Tentative Subject Code Template

1st and 2nd Semester, 1st Year P.G

SEMESTER	COURSE CODE	NAME OF THE COURSE
I	CH 1812	ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY
I	CH 1813	CONCEPTS IN INORGANIC CHEMISTRY
I	CH 1814	QUANTUM CHEMISTRY AND GROUP THEORY
I	CH 1815	ANALYTICAL CHEMISTRY
I	CH 1816	ORGANIC LABORATORY TECHNIQUES -I
I	CH 1817	INORGANIC QUANTITATIVE ANALYSIS AND PREPARATIONS
II	CH 2819	ORGANIC REACTION MECHANISMS AND HETEROCYCLICS
II	CH 2820	MAIN GROUP ELEMENTS AND NUCLEAR CHEMSITRY
II	CH 2821	MOLECULAR SPECTROSCOPY
II	CH 2822	ORGANIC LABORATORY TECHNIQUES -II
II	CH 2823	INORGANIC SEMIMICRO QUALITATIVE ANALYSIS
II	CH 2824	SEMINAR AND PROJECT
II	CH 2955	BIO-ORGANIC CHEMISTRY
II	CH 2956	MEDICINAL CHEMISTRY
II	CH 2957	CATALYSIS

CH 1812 : ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY

Semester: I Credits : 4

Category Major Core (**MC**) No. of hrs: 60 (5hrs/wk)

Objectives:

1. *To understand the path, feasibility and mechanism of a reaction.*
2. *To suggest synthetic route for simple organic compounds based on stereochemistry.*
3. *To understand the techniques involved in the determination of mechanism of reactions and to propose methods to determine the mechanism of reaction*
4. *To understand the concept of stereochemistry and reaction mechanism.*

Unit-1: Mechanisms and Methods (10 hrs)

1.1 Types of mechanism, reagents and reactions.

1.2 Thermodynamic and kinetic requirements of reactions; Baldwin rules for ring closure; Hammond postulate; microscopic reversibility and Marcos theory

1.3 *Methods of determining mechanism*: Non-kinetic methods: identification of products and intermediates; isotopic labeling; stereo chemical evidences; isotopic effects; cross-over experiments, trapping of intermediates. Kinetic methods - relation of rate with the mechanism of reaction.

Self study:

Acids and bases; Bronsted theory; proton transfer reactions; measurement of solvent acidity; hard and soft acids and bases; effect of structure and medium on the strength of acids and bases.

Unit-2: Rearrangement Reactions (10 hrs)

2.1 *Types of rearrangements*: Nucleophilic; free radical and electrophilic reactions.

2.2 *Mechanisms*: Nature of migration; migratory ability and memory effects, ring enlargement and ring contraction rearrangements

2.3 *Reactions*: Wagner-Meerwin and related reactions, Benzil-benzilic acid, Favorskii, Hoffmann and related rearrangements, Beckmann, Neber, Baeyer-Villiger, Stevens, Claisen rearrangements, boron-carbon migration, Non-1,2-rearrangements, Fischer-indole synthesis, Arndt-Eistert synthesis,

Self study:

Longer nucleophilic, carbene and dienone-phenol rearrangements.

Unit-3: Oxidation and Reduction Reactions. (10 hrs)

3.1 *Mechanisms*: direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination and formation of ester intermediates

3.2 *Oxidation Reactions*: Hydrogen elimination; oxidation of alcohols and amines; Reactions involving cleavage of C-C bonds: cleavage of double bonds; oxidative decarboxylation.

3.3 *Reduction Reactions*: Replacement of oxygen by hydrogen - Wolff Kishner and Clemmenson reductions; Removal of Oxygen from substrate; Reduction with cleavage; MPV reductions.

Self study:

Oxidative and reductive coupling reactions

Unit-4: Stereochemistry-I (15 hrs)

4.1 Optical isomerism due to asymmetric and dissymmetric carbon atoms.

4.2 *Racemic modifications*: Racemisation by thermal, anion, cation, reversible formation; Epimerisation, mutarotation

4.3 *Cram's and Prelog's rules*; D, L, R, S-notations; Cahn-Ingold-Prelog rules, absolute and relative configurations; configurations of allenes, spiranes, biphenyls, cyclooctene and helicene.

4.4 Criteria for optical purity; Resolution of racemic modifications; asymmetric transformations; asymmetric synthesis; destruction.

4.5 Geometrical isomerism: E, Z notations, geometrical isomerism in C=C and cyclic systems.

Unit-5: Stereochemistry-II (15 hrs)

5.1 Conformation and reactivity of acyclic systems; intramolecular rearrangement; neighbouring group participation; Curtin-Hammett principle

5.2 Stability of six and seven-membered rings; mono and disubstituted cyclohexanes; conformation and reactivity in cyclohexane systems.

5.3 Fused and bridged rings; bicyclic and poly cyclic systems; decalins and Brett's rule.

5.4 Optical rotation and optical rotatory dispersion; conformational asymmetry, ORD curves; octant rule; configuration and conformation; Cotton effect; axial haloketone rule; Determination of configuration

5.5 Stereoselective and stereospecific synthesis.

Self study:

Specific and molar rotations; polarimetry; Fischer, Newmann and Sawhorse notations; optical isomerism of lactic and tartaric acids.

Text books

1. J. March and M. Smith, *Advanced Organic Chemistry*, 5th edn, John-Wiley and Sons. 2001.
2. E. S. Gould, *Mechanism and Structure in Organic Chemistry,* Holt, Rinehart and Winston Inc., 1959.
3. P. S. Kalsi, *Stereochemistry of carbon compounds*, 3rd edn, New Age International Publishers, 1995.

References

1. E. L. Eliel, *Stereochemistry of Carbon Compounds*, Tata-McGraw Hill, 2000.
2. I. L. Finar, *Organic Chemistry. Vol-2*, 5th edition, Pearson Education Asia, 1975
3. I. L. Finar, *Organic chemistry, Vol-1,* 6th edition, Pearson Education Asia, 2004

4. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part-A and B,* 4th edn, Kluwer Academic / Plenum Publishers. 2000.

5. S. H. Pine, *Organic Chemistry, 5th edn*, McGraw Hill International Edition, 1987.

6. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.

7. D. Nasipuri, *Stereochemistry of Organic Compounds, 2nd Edn*, New Age Publishers, 2005.

CH 1813: CONCEPTS IN INORGANIC CHEMISTRY

Semester : I — Credits : 4

Category : Major Core (MC) — No. of Hours : 60 (5 hrs/wk)

Objectives

1. *To understand the different kinds of chemical forces in molecules.*
2. *To identify the nature of chemical bond in a given inorganic compound.*
3. *To predict the nature and topology of inorganic compounds.*
4. *To know the existence of compounds through weak chemical forces.*
5. *To identify relevant inorganic compounds for specific applications.*

Unit-1: Atomic Structure and Periodic Table (7 hrs)

1.1 *Modern views on atomic structure*: Wave mechanical description of electron and orbitals-radial density functions and orbital energies, angular functions and orbital shapes.

1.2 *Slater orbitals and their uses*: Computation of effective nuclear charge and radii of atoms and ions.

1.3 *Modern periodic table*: Periodic properties, trends and the underlying reasons.

Self study

(a)Study the trend in the atomic and ionic radii, ionization potential, and electron affinity along the period of the periodic table.

(b) Electronic configuration: the exchange energy and *Aufbau* principle.

Unit-2: Ionic Compounds (18 hrs)

2.1 Packing of ions in crystals and crystal structures-*ccp*, *hcp*, *bcc*, and *fcc*.

2.2 *Radius ratio and structure of ionic lattices*: Geometrical method of computing radius ratio, radius ratio and coordination number, stoichiometry and crystal structures.

2.3 *Lattice energy*: Born-Lande equation, modified Born-Lande equation, factors affecting lattice energy.

2.4 *Born-Haber cycle*: Thermochemical calculations, radii of nonspherical ions, solubility and thermal properties of ionic compounds as a function of U_o and ΔH_f.

2.5 *Polarization in ionic compounds*: covalency and Fajans rules, effects of polarization.

2.6 Crystal defects: Schottky defects, controlled valency, *F*-center, and Frenkel defect.

2.7 Nonstoichiometric compounds-, interstitial-, and electron deficient compounds.

Self study

(a)Layer lattices, applications, and properties of crystal defect.

(b) Thermodynamic parameters which affect lattice energy and factors which affect ionic radii.

(c)Predicting the existence of certain ionic compounds and the nonexistence of hypothetical compounds from thermochemical calculations.

Unit -3: Covalent Bond (18 hrs)

3.1 *Molecular topologies*: Shared and lone pairs and Lewis structures, isoelectronic and isolobel relationships, hybridization and geometry, VSEPR model, and Bent's rule.

3.2 *Molecular Orbital Theory*: Symmetry of molecular orbitals formed from atomic orbital overlap, Extended Huckel theory of Hartree-Fock approximation (SCF), LCAO-MO model, TASO, LUMO, and HOMO concepts in bonding.

3.3 MO energy level diagrams of homodiatomic and heterodinuclear molecules (CO, NO, and HCl).

3.4 *Bonding in metals*: Packing of atoms in metals, band theory of metals and metallic properties, insulators, and semiconductors.

Self study

(a)Qualtitative MO energy level diagram of heterodiatomic molecules and concept of electronegativity.

(b) TASO, LUMO, and HOMO in MO formation and reactivity of molecules.

Unit-4: Weak Chemical Forces (7 hrs)

4.1 *van der Waals forces*: Inclusion compounds-layer, channel, and cage structures (gas hydrates and clathrates).

4.2 *Hydrogen bonding*: Types, associated molecules, and molecular self assembly.

4.3 Supramolecular architectures formed by weak chemical forces.

Self study

(a)Structural features of zeolites and clathrates.

(b)Nature and importance of supramolecular assemblies formed by van der Waals forces and H-bonding.

Unit-5: Acid-base theory and Solvent Systems (10 hrs)

5.1 *Acid-Base theories*: Bronsted-Lowry, Lux-Flood, Usanovich, Lewis, and solvent system. definitions, measures of acid-base strength, acid-base interactions, hard and soft acid and bases, classification, HSAB principle, levelling effect, symbiosis, proton sponges.

5.2 *Non aqueous solvents*: Classification-protonic and aprotic solvents, super acids, molten salts as solvents, and ionic liquids.

Self study

(a)Classification of acids and bases by *class-a* , *class-b*, and *borderline*.

(b) Use of ionic liquids in synthesis. Reactions in liquid ammonia and liquid SO_2.

(c)Strengths of protonic acids: Binary acids, oxo acids, pure acids and relative acidities, Properties of perchloric acid, fluorosulfuric acid, trifluoromethanesulfonic acid.

Text Books

1. F.A.Cotton, G.Wilkinson, C.A. Murillo and M.Bochmann, . *Advanced Inorganic Chemistry*; 6th ed.; Wiley Interscience: New York, **1988**.

2. K.F.Purcell and J.C. Kotz, *Inorganic Chemistry*; Saunders: Philadelphia, **1976**.

3. J.E.Huheey, E.A. Keiter and R.L. Keiter , *Inorganic Chemistry*; 4th ed.; Harper and Row: NewYork, **1983**.

References

1. T.Moeller, . *Inorganic Chemistry, A Modern Introduction*; John Wiley: New York, **1982**.

2. D.F.Shriver , P.W..Atkins and C.H. Langford; *Inorganic Chemistry*; 3rd ed.; Oxford University Press: London, **2001**.

3. G.H.Stout and L.H.Jenson, *X-Ray Structure Determination*; 2nd ed.; John Wiley & Sons: New York, **1989**.

4. A.R.West, *Solid State Chemistry and its Applications*; John Wiley & Sons: New York, **1989**.

5. G.Rhodes, *Crystallography Made crystal Clear*; Academic Press, Inc.: New York, **1993**.

6. C.Hammond, *The Basics of Crystallography and Diffraction*; Oxford University Press; **1997**.

7. L.Smart and E.Moore, *Solid State Chemistry, An Introduction*; 2nd ed.; Nelson Thornes Ltd.: Cheltenham, **1996**.

CH 1814: QUANTUM CHEMISTRY AND GROUP THEORY

Semester : I **Credits : 4**

Category : Major Core (MC) **No. of Hours : 60 (5 hrs/wk)**

Objectives:

1. *To understand the physical and mathematical aspects of quantum mechanics.*
2. *To familiarize with the required mathematics for solving quantum mechanical problems.*
3. *To understand the quantum mechanical approach to the atomic and molecular electronic structure.*

Unit 1: Mathematics for Quantum Mechanics and Postulates of Quantum Mechanics (9hrs)

1. 1 *Coordinate systems*: Cartesian, spherical polar, cylindrical and elliptical. Real and complex functions: Odd, even, orthogonal and normalized functions. Differential equations: order and degree. Solutions to typical differential equations.

1.2 *Operators*: linear, differential, Hermitian and Hamiltonian operators

1.3 Eigen functions and Eigen values

1.4 *Failure of classical mechanics*: Black body radiation, photo electric effect, and Compton effect. The need for Quantum Mechanics.

1.5 Postulates of Quantum of Mechanics and Schrodinger wave equation

Unit 2: Some Quantum mechanical models and their applications (12 hrs)

2.1 *Particle in a box* (1D and 3D). Degeneracy and its application to linear conjugated molecular systems.Free particle. Bohr's correspondence principle. *Quantum Mechanical tunneling*: Tunneling in some typical chemical reactions, inversion of ammonia, proton transfer reactions.

2.2 *Rigid Rotor*: Wave equation and solution. Calculation of rotational constants and bond length of diatomic molecules.

2.3 *Harmonic Oscillator*: Wave equation and solution. Anharmonicity, force constant and its significance

Unit 3: Application of Quantum Mechanics to Hydrogen and poly electron atoms (14 hrs)

3.1 *Hydrogen atom and Hydrogen like ions*: Solution to hydrogen and hydrogen like wave equation. Radial and angular functions.Quantum numbers n, l, m and s & their importance. Radial distribution functions and hydrogen like orbital and their representation.

3.2 *Approximation Methods*: Variation method- Trial wave functions, variational integral and its application to particle in a 1D box.

Perturbation method and its application. Hartree-Fock Self Consistent Field Method.

3.3 *Quantum mechanical treatment of angular momentum* - Simultaneous measurement of some properties: Evaluation of commutators such as $[x, p_x]$, $[x, p_x^2]$, $[L_x, L_y]$ and $[L_x^2, L_x]$ and their significance.

3.4 *Helium atom*: Electron spin, Pauli Exclusion Principle and Slater determinant. Derivation of atomic term symbols.

Unit 4: Molecular Quantum Mechnaics and Chemical bonding (11 hrs)

4.1 *Hydrogen molecule*: Molecular orbital theory and Heitler-London (VB) treatment. Energy level diagram.

4.2 *Hydrogen molecular ion*: Use of linear variation function and LCAO methods.

4.3 *Electronic structure of conjugated systems*: Huckel method applied to ethylene, allyl systems, butadiene and benzene.

Unit 5: Group theory and its applications. (14 hrs)

5.1 Group and subgroup. Symmetry elements and operations. Classification of molecules into – non axial, axial,and dihedralpoint groups.

5.2 Matrix representations of symmetry operations. Reducible and irreducible representations, classes of operations.

5.3 *Great orthoganility theorem*: Reduction formula. Construction of character table for C_{2v} and C_{3v} point groups.

5.4 Applications of group theory to molecular vibrations (IR and Raman) and chemical bonding.

Text books

1. N. Levine, *Quantum Chemistry*, IV edition. Allyn& Bacon Inc.. **1983**.
2. A. Vincent- *Molecular Symmetry and Group Theory*. A Programmed Introduction to Chemical Applications. John and Willy & Sons Ltd. **1977**.
3. D.A. McQuaric and J. D. Simon.*Physical chemistry - A Molecular Approach*, Viva Books Pvt. Ltd.. New Delhi. **1998**.
4. D. A. McQuarie, *Quantum Chemistry*. Viva Books PW. Ltd..New Delhi. **2003**.
5. T.Engel and R.Philip , *Quantum Chemistry And Spectroscopy*,5th , ed., Pearson, New Delhi, **2006**.
6. F. A. Cotton, *Chemical Applications of Group Theory*. 2nd ed..John Wiley & Sons, **1971**.
7. K. V. Raman, *Group Theory and its Applications to Chemistry*, Tata McGraw-Hill, New Delhi, **1990**.

References

1. R. K. Prasad. *Quantum Chemistry through problems and Solutions*, New Age International Publishers- New Delhi. **1997**.
2. R.P. Rastogi and V.K. Srivastava.*An Introduction to Quantum Mechanics of Chemical Systems*.Oxford&: IBH Publishing Co.. New Delhi_ **1986**,
3. R.L. Flurry. Jr. *Symmetry Group Theory and Chemical Applications.*PrenticeHall.Inc.. **1980**.
4. P.W. Atkins and J. de Paula. Atkins' *Physical Chemistry*, VII ed. Oxford University Press. **2002**.
5. J. M. Hollas, *Symmetry in Molecues*, Chapman and Hall, London,**1972**.
6. H. Eyring, J. Walter and E. Kimball, *Quantum Chemistry*, Wiley International Edition, John Wiley, London, **1989**.
7. W. J Moore, *Physical Chemistry,* Longman, 5th ed., London, **1974**.
8. G. W. Castellan, *Physical Chemistry,* Addison-Wesley, 4th ed., London, **1996**.

CH 1815: ANALYTICAL CHEMISTRY	
Semester: I	Credits: 4
Category: Major core (MC)	No. of hrs: 60 (5 hrs/wk)

Objectives:

1. *To understand the concepts of data analysis.*
2. *To learn the basic analytical methods and to have a sound knowledge of chemistry involved in an chemical analysis.*
3. *To know the principle and instrumentation of different analytical techniques.*

Unit-1: Data analysis (10 hrs)

1.1 *Errors*: Precision and accuracy, Classification of errors, minimisation or elimination of errors.

1.2 *Statistical methods*: Treatment of random errors, reliability of results, rounding up of results from chemical computation, confidence interval, comparison of results-students t-test, F-test and linear regression for deriving calibration plots.

Self Study: Normal error curve and its importance.

Unit-2: Chromatography (10 hrs)

Principle and instrumentation of

2.1 Gas chromatography: carrier gas, columns, detectors- hot-wire detector, flame ionisation detector, photo ionisation detector and ECD. Determination of C,H,N and S.

2.2 HPLC: Column, solvent delivery system, sample injections, Detectors. Advantages of HPLC. Applications of HPLC in the separation of cations, and lipids. Elementary concepts of UPLC.

2.3 Electrophoresis and capillary electrophoresis.

Self Study: Principle of paper, TLC and column chromatography.

Unit-3: Titrimetric methods of analysis (10 hrs)

3.1 Difference between titrimetic and volumetric analysis, Principle and reactions involved in acid-base, redox, complexometric and precipitation titrations, Different methods of expressing concentration terms, calculations involving stoichiometry- acid base and redox systems.

3.2 Acid-base titrations in nonaqueous solvents: Principle, Properties – acidic and basic properties, autoprotolysis constant of solvents, dielectric constant and its effect on solvent behaviour. Detection of equivalence point – titrations in ethylene diamine, glaciel acetic acid, methanol and ethanol.

Unit-4: Thermal and electroanalytical methods (15 hrs)

4.1 *Thermogravimetry*: Principle, factors affecting thermogram, instrumentation and thermal decomposition of $CaC_2O_4.H_2O$ and $CuSO_4 .5H_2O$. Differential techniques: Instrumentation, experimental, instrumental factors of DTA. Thermal behaviour of $CuSO_4 .5H_2O$ by DTA. Principle and determination of purity of pharmaceuticals, phase transition studies by DSC.

4.2 *Electrogravimetry*: Principle, instrumentation, deposition and separation. Electrolysis at constant current and estimation of copper.

4.3 *Coulometry*: controlled potential coulometry, Principle and separation of nickel and cobalt, coulometric titration, instrumentation - Estimation of Sb(III).

4.4 *Potentiometry*: Potentiometric titration, equivalence point potential for (i) Fe^{2+}/ Fe^{3+}- Ce^{3+}/Ce^{4+} system (ii) Fe^{2+}/ Fe^{3+}- $MnO_4^-,H^+/Mn^{2+}$ system, determination of concentration of the species at the equivalence point. Ion selective electrodes, coated/modified electrodes, Biochemical electrodes. Solid state ion selective detectors.

4.5 *Voltammetry*: D.C and A.C. polarography, principle, Ilkovich equation, instrumentation, role of supporting electrolyte, polarographic maximum. cyclic voltammetry, anodic and cathodic stripping voltammetry.

Unit-5: Spectrometry (15 hrs)

5.1 *Spectrophotometry*: Beer Lambert 's law , spectrophotometric titrations, determination of Fe (III) with EDTA and determination of Fe (III) in the presence of aluminium.

5.2 *Atomic Absorption Spectroscopy*: Principle, instrumentation- Burner, furnace, resonance line source, detectors. Spectral and chemical interferences, determination of alkali metals in blood serum, Determination of lead in petrol. Principle of Inductively coupled plasma (ICP).

5.3 *Flame Spectrometry*: Principle, instrumentation and interferences, determination of alkali metals, Determination of iron in non-ferrous alloys.

5.4 *Turbidimetry*: Principle, instrumentation - determination of sulphate and phosphate

5.5 *Fluorimetry*: Principle, relationship between excitation spectra and fluorescence spectra, factors affecting fluorescence emission, determination of quinine in tonic water and determination of codeine and morphine in a mixture.

Text Books:

1. Douglas A. Skoog, Donald M. West and F. James Holler, Fundamentals of analytical Chemistry, Harcourt Asia Pvt. Ltd., **2001**.
2. R.A. Day, Jr. and A.L. Underwood, Prentice-Hall of India, **2001**.
3. H. Kaur, Instrumental methods of chemical analysis, Pragati Prakashan Publishers, **2003**.
4. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, Longman Scientific and Technical, **1989**.

References:

1. D. A. Skoog, D.M. West and F. J. Holler, *Analytical Chemistry An Introduction*. Saunders College Publishers, **1990**.

2. J. Mendham, R.C. Denney, J.D. Barnes and M. Thomas, *Vogel's Text book of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd.. **2004**.

3. J.G. Dick, *Analytical Chemistry.* Sir George Williams University. McGraw-Hill Book Company, New. York. **1973**.

4. H.H. Willard, L.L. Merritt, J.A. Dean and F.A. Seattle, *Instrumental methods of analysis,* 5th Ed., Harcourt Asia Pvt. Ltd., India, 2001.

CH 1816: ORGANIC LABORATORY TECHNIQUES-I

Semester : I	Credits : 2
Category : Major core (**MC**)	No. of Hours : 50 (4 hrs/wk)

Objective:

To develop analytical skill in (i) separation of organic mixture (ii) organic qualitative analysis and (iii) organic preparations involving two or three stages.

1. **Separation and analysis**: Two component mixtures
2. **Preparations**: Two or three stage processes involving nitration, halogenation, diazotization, rearrangement, hydrolysis, reduction, alkylation and oxidation

A. Two stage preparations

a) p-Bromoacetanilide from Aniline

b) p-Nitroaniline from Acetanilide

c) 1,3,5-Tribromobenzene from Aniline

d) Acetyl salicyclic acid from Methyl salicylate

e) Benzilic acid from Benzoin

f) m-Nitroaniline from Nitrobenzene

g) β-Naphthol from Naphthalene

B. Three stage preparations

a) 1-Bromo-2-(bromomethyl)naphthalene

b) Sulphanilamide from acetanilide

Text books

1. N.S. Gnanapragasam and G. Ramamurthy, *Organic Chemistry – Lab manual*, S. Viswanathan Co. Pvt. Ltd, **1998**.
2. J.N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, S. Chand and Co., 1987

References

3. Vogel's *Text book of Practical Organic Chemistry*, 4th Edition, ELBS/Longman, England, **1984**.

CH 1817: INORGANIC QUANTITATIVE ANALYSIS AND PREPARATIONS

Semester: I — Credits: 2
Category: Major core (MC) — No. of hrs: 50 (4 hrs/wk)

Objectives

1. *To impart the skill in quantitative estimation of metal ions by colorimetric methods and complexometric titration.*
2. *To identify the methodology to quantitaively separate and estimate mixture of metal ions.*
3. *To identify the methodology to estimate a metal ion in the presence of another metal ion.*
4. *To improve the skill in preparations of metal complexes.*

1. Colorimetry (visual**)**

1.1 Estimation of iron

1.2 Estimation of nickel

2. Complexometric Titration

2.1 Estimation of zinc, nickel, aluminium, and calcium.

2.2 Estimation of mixture of metal ions-pH control, masking and demasking agents.

2.3 Determination of calcium and lead in a mixture (pH control)

2.4 Determination of manganese in the presence of iron

2.5 Determination of nickel in the presence of iron

3. Gravimetry and Titrimetry

3.1 Determination of nickel by gravimetry and copper by titrimetry in a mixture.

3.2 Determination of barium by gravimetry and calcium by complexometry in a mixture.

4. Preparations and estimation of one metal ion in one experiment:

4.1 Potassium tris(oxalato)ferrate(III)

4.2 Hexaamminenickel(II) tetrafluoroborate

4.3 Potassium tetrachlorocuprate(II)

4.4 Tris(thiourea)(sulfato)zinc(II).

Text book

1. G.H.Jeffery, J.Bassett, J.Mendham and R.C.Denney, *Vogel's Textbook of Quantitative Chemical Analysis*; 5th ed., ELBS, **1989**.

References

1.J.D.Woollins, *Inorganic Experiments*; VCH: Weinheim, **1994**.

2. G.Pass, and H.Sutcliffe, *Practical Inorganic Chemistry*; Chapman Hall, **1965**.

3. W.G.Palmer, *Experimental Inorganic Chemistry*; Cambridge University Press, **1954**.

CH 2819: ORGANIC REACTION MECHANISMS AND HETEROCYCLICS

Semester : II | Credits : 4

Category : Major core (**MC**) | No. of hrs: 60 (5 hrs/wk)

Objectives:

1. *To understand the mechanism of organic chemical reactions.*
2. *To appreciate the concept of substitution, addition and elimination reactions and their reaction mechanisms.*
3. *To comprehend the importance of heterocyclic compounds.*

Unit-1: Aromatic and Aliphatic Electrophilic Substitution (15 hrs)

1.1 Aromaticity of non-benzenoid and heterocyclic compounds - Aromatic electrophilic substitution: Mechanism, orientation and reactivity - Quantitative treatment of reactivity in the substrates and reactivity of the electrophiles. Selectivity relationship: Hammett and Taft equations, the effect of the leaving group, Linear Free energy relationship.

1.2 Reactions involving a) Nitrogen electrophiles: nitration, nitrosation and diazonium coupling b) Sulphur electrophiles: sulphonation c) Halogen electrophiles: chlorination and bromination d) Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

1.3 *Aliphatic substitution Mechanisms*: S_E2 and S_Ei, S_E1; Substitution by double bond shifts; other mechanism: addition-elimination and cyclic mechanism.

1.4 *Hydrogen as electrophile*: (a) Hydrogen exchange; hydro-dehydrogenation; keto-enol tautomerism. b) Halogen electrophiles: Halogenation of aldehydes and ketones; carboxylic acids c) Nitrogen electrophiles: aliphatic diazonium coupling; direct formation of diazo compounds; direct amination; insertion by nitrenes. d) sulphur electrophiles: sulphonation, sulphenylation. e) carbon electrophiles: acylation; alkoxy carbonyl alkylation; alkylation; Stork-enamine reaction; insertion by carbene.

Self study:

Kolbe-Schmitt reaction, amidation with isocyanates, hydroxyalkylation, haloalkylation. Metal electrophiles, cleavage of alkoxides.

Unit-2: Aromatic and Aliphatic Nucleophilic Substitution (15 hrs)

2.1 *Mechanisms*: S_NAr, S_N1 and Benzyne mechanisms. - Reactivity, Effect of structure, leaving group and attacking nucleophile.

2.2 *Reactions*: O and S-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet-Hauser and Smiles rearrangements.

2.3 S_N1, ion pair, S_N2 and neighbouring group mechanisms. Nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon.

2.4 Reactivity: Effect of substrate, attacking nucleophile, leaving group and the medium - Swain-Scott, Grunwald-Winstein relationship - Ambident nucleophiles

Self study:

Hydrolysis of alkyl halides, acyl halides, anhydrides, carboxylic esters and amides. Goldberg and Rosenmund-von Braun reactions, Stephens-Castro coupling.

Unit-3: Elimination and Free Radical Reactions (10 hrs)

3.1 E2, E1, E1cB and E2C mechanisms. - Syn eliminations - E1-E2-E1cB spectrum. Orientation of the double bond: Hoffmann and Saytzeff rules
Reactivity: Effect of substrate, attacking bases, leaving group and medium. Mechanisms and orientation in pyrolytic eliminations.

3.2 Long Lived and short lived radicals - Detection of radicals and characteristics of free radical reactions and free radical rearrangements.
Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

Self study:

Chugaev reaction, Hofmann degradation, Cope elimination, Bamford-Stevens reaction, epi-oxy elimination and Sandmeyer reactions.

Unit-4: Addition to Carbon Multiple Bonds (10 hrs)

4.1 Mechanism: Electrophilic, nucleophilic, free radical addition.
4.2 Orientation and Reactivity: Stereochemical orientation, addition to cyclopropane rings.
4.3 Reactions: Addition to double and triple bonds.
4.4 Carbenes and their addition to double bonds.
4.5 Stereochemical aspects of addition reactions.

Self study:

Stork-Eschenmoser hypothesis, Nazarov cyclization, Michael and Koch reactions. Mechanistic study with specific examples, factors influencing addition reaction.

Unit-5: Heterocyclic Chemistry (10 hrs)

5.1 Nomenclature, reactivity, aromaticity, spectral properties.
5.2 Synthesis and reactions of indole, isoindole oxazole, imidazole, thiazole, pyridines, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid and xanthines.

Self study:

Synthesis and reactions of five membered (pyrrole, thiophene, furan) and six membered heterocyclic compounds (pyridine), fused rings (quinoline and isoquinoline)

Text books

1. J. March and M Smith, *Advanced Organic Chemistry*, 5th edn, John-Wiley and sons, 2001.
2. I. L. Finar, *Organic Chemistry* Vol-2, 5th edn, Pearson Education Asia, 1975.
3. I. L. Finar, *Organic Chemistry* Vol-1, 6th edn, Pearson Education Asia, 2004.
4. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Part A and B, 4th edn, Kluwer Academic/Plenum Publishers, 2000.

References

1. S. H. Pine, *Organic Chemistry*, 5th edn, McGraw Hill International Edn, 1987.
2. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
3. E.S. Gould, *Mechanism and structure in organic chemistry*, Holt, Rinehart and Winston Inc., 1959.
4. T. L. Gilchrist, *Heterocyclic Chemistry*, Longman Press, 1989.
5. J. A. Joule and K. Mills, Heterocyclic Chemistry, 4th Edn, John-Wiley, 2010.

CH 2820: MAIN GROUP ELEMENTS AND NUCLEAR CHEMSITRY

Semester : II **Credits : 4**

Category : Major Core (MC) **No. of Hours : 50 (4 hrs/wk)**

Objectives

1. To know the structure and bonding in inorganic chains, rings, and cages.
2. To identify ligands of main group elements and complexing agents for main group metals.
3. To identify specific reagents of main-group elements used in synthesis.
4. To understand theory of radioactivity and applications of radioisotopes.
5. To know the working principle and safety features of nuclear reactors.

Unit-1: Inorganic chains, rings, and cages (20 hrs)

1.1 Catenation and heterocatenation: ; Allotropes of carbon, graphite, diamond, fullerenes and carbon nanotubes. Heterocatenation - by coupling cyclic silicon and phosphorous compounds.

1.2 Alkali and alkaline earth metal complexes: complexes of β-diketones, crown ethers, cryptands, and calixarenes; biological roles of alkali and alkaline earth metal ions and ionophores.

1.3 Electron defficient, electron precise, and electron rich compounds: Boranes and carboranes: synthesis of neutral boron hydrides, polyhedral borane anions and dianions, structure of polyhedral boranes-*nido*-, *arachno*-, and *closo*-frameworks, PSEPT (Wade's rules) and polyhedral geometries; carboranes-synthesis and polyhedral geometries, metalloboranes, and metallocarboranes. Silanes and cyclopolysilanes, hydrometallation-hydroboration and hydrosilylation. Hydroboration reaction as precursor for metalloborane and heteroborane clusters.

1.4 Boron-nitrogen compounds: azaboranes, pyrazaboles, borazines, and B-N clusters.

1.5 Silicates: classification-orthosilicates, noncyclic silicate anions, cyclic silicate anions, infinite chain anions, infinite sheet anions, framework minerals, and zeolites-typical examples and structure, cyclic siloxanes

1.6 Poly acids: structure of isopoly and heteropoly anions and polycations of W and Mo.

1.7 P-N and P-S compounds: polyphosphazene, cyclophosphazenes, and cyclic aminophosphanes, phosphorus-oxide and phosphorus-sulfide cages.

1.8 Cyclic sulfur-nitrogen compounds: tetrasulfur-tetranitride, polythiazyl, and S_xN_y compounds.

Self study.

(a) Synthesis and uses of polyanions and cations.
(b) Natural and synthetic zeolites and application of zeolites as catalysts.

Unit-2: Main group organometallics and reagents and synthesis (10 hrs)

2.1 Organometalics of Li, Be, and Mg: synthesis and applications.

2.2 Organometalics of Si and Al: silsesquioxanes, aryl- and alkyl silicon halides, aluminium alkyls.

2.3 Specific reagents of main-group elements: fluorinating agents-ClF, ClF_3, and BrF_3 (harsh); SF_4, SbF_3, and SbF_5 (moderate) and organometal reagents-Grignard reagents, organolithium, diorganomercury, and diorganomagnesium.

Self study

(a) Special techniques for the synthesis of inorganic compounds: the chemical vacuum line, plasmas, photochemical apparatus, and electrolysis.
(b) Synthetic importance of diborane, boranes, PCl_3, and silylating agents.
(c) Illustrative examples of N and P ligands.

Unit-3:Halogen and noble gas chemistry (10 hrs)

3.1 Halogen oxides and oxo compounds: Dichlorine monoxide, chlorine dioxide, dibromine monoxide, and iodine pentoxide-preparation and properties; halogen oxyfluorides trioxohalofluorides) and ionic oxyhalogen species.
3.2 Xenon oxides and fluorides: Xenon trioxide, difluoride, tetrafluoride, xenon oxofluoride.
3.3 Halogen compounds of nitrogen: nitrogen trifluoride, tetrafluorohydrazine, dinitrogen difluoride, haloamines, oxohalides, and nitrogen trifluoride oxide.
3.4 Sulfur fluorides: Synthesis and reactivity of disulfur difluoride, sulfur tetrafluoride, substituted sulfur fluorides.

Self study

(a) Structure of halogen oxides and halogen oxo compounds with the aid of VSEPR model.
(b) Reactivity of the halides of N, S, and Xe and applications.

Unit-4: Radiochemistry (5 hrs)

4.1 The nucleus: Structure of nucleus, quadrupolar nucleus, factors affecting nuclear stability binding energy per nucleon, *n/p* ratio, magic number, odd-even rule. - nuclear models-liquid drop model, shell model, collective model,
4.2 Radiochemistry: Natural and induced radioactivity; radioactive decay-α-decay, β-decay, ν-decay; neutron emission, positron emission, electron capture; Geiger-Nattal rule, radioactive displacement law, radioactive series.
4.3 Measurement of radioactivity: ionization chamber, GM counters, scintillation counters.

Self study

(a) Types of nuclei-isotopes, isotones, isobars, nuclear isomers. Radioactive isotopes and radioactive decay series.
(b) Half life period, lifetime, decay constant -relationship between them.

Unit-5: Nuclear Reactions (5 hrs)

5.1 Types of nuclear reactions: Spallation, fusion-hydrogen bomb, stellar energy, nuclear fission-theory of nuclear fission; chain reaction, nuclear cross section,, critical mass; atom bombs, nuclear fission reactors, breeder reactors - fuels used in nuclear reactors, moderators, coolants; nuclear fusion; separation of isotopes, nuclear reactors in India.
5.3 Reprocessing of spent fuels: Nuclear waste streams from nuclear reactors, sequestering agents for radioisotopes, solvent extraction, ionic liquid technology.

5.4 Applications: Dating of objects-principles and applications, neutron activation analysis, isotopic dilution and labeling studies, nuclear medicine-^{99m}Tc radiopharmaceuticals.

Self study

(a) Isotopes used in nuclear fission reactions.
(b) Radioisotopes used in noninvasive imaging techniques in nuclear medicine.

Text books

1. F.A.Cotton, G. Wilkinson,C.A. Murillo and M.Bochmann, *Advanced Inorganic Chemistry*; 6th ed.; Wiley Interscience: New York, **1988**.
2. J. E.Huheey, E.A.Keiter and R.L.Keiter, *Inorganic Chemistry*; 4th ed.; Harper and Row: New York, **1983**.
3. D.F. Shriver, P.W. Atkins and C.H. Langford,. *Inorganic Chemistry*; 3rd ed.; Oxford University Press: London, **2001**.
4. K.F.Purcell and J.C. Kotz, *Inorganic Chemistry*; Saunders: Philadelphia, **1976**.

References

1. T.Moeller, *Inorganic Chemistry, A Modern Introduction*; John Wiley: New York, **1982**.
2. H.J.Arnikar, *Essentials of Nuclear Chemistry*, 4th ed., New Age International, New Delhi, **1995**.
3. A.K.Srivatsava,and P.Jain, P. *Essential of Nuclear Chemistry*, S. Chand, New Delhi, **1989**.
4. G. Friedlander, G.; Kennedy, W.and J.M. Miller *Nuclear and Radiochemistry*; 2nd ed.; John Wiley and& Sons Inc., **1964**.

5. S. Glasstone, . *Source Book on Atomic Energy*; 2nd ed.; Van Nostrand Co. Inc., New Jersey, **1958**.

CH 2821 MOLECULAR SPECTROSCOPY

Semester: II | Credits : 4

Category: Major Core (**MC**) | No. of Hours : 60 (5 hrs/wk)

Objectives:

1. To learn the quantization of energy and interaction of electromagnetic radiation with matter.

2. To understand the fundamentals of different branches of spectroscopy.

3. To elucidate the structures of molecules using different spectral techniques.

Unit-1: Rotational and Vibrational Spectroscopy (15 hrs)

1.1.*Diatomic molecules as rigid rotors:* intensity of spectral lines, selection rules, effect of isotopic substitution. *Diatomic molecules as non-rigid rotors:* centrifugal distortion constant, rotational spectra of linear and symmetric top polyatomic molecules.

1.2.*Vibrating diatomic molecule:* energy of diatomic molecules, simple harmonic oscillator-energy levels, transitions, selection rules. Anharmomic oscillator - energy levels, selection rules. Diatomic vibrating rotator - P, Q, R branches.

1.3.*Vibrations of polyatomic molecules:* Symmetry and fundamental vibrations, overtones, combination, difference bands. Influence of rotations on the spectra of polyatomic molecules - parallel and perpendicular vibrations in linear and symmetric top molecules.

1.4.*Interpretation of IR spectra of organic and inorganic compounds*: Frequencies of various functional groups containing oxygen , nitrogen and hydrocarbons. Factors affecting the fundamental vibrational frequencies. Linkage, geometrical isomers, coordinated and lattice water. NO_3^-, ClO_3^-, ClO_4^-, and SO_4^{2-}.

1.5.*Raman Effect:* Rayleigh and Raman scattering, Stokes' and anti-Stokes' radiation, molecular polarizability, selection rules.

1.6.*Raman spectra:* Rotational Raman spectra - linear molecules, symmetric top and spherical top molecules. Vibrational Raman spectra - symmetry and Raman active vibrations, rule of mutual exclusion. Rotational fine structure. Structure determination from Raman and Infra-red.

Unit 2: Electronic spectroscopy (9 hrs)

2.1.*Electronic spectra of diatomic molecules:* Born-Oppenheimer approximation, Franck-Condon Principle, selection rules, intensity of electronic transition, vibronic coupling, types of electronic transitions.

2.2.*Characterization of organic compounds:* application of Woodward-Fieser rules to conjugated dienes, α,β - unsaturated carbonyl compounds, benzene and its substituted derivatives, polycyclic aromatic hydrocarbons, polyenes, poly-ynes, and heterocyclic compounds.

2.3.*Charge transfer transitions:* intensity, electronic spectra of charge transfer complexes of organic compounds, charge transfer transitions in inorganic and coordination compounds.

2.4.*Photoelectron spectroscopy (PES):* principle of PES and ESCA.

Unit-3: Mass spectroscopy (6 hrs)

3.1. *Determination of molecular formula*: molecular ion, nitrogen rule, isotope peaks, metastable ions, Mc Lafferty rearrangement, Retro Diels Alder reaction.

3.2.*Fragmentation:* Basic fragmentation types and rules, Fragmentation patterns of hydrocarbons, oxygen and nitrogen containing organic compounds and carbonyl compounds.

Unit-4 : Magnetic Resonance Spectroscopy (NMR and EPR) (20 hrs)

4.1 Theory of NMR spectroscopy: nuclear spin, magnetic nuclei, nuclear magnetic moment, NMR transition, Bloch equations, relaxation mechanisms.

4.2 Parameters of NMR: chemical shift, shielding and deshielding, factors affecting chemical shift-inductive effect, anisotropy, hydrogen bond. Region of proton chemical shift in organic molecules, chemical shift equivalence and magnetic equivalence. NMR of paramagnetic compounds: Shift reagents in NMR.

4.3 Spin-spin splitting: mechanism of spin-spin splitting, application of spin-spin splitting to structure determination. Coupling constants: mechanism of coupling, geminal coupling, vicinal coupling, variation of coupling constants with bond angle, dihedral angle, ring size, hetero atom. Long-range coupling, aromatic coupling, virtual coupling.

4.4 FT and 2D NMR spectroscopy: principle of FT-NMR, FID. Introduction of 2D techniques: COSY and HeteroCOSY. ^{13}C, ^{19}F, ^{31}P NMR- spectra of typical examples.

4.5 Electron paramagnetic resonance spectroscopy: theory of EPR, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems.

4.6 *EPR spectra of anisotropic systems:* anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupolenucleii. EPR spectra of systems with more than one unpaired electrons: Zero-field splitting, causes of ZFS, ZFS and EPR transitions. EPR of triplet naphthalene, copper salen complex and high-spin Mn(II) complexes.

4.7 Structural elucidation of organic compounds by combined spectral techniques.

Unit-5: NQR and Mossbauer Spectroscopy (10 hrs)

5.1 *Principle of NQR spectroscopy*: nuclear charge distribution and quadrupole moment, quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, asymmetry parameter, quadrupole energy levels, transitions in spherical and axially symmetric fields, effect of magnetic field.

5.2 *Applications of NQR spectroscopy*: quadrupole coupling constant and its interpretation, structural information from NQR spectra of haloorganic compounds and complexes, point group symmetry, phase transitions, chemical bonding and hydrogen bonding.

5.3 *Principle of Mössbauer spectroscopy*: Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mössbauer spectra of high and low-spin Fe and Sn compounds.

Text books

1. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th ed., Tata McGraw Hill, New Delhi, **2000**.
2. R. M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th ed., John Wiley & Sons, New York, **2003**.
3. W. Kemp, *Applications of Spectroscopy*, English Language Book Society, **1987**.
4. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*.
5. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry,* 4th ed., Tata McGraw-Hill Publishing Company, New Delhi, **1988**.
6. D. Pavia, G. M. Lampman, and G.S. Kriz , *Introduction to Spectroscopy*, 3rd ed., John Vondeling, Florida, **2006**.
7. K. V. Raman, R. Gopalan and P. S. Raghavan, *Molecular Spectroscopy*, Thomson and Vijay Nicole, Singapore, **2004**.

8.R. S. Drago, *PhysicaI Methods in Chemistry*; Saunders: Philadelphia, **1977**.

References

1. P. Atkins and J. de Paula, *Physical Chemistry*, 7th ed., Oxford University Press, Oxford, **2002**.
2. I. N. Levine, *Molecular Spectroscopy*, John Wiley & Sons, New York, **1974**.
3. A. Rahman, *Nuclear Magnetic Resonance-Basic Principles*, Springer-Verlag, New York, **1986**.

4. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and coordination Compounds*, Part B: 5th ed., John Wiley& Sons Inc., New York, **1997**.
5. J. A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance*; Wiley Interscience: **1994**.
6. L.D. Field, S. Sternhell, and J. R. Kalman, *Organic Structures from Spectra*, 3rd ed., John Wiley & Sons Ltd England, **2003**.
7. J. W. Akitt, *NMR and Chemistry*, 3rd., ed Chapman & Hall, London,**1992**.
8. Jack K. Becconsall *Basic ond and two dimensional NMR Spectroscopy*, 4th., ed, Wiley – VCH, **2005**.
9. R. V. Parish, *NMR, NQR, EPR, and Mossbauer Spectroscopy in inorganic chemistry*, Ellis Horwood, London.
10. G. M. Bancroft, *Mössbauer spectroscopy*, Mc Graw Hill, London, 1973.

CH 2822 : ORGANIC LABORATORY TECHNIQUES -II

Semester: II	**Credits: 3**
Category: Major Core (MC)	**No. of Hours: 50 (4 Hrs/Wk)**

Objectives:

1. *To develop analytical skill in organic quantitative analysis*
2. *To understand the techniques involved in estimations of organic compounds.*

Unit 1: Estimations

a) Phenol and aniline
b) Ketones (ethyl methyl ketone)
c) Sugars (Glucose)
d) Ascorbic acid (Vitamin-C tablets)
e) Amino groups (aniline)
f) Nitro groups (aromatic nitro compounds)
g) Amino acids (Glycine)

Unit 2: Extraction and estimation

a) Caeffine from coffee
b) Nicotine from tobacco leaves
c) Citric acid from citrus fruits

Unit 3: Separation of components of a mixture (Demonstration)

a) Thin layer chromatography
b) Column chromatography
c) Paper chromatography.

Text Books

1. N. S. Gnanapragasam and G. Ramamurthy, *Organic Chemistry – Lab manual*, S. Viswanathan Co. Pvt. Ltd, 1998.
2. J. N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, S. Chand and Co., 1987

Reference

1. Vogel's *Text book of Practical Organic Chemistry*, 4th Edn, ELBS/Longman, England, 1984.

CH 2823 : INORGANIC SEMIMICRO QUALITATIVE ANALYSIS

Semester: II | Credits: 3

Category: Major Core (**MC**) | No. of Hours: 50 (4 hrs/wk)

Objectives

1. *To study the principle of distribution of common and rare metal ions in diffferent groups.*
2. *To know the inter- and intra group precipitation and separation of metal ions.*
3. *To improve the skill in the qualitative analysis of rare metal ions in different groups.*
4. *To identify the methodology to analyse a metal ion in the presence of another metal ion.*

1. Theoretical Principles

1.1 Classification of cations into groups, group reagents

1.2 Inter group and intragroup separations

1.3 Confirmatory test for cations -the reaction and the product

2. Analysis of mixture of cations

Analysis of a mixture of four cations containing two common and two rare cations.

Rare cations:

Group-I: W and Tl

Group-II: Se, Te and Mo

Group-III: Tl, Ce, Th, Zr, V and Cr.

Group-VI : Li and Na

Text Books

1. V. V. Ramanujam, *Inorganic Semimicro Qualitative Analysis*; 3rd ed., The National Publishing Company, Chennai, **1974**.
2. *Vogel's Text book of Inorganic Qualitative Analysis,* 4th Ed, ELBS, London, **1974**.

CH 2955: BIO-ORGANIC CHEMISTRY

Semester : II | Credits : 3

Category : Subject Elective (**SE**) | No. of hrs / wk: 50(4 Hrs/Wk)

Objectives:

1. *To enable the student to understand and appreciate the importance of biomolecules.*
2. *To understand the techniques involved in the extraction and methods of determination of structure of natural products.*

Unit - 1: Carbohydrates **(**10hrs**)**

1.1 Configuration and conformations of monosaccharides, anomeric effect, epimerization and mutarotation. Determination of ring size of monosaccharides.

1.2 Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose and maltose.

1.3 Industrial and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, cytosine, crysin.

1.4 Glycolysis and its reversal; TCA cycle. Relation between glycolysis and respiration.

Unit - 2: Proteins and nucleic acids **(**12hrs**)**

2.1 Classification – properties - 3D structure of protein; Determination of C and N-terminal amino acid sequence – denaturation and renaturation of proteins.

2.2 Separation and purification of proteins – dialysis – gel filtration - electrophoresis.

2.3 Catabolism of amino acids: transamination, oxidative deamination, decarboxylation and urea cycle.

2.4 Introduction, structure and synthesis of nucleosides and nucleotides, protecting groupsforhydroxy group in sugar, amino group in the base and phosphate functions.

2.5 Methods of formation of internucleotide bonds: Structure of RNA and DNA, Crick-Watson model.

2.6 Solid phase synthesis of oligonucleotides. Role of nucleic acids in the biosynthesis of proteins.

Unit - 3: Alkaloids and terpenoids **(**10hrs**)**

3.1 General methods of structural elucidation of alkaloids.

3.2 Structural elucidation of papaverine and cocaine; synthesis and functions of atropine, heptaphylline, morphine.

3.3 General methods of determination of structure of terpenoids.

3.4 Structural elucidation of cadinene, vitamin A, abietic acid; synthesis and functions of gibberelic acid, zingiberine and squalene

Unit 4: Steroids (10hrs)

4.1 Conformations of stereoids - molecular rearrangements (acid, base catalysed, and photochemical).

4.2 Synthesis of steroids – ring forming reaction and control of ring junction stereochemistry.

4.3 Synthesis and functions of cholesterol, androgens, oestrone, progesterone and cortisone.

Unit - 5: Anthocyanins and flavonoids **(**8hrs)

5.1 General nature and structure of anthocyanins.

5.2 General methods of synthesizing anthocyanidins.
5.3 Structural elucidation of cyanidin chloride, pelargolidin chloride, Hirsutidin chloride.
5.4 Flavones – flavonols – isoflavones.
5.5 Biosynthesis of flavonoids.

Text books

1. T. K Lindhorst, *Essentials of Carbohydrate Chemistry and Biochemistry*, Wiley VCH, **2007**.
2. G. K. Chatwal, *Organic Chemistry on Natural Products,* Vol. 1, Himalaya Publishing House, Mumbai, **2009**.
3. G. K. Chatwal, *Organic Chemistry on Natural Products, Vol. 2*, Himalaya Publishing House, Mumbai, **2009**.
4. O. P. Agarwal, *Chemistry of Organic Natural Products, Vol. 1,* Goel Publishing House, Meerut, **1997**.
5. O. P. Agarwal, *Chemistry of Organic Natural Products, Vol. 2,* Goel Publishing House, Meerut, **1997**.
6. I. L. *Finar, Organic Chemistry Vol-2, 5thedn, Pearson* Education Asia, **1975**.

References

1. I. L. Finar, *Organic Chemistry Vol-1, 6thedn*, Pearson Education Asia, **2004**.
2. Pelletier, *Chemistry of alkaloids*, Van Nostrand Reinhold Co, **2000**.
3. Shoppe, Chemistry of the steroids, Butterworthes, **1994**.

CH 2956 MEDICINAL CHEMISTRY

Semester: II	No. of Credits: 3
Category: SE (Subject Elective)	Total Hrs: 50 (4 hrs/wk)

Objectives:

1. *To understand the medicinal properties of various functional groups.*
2. *To learn the different types of drugs and their modes of action.*
3. *To learn drug design and structure activity relationship in terms of physico-chemical properties.*

Unit-1: Drugs – Introduction (10 hrs)

1.1 *Nature and sources of drugs*: Terms and terminology used in pharmaceutical chemistry. Classification and nomenclature of drugs, biological, chemical & trade name (commercial). Generic and proprietry drugs.

1.2 *Pharmaceutical aids:* Organic pharmaceutical aids. Preservatives, antioxidants, sesqustrants, emulsifying agents, colouring, flavouring and sweetening agent, stabilizing and suspending agents – ointment bases and related agents and solvents.

1.3 *Chemical structure and pharmacological activity:* Effects of some functional groups – unsaturation chain length, isomerism, halogens – amino group, nitro and nitrite compound – nitrite acidic group, aldehyhyde and ketone group, hydroxyl group, alkylsp. etc. Mechanism of drug action and metabolism of drugs-Chemical pathways and factors.

Self-Study:

a) *Different types of chemical poisons in environment* - Biological response to drugs.

b)*Blood-composition* of blood, blood grouping and matching, haematological agents-coagulants, anticoagulant drugs.Biochemical analysis of Urine, Serum, Blood Urea, Bile Pigment.

Unit-2: Drugs and Mode of Action (10 Hrs)

Pharmacological classification of drugs-

2.1 *Sulphanamides*: Properties, mechanism of action of sulpha drugs - Synthesis of sulphanilamide, Sulphadiazine, Sulphapyridine

2.2 *Anticovulsant agents*: – Hydantion, Barbiturates, Valium(Diazepan). Analgesics, antipyretic and anti-inflammatory agents – Narcotic analgesic: Morphine, Codine – Structure activity relationship of morphine – Synthetic analgesic – Pethadine, Benzomorphan, non-narcotic analgesics - Nalorphine, Aspirin

2.3 *Anaesthetics*: Local anaesthetics – Requisites – benzocaine, Procaine – Synthesis – Advantages & Disadvantages,

2.4 *Antiseptics & Disinfectants*: Distinction between antiseptics and disinfectants, standardisation phenol coefficient

2.5 *Antibiotics*: Classification based on the spectrum of biological action of antibiotics and the chemical structure. Penicillin, Streptomycine – Structure, properties, structure and activity relationship.

Self-Study:

a) Cancer and Antineoplastic drugs - drugs.

b) Diabetes and hypoglycemic drugs- chemical structure of insulin, hypoglycaemic agents.

Unit -3: Drug Designing (10Hrs)

3.1 Physicochemical properties evolved in the design, preparation of dosage forms. solubility and partition coefficients – cut-off point, Meyer Overton theory, Ferguson principle, bio-

activities, Hammett sigma values – steric factors partition coefficients π values – surface activity.

3.2 *Pharmacokinetics*: Close, dosage forms and routes to drug administration, factors influencing dosage and drug action –Tolerance. Pharmacokinetic factors – Administration, absorption, distribution, metabolism and excretion of drugs. Pharmacokinetics – drug plasma concentration, first-order and zero-order, kinetics. Volume of distribution (1/2), half-life (1/2), drug dosage, therapeutic drug monitoring.Pharmacodynamics-receptor binding, effects on the body, desired activity and undesirable effect.

3.3 *Quantitative Structure-Activity Relationship (QSAR):* Mathematical models, Linear Free Energy Relationships. Substituent effect analysis: mechanism of drug action, active site studies, drug design. LCAO – MO –SCF, Semi empirical and HMO methods and application of quantum chemistry to simple biological problems.

Self-Study:

a)chelation – importance of chelation in medicine, design of antibacterial and antifungal agents,

b) physiochemical properties involved in the design- Hydrogen ion concentration, pH and buffers. Colloidal state, membrane phenomena, osmosis, adsorption surface tension, viscosity, ionization constants,

Unit-4: Bioavailability of Drugs (15 hrs)

4.1 *Drug absorption and drug disposition*: Factors affecting drug absorption including physicochemical, biological and pharmaceuticals. Passive and active diffusion

4.2 *Bioavailability:*Factor affecting the drug bioavailability, rate of dissolution, pH and drug absorption, particle size, clinical application. Invivo-Invitro correlation of rate of dissolution.

4.3 *Drug release*: Drug delivery systems- oral controlled release. Commercially marketed oral osmotis systems (any four), sustained release of drugs. Mechanism of DDS entering the main stream – A brief survey of applications of pharmaco kinetic in clinical situations.

4.4 *Prodrugs and drug delivery system*: Ideal drug carriers, characteristic properties of carriers, types and utility of prodrugs, examples for - carrier linkages of various functional groups, ester, enol, phosphonate, mannich bases, sulphonamides producing site specificity, mechanism of prodrugs, activation of prodrugs for site specificity, antibody directed Abzyme prodrug therapy (ADAPT), antibody targeted chemotherapy, reversible redox drug delivery system to CNS.

4.5 Targeted delivery systems -macromolecular delivery systems, synthetic polymers, role of dendrimers , spacer and ampicillin, advantatages and disadvantages of macromolecules in DDS. Nano medicines -application of quantum dots and ligand targetted accumulation of liposomal DDS as diagnostic sensor in the treatment of cancer and nanonephrology.

Self-Study:

a) Storage of pharmaceutical substances – Capsule– hard gelatin capsules, soft gelatin capsules, encapsulation.

Unit-5: Screening and testing of drugs (5 hrs)

5.1 *Screening of drugs*- Principles of screening methods, clinical trial, screening methods for evaluation of anti- inflammatory, analgesics, antipyretics, antiulcer, anticonvulsants, antidiabetic, diuretic and drugs active on CNS.

5.2 Basic concept of quality assurance & requirement of GMP (WHO, USFDA, MHRA) ISO and ICH requirements of quality GLP Guidelines GCP

5.3 *Biological testing of drugs*: Testing drugs in vitro – enzyme inhibition, receptor studies, efficacy microbiological testing, screening & testing by NMR testing drugs in Vivo: test systems: drug potency therapeutic ratio.

Self study:

a) Registration of drugs for importing and manufacturing in India, DCCI and CDSCO.

b) Introduction to IND, NDA, ANDA for Registration in USA.

Test Books

1. J. Ghosh, *A Textbook of Pharmaceutical Chemistry*, New Delhi: S. Chand & Company, **1999**.
2. P. Parimoo, *A Textbook of Medical Chemistry*, New Delhi: CBS Publishers.**1995**.
3. S. Ramakrishnan, K. G. Prasannan and R. Rajan, *Textbook of Medical Biochemistry*, Hyderabad: Orient Longman. 3rd edition, **2001**.

References

1. F. S. K. Barar, *Essential of Pharmacotherapeutics*, New Delhi: S. Chand & Company, **2000**.
2. S. N. Pandeya and J. R. Dimmock, *An Introduction to Drug Design*, New Delhi: New Age International. 1997.
3. G. Patrick, *Medical Chemistry*, New Delhi: Viva Books, **2002**.
4. Richard B. Silverman. *The organic chemistry of drug design and drug action*, 2nd ed., Academic Press, **2004**.

CH 2957 CATALYSIS

Semester : II Credits: 3

Category: Subject elective (SE) No. of hrs: 50 (4hrs/wk)

Objectives:

1. To understand the basic concepts of catalysis
2. To know the different methods of catalysis
3. To learn the various techniques and mechanisms involved in catalysis.

Unit -1: Introduction to catalysis (7 hrs)

1.1 Activity, selectivity, promoters, stabilisers and poisons, Catalysts deactivation, Turn over number, inhibitors.

1.2 *Thermodynamic consideration in catalysis:* Energy factor , significance of activation parameters and application to kinetic systems.

1.3 Physical adsorption-Unimolecular adsorption- types of adsorption isotherms, Multimolecular adsorption-BET method, Harkins-Jura equation.

1.4 Chemisorption of gases on metals and oxides

Unit - 2 : Homogeneous and Heterogeneous Catalysis (12 hrs)

2.1 Acid-base catalytic reactions, protolytic and protropic mechanisms, activation energy of the processes, catalytic activity and acid-base strength, acidity functions: Hammett-Zucker treatments, linear free energy relationships.

2.2 Homogeneous catalysts for the polymerization of olefins, oxidative dehydrogenation, Ethyl benzene to styrene, Ziegler-Natta polymerization.

2.3 Partial oxidation: n- butane to maleic anhydride, propylene to acrolene, Fisher-Tropsch synthesis, catalytic reaction of cracking, shape selective catalysis: Zeolites-Alkylation of aniline with alcohols.

2.4 Catalysts for the production of petrochemicals- production of aromatics, para-xylene, cumene, linear alkylbenzenes and methanol.

2.5 Phase transfer catalysis – Rhodium water soluble catalyst systems with carboxylated and sulfonated phsphines for hydroformylation reactions.

Unit - 3: Photocatalysis and Electrocatalysis (10 hrs)

3.1 Thermal and photochemical reactions between H_2-Cl_2 and H_2-Br_2 and H_2- I_2 reactions, fluorescence, phosphorescence and quenching-Stern-Volmer equation.

3.2 Photocatalytic studies using non-stiochiometric oxides such as n-type and p-type semiconductors (TiO_2, ZnO, Cr_2O_3, doped and coupled semiconductors for the degradation of dyes)

3.3 Solar energy conversion, electrochemical cells, photoelectrolysis of water and photocatalytic reactions

3.4 Photocatalytic reduction of dinitrogen, photocatalysis for organic reactions-oxidation, reduction, polymerization, substitution and isomerization reaction using TiO_2.

Unit -4: Biocatalysis: Mechanism and Application (11 hrs)

4.1. *Mechanisms*: Covalent catalysis, acid-base and metal-ion catalysis, entropy and geometric effects, structural complementary of the active site to the transition state, prevention of the side reactions, the size of the enzymes

4.2 *Applications of enzymes in organic synthesis*: Oxidoreductase: Oxidation - Alcohols, epoxides, sulfoxides, amino acids, lactones, Oxidoreductase: Reduction-α-hydroxyamino acid, Transferase: Amino acids, amines.

Unit -5: Techniques in Catalysis (10 hrs)

5.1 Structural characterization-BET surface area method, pore volume, and pore size distribution-BJH method, t-plot method, XRD, SEM, TEM, AFM, STM, TPR and TPD

5.2 Special relevance to metal oxides with different structures

Text Books

1. B. Viswanathan, S. Sivasanker and A.V. Ramaswamy, *Catalysis*: *Principles and Applications*, Narosa Publishing House, New Delhi, **2004**

2. G.C. Bond, *Heterogeneous catalysis: Principles and applications*, Oxford University Press, Ely House, London W.I, **1974**.

References

1. V. Murugesan, A. Banumathi and M. Palanichamy, *Recent Trends in Catalysis*, Narosa Publishing House, New Delhi, **1999**
2. K.J. Laidler, *Chemical Kinetics*, Tata Mcgraw-Hill Publishing Company Ltd, New Delhi,**1973**
3. D.K. Chakrabarty, *Adsorption and Catalysis by solids*, Wiley Eastern Limited, New Delhi, **1991**.
4. J.M Thomas, W.J. Thomas, *Principles and practice of Heterogeneous Catalysis*, Wiley-VCH, New York, **1996**.