CHEMISTRY

DSC-3:Analytical and Organic Chemistry-II

Contact Hours: 56 **Work load: 4 Hours/Week.**

Credit Points :4

Evaluation: Continuous Internal Assesment-40 Marks

Semester End Examination -60 Marks

Course Objectives:

1) Interrelationship among frequency, wavelength and wave number and importance of validation parameters of an instrumental method will be taught
2) Principle, instrumentation and applications of spectrophotometry, nephelometry and turbidometry will be taught
3) Fundamentals of separation methods and principles of paper, thin layer and column chromatography will be taught
4) Principle, types and applications of solvent extraction will be taught
5) Principle and mechanism of ion-exchange, types of resins and domestic and industrial applications of ion-exchange chromatography will be taught
6) The concept of mechanism and its importance will be taught to the student
7) Concept and importance of intermediates in organic chemistry will be taught taking proper examples
8) The various techniques for identification of reaction mechanism will be taught to the student taking proper examples
9) Concept of stereochemistry and its importance will be taught.
10) The various projection formulae and the techniques of designating the molecules into R, S, D, L will be taught taking proper examples
11) The theory and concept of Cis-, Trans- isomerism and its importance and the techniques to differentiate between them will be taught taking examples

Course Specific Outcomes

After the completion of this course, the student would be able to

1) Understand the importance of fundamental law and validation parameters in chemical analysis
2) Know how different analytes in different matrices (water and real samples) can be determined by spectrophotometric, nephelometric and turbidometric methods.
3) Understand the requirement for chemical analysis by paper, thin layer and column chromatography.

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4) Apply solvent extraction method for quantitative determination of metal ions in different samples
5) Utilize the ion-exchange chromatography for domestic and industrial applications
6) Explain mechanism for a given reaction.
7) Predict the probable mechanism for an reaction
   Eexplain the importance of reaction intermediates, its role and techniques of generating such intermediates
8) Explain the importance of Stereochemistry in predicting the structure and property of organic molecules.
9) Predict the configuration of an organic molecule and able to designate it.
10) Identify the chiral molecules and predict its actual configuration

Unit-I

Quantitataive analysis-Instrumental methods

Electromagnetic spectrum, absorption of electromagnetic radiation, Definition and units of frequency, wavelength, wave number, Beer's law, Beer-Lambert law derivation, deviations from Beer's law, limitations, construction of calibration graph (Plot of absorbance versus concentration), Evaluation Procedures- standard addition, Internal standard addition, validation parameters-detection limits, sensitivity, dynamic/linearity range, Instrumentation, single beam and double beam spectrophotometers, quantitative applications of colorimetry (determination of Fe, Mo, Cu, Ti and PO_4^{3-}) and numerical problems on application of Beer's law. **10 hrs**

Nephelometry and Turbidimetry: Introduction, principle, instrumentations of nephelometry and turbidimetry; effects of concentration, particle size and wavelength on scattering; choice between nephelometry, applications of nephelometry and turbidimetry (determination of SO_4^{2-} and PO_4^{3-}) **4 hrs**

Unit-II

Separation methods

Fundamentals of chromatography: General description, definition, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of stationary and mobile phase and nature of adsorbents. Principles of paper, thin layer, column chromatography. Column efficiency, factors affecting the column efficiency, van Deemter's equation and its modern version. **3hrs**

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Paper chromatography: Theory and applications

Thin layer chromatography (TLC): Mechanism, R_f value, efficiency of TLC plates, methodology–selection of stationary and mobile phases, development, spray reagents, identification and detection, qualitative applications. **4 hrs**

Solvent Extraction: Types- batch, continous, efficiency, selectivity, distribution coefficient, Nernst distribution law, derivation, factors affecting the partition, relationship between % extraction and volume fraction, Numerical problems on solvent extraction. Solvent extraction of iron and copper. **4hrs**

Ion exchange chromatography: resins, types with examples- cation exchange and anion exchange resins, mechanism of cation and anion exchange process and applications of ion-exchange chromatography (softening of hard water, separation of lanthanides, industrial applications). **03Hrs**

Unit-III

Reaction Intermediates: Generation, Stability and Reactions of,

i) Carbocations: Dienone-phenol; and Pinacol-Pinacolone Rearrangement.
ii) Carbanions :PerkinReaction,Aldolcondensation,Claisen-Schmith condensation.
iii) Free Radicals : Sandmeyer Reaction
iv) Carbenes and Nitrenes: Singlet and Triplet states, their relative stability and reactions
v) Arynes: Formation,detection etc. **8 hrs**

Methods for Identifying Reaction Mechanism:
Product analysis, Isolation and Identification of Intermediates, Stereochemical Evidences,Effect of Catalyst,crossover Experiments,Isotopic studies,Kinetic Studies. **6 hrs**

Unit-IV

Stereochemistry of Organic Compounds:
Fischer projection,Newmann and Sawhorse projection formulae and thei interconversions.
Geometrical isomerism : Cis-trans and syn-anti isomerism, E/Z notations with C.I.P rules.
Optical Isomerism :Optical activity, Specific rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral centres, Diasteroisomers, meso structures, Racemic mixtures and Resolution, Relative and absolute configuration, D/L and R/S designations **14 hrs**

References :

1) Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, Saunders College Publishing, New York (2005).
2) Analytical Chemistry, G.D. Christian, 6th edition, Wiley-India (2007).

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3) Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, PHI Learning Pvt Ltd.NewDelhi(2009).
4) Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D.Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, Pearson Education Pvt.Ltd.(2007).
5) Organic Reaction Mechanism by V.K.Ahluwalia and R.K.Parashar (Narosa Publishers)
6) Organic Chemistry by S.M.Mukherji,S.P.Sinh and R.K.Kapoor (Narosa Publishers)
7) Morrison R.N and Boyd R.N,OrganicChemistry,Darling Kindersley(India)Pvt.Ltd.(Pearson Education)
8) Finar I.L,Organic Chemistry(Volume I); Finar I.L (Volume II) Stereochemistry and the Chemistry of Natural Products.,Dorling Kindersley(India)Pvt.Ltd.(Pearson Education)
9) Kalsi P.S.Stereochemistry,conformation and Mechanism,New age International
10) Eliel E.L and wilenS.H,Stereochemistry of Organic Compounds,Wiley,(London)

PRACTICALS

Credit Points: 2 **Teaching Hours:4 hrs**

Evaluation : ContinuousInternal Assessment-20 marks

Semester End Examination :30 marks

Course Objectives

1) To impart skills related to preparation of stock and working solutions and handling of instrumental methods
2) To know the principle of colorimetric analysis and construction of calibration plot
3) To understand the chemistry involved in colorimetric determination of metal ions and anions
4) To determine R_f values of different metal ions present in a mixture
5) To impart knowledge on the importance of functional groups in organic compounds.
6) Techniques to identify the functional groups in an compound by performing physical and chemical tests
7) To record its melting point/boiling point.
8) To prepare suitable derivative for that compound and to characterize it.

Course Specific outcomes

After the completion of this course, the student would be able to

1) Understand the importance of instrumental methods for quantitative applications

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2) Apply colorimetric methods for accurate determination of metal ions and anions in water or real samples

3) Understand how functional groups in an compound is responsible for its characteristic property

4)Learn the importance of qualitative tests in identifying functional groups.

5)Learn how to prepare a derivative for particular functional groups and how to purify it

PART-A (Analytical Chemistry)

1) Colorimetric determination of copper using ammonia solution
2) Colorimetric determination of iron using thiocyanate solution
3) Colorimetric determination of nickel using DMG solution
4) Colorimetric determination of titanium using hydrogen peroxide
5) Colorimetric determination of nitrite in a water sample (diazo coupling Reaction/Griess reagent
6) Colorimetric determination of phosphate as ammonium phosphomolybdate
7) Determination of R_f values of two or three component systems by TLC
8) Separation of different metal ions by paper chromatography/ Solvent extraction of iron using oxine solution **(demonstration)**

PART-B(Organic Chemistry)

Qualitative analysis of bifunctional Organic compounds such as 1)Salycilic acid ,p-Nitro benzoic acid,Antranilicacid,p-Chloro benzoic acid 2) o-Cresol,p-Cresol,Resorcinol,o-Nitrophenol,p-nitophenol 3)o-Nitro aniline,p-Nitroaniline,p-Toluidine,p-Chloroaniline,p-Bromoaniline, 4)Ethyl Salicylate, Salicylaldehyde, Actophenone,p-Dichlorobenzene,p-Nitro toluene,,Benzamide etc.(Atleast 6-8 compounds to be analysed in a semester)

References

1)Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D.Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, Pearson Education Pvt.Ltd.(2007)

2) Vogels Text Book of Qualitative Chemical Analysis,ELBS

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BSc Semester III – Chemistry (Hons) with Analytical/ Organic/ Inorganic/ Physical Specialization

Title of the Course: Open Elective-3: ATOMIC STRUCTURE,BONDING AND CONCEPTS IN ORGANIC CHEMISTRY

Contact Hours: 42 **Workload: 3 hours per week**
Credit Points: 3
Evaluation: Continuous Internal Assessment - 40 marks
Semester End Examination - 60 marks

Course Objectives:

- To develop an understanding of principles of Atomic structure
- To know the importance of quantum numbers, writing of electronic configurations and represention of orbitals
- To develop an understanding of the periodic trends
- To understand the nature of bonding and to predict the shapes of molecules
- To construct MO energy level diagrams and predict the properties of molecules
- To understand the formation of sigma and pi bonds and the bond strength.
- To study the classification of organic reactions
- To learn nomenclature preparation and reactions of alkanes,alkenes,alkynes and stability of alicyclic compounds

COURSE CONTENT

Unit I: Atomic Structure and Periodic Properties

History of an atom. Idea of de Broglie matter waves. Heisenberg uncertainty principle. Schrödinger wave equation, significance of wave functions, Bohr's model of hydrogen atom and its limitations. Quantum numbers and their importance, atomic orbitals and shapes of s, p, d orbitals , Multi-electron atoms, Aufbau and Pauli exclusion principle and Hund's multiplicity rule- Electronic configurations of the elements (atomic no. up to 30), effective nuclear charge and shielding.

(8 hours)

Periodic Properties

Atomic radius, Covalent, ionic and van der Waal radii-explanation with examples. Definition and periodicity of the following properties - ionic radii, ionisation potential, electron affinity and electronegativity, methods of determination of electronegativity. Factors affecting the values of ionisation energy. **(6hours)**

Unit II: Chemical Bonding

Ionic Solids– Ionic structures(NaCl, CsCl, TiO_2, ZnS), radius ratio rule and coordination number, limitation of radius ratio rule, lattice energy and Born-Haber cycle, solvation energy and solubility of ionic solids, polarizing power and polarisability of ions, Fajan's rule and their consequences. **(4 hours)**

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Covalent Bond – Valence bond theory and its limitations, directional characteristics of covalent bond, various types of hybridization with examples and shapes of simple inorganic molecules and ions. Shapes of NH_3, I_3^+, I_3^-, SF_4, ClF_3, IF_5, ICl_2^- and H_2O using valence shell electron pair repulsion (VSEPR) theory, linear combination of atomic orbitals (LCAO), bonding, nonbonding and antibonding molecular orbitals, physical picture of bonding and antibonding wave functions. Applications of MO theory to explain the stability of homo dinuclear (He_2, N_2, O_2, F_2, C_2) and hetero dinuclear (NO and CO) molecules. Comparison of M.O. and V.B. Models.

(7hours)

Metallic bond-free electron, Band theory-electrical properties of metals, semiconductors and insulators.

Weak interactions – Hydrogen bonding and its consequences, van der Waals forces.

(3 hours)

Unit III: Bonding and molecular structure and hydrocarbons

Bonding and molecular structure: Introduction to organic chemistry,atomic orbitals,sigma and pi bond formation-molecular orbital [MO]method,sp,$sp^2$and sp^3 hybridization,bond length,bond dissociation energies and bond angles(open chain and cyclic compounds).Electronegativity and polarity of the bonds.Classification and reactions of organic compounds(with examples). **7 Hours**

Alkanes,Alkenes and Alkynes

Definition,Nomenclature,preparations (any two methods)

Reactions: Electrophilic, nucleophilic and free radical addition reactions

Alicyclic compounds:

Nomenclature,preparation and stability of cyclopropane, cyclobutane, cyclopentane and cyclohexane. **7 Hours**

Reference Books:

1. ConciseInorganicChemistry, J. D. Lee, ELBS,1996.
2. Inorganic Chemistry, A. K. Das
3. Inorganic Chemistry: PrinciplesofStructureandReactivity,Huheey, J. E., Keiter, E.A., Keiter, R.L. & Medhi, O. K.PearsonEducationIndia,2006.
4. InorganicChemistry,Shriver,D.F.&Atkins,P.W.OxfordUniversityPress.
5. Schaum's Outline Series Theory and Problems of Organic Chemistry.SI (metric) edition Herbert Meislich,Howard Nechamkin and Jacob Sharefkin.
6. Organic chemistry. Robert T.Morrison Robert N. Boyd,6thEdition
7. Organic Chemistry Volume-1, I.L.Finar

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COURSE OUTCOME:

On completion of the course the student will learn and be able to understand/explain

- the concept of atomic structure, significance of quantum numbers, filling of electrons of atoms/ions in various orbitals as per rules
- the trends in periodic properties
- the structures of ionic solids, applications of B-H cycle, solubility of compounds and consequences of polarization of ions
- the shapes of molecules/ions based on VSEPR theory
- the construction of MO energy level diagrams and prediction of properties of molecules/ions like bond order, bond energies, bond lengths and magnetic properties.
- the formation of sigma and pi bonds and the bond strength
- the classification of organic reactions
- nomenclature preparation, and reactions of alkanes,alkenes,alkynes and stability of alicyclic compounds.

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