (c) Ratio method, (iv) Standard addition method

References:

Theory:

1. Willard, H.H.(1988),**Instrumental Methods of Analysis**, 7th Edition, Wardsworth Publishing Company.
2. Christian, G.D.(2004),**Analytical Chemistry**, 6th Edition, John Wiley & Sons, New York.
3. Harris, D. C.(2007),**Quantitative Chemical Analysis**,6th Edition, Freeman.
4. Khopkar, S.M. (2008), **Basic Concepts of Analytical Chemistry,** New Age International Publisher.
5. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), **Principles of Instrumental Analysis,** Thomson Asia Pvt. Ltd.

Practical:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C.(1989),**Vogel's Textbook of Quantitative Chemical Analysis**,John Wiley and Sons.

Teaching Learning Process:

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- Teaching through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

Assessment Methods:

- Presentations by individual student/ small group of students
- Class tests at periodic intervals.
- Written assignment(s)
- Objective type chemical quizzes based on contents of the paper.
- End semester university theory and practical examination.

Keywords:

Separation techniques, Solvent extraction, Ion-exchange, Optical methods, Flame Atomic Absorption and Emission Spectrometry, indeterminate errors, statistical test of data; F, Q and t tests. TGA.

Course Code: CHEMISTRY –DSE-5
Course Title: Molecular Modelling and Drug Design
Total Credits: 06   (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

Objective of this course is to make students learn the theoretical background of principles of computational techniques in molecular modelling, evaluation and applications of different methods for various molecular systems, energy minimization techniques, analysis of Mulliken Charge & ESP Plots and elementary idea of drug design.

Learning Outcomes:

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

- Understand theoretical background of computational techniques and selective application to various molecular systems.
- Learn Energy minimization methods through use of different force fields.
- Learn ESP Plots by suitable soft wares, electron rich and electron deficient sites,
- Compare computational and experimental results and explain deviations.
- Carry out Molecular dynamics (MD) and Monte Carlo (MC) simulations on several molecules and polymers.
- Learn QSAR properties and their role in molecular modelling, cheminformatics and drug discovery.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.