DEPARTMENT OF CHEMISTRY

M. Sc. Chemistry

P.G. PROGRAMME

SYLLABUS

Effective from the Academic Year 2012-2013

Loyola College (Autonomous)

Chennai- 600 034

LOYOLA COLLEGE (AUTONOMOUS)
CHENNAI - 600 034.

DEPARTMENT OF CHEMISTRY

M.Sc (*Chemistry*) Restructured Syllabus Effective from 2012-2013-CONTENTS

LOYOLA COLLEGE (AUTONOMOUS)
CHENNAI - 600 034.

M.Sc. (Chemistry) TEMPLATE: Effective from 2012-2013

Major Core (**MC**) h/Cr	Elective Subject (**ES**) h/Cr	Inter Disciplinary (**ID**) h/Cr	Self-study (SSP) h/Cr	Life skills Training (LST) h/Cr	Extension Activities	
812:OrgRxn.Mech&Stero. 5/4 **813**:Concpts in InorgChem5/4 **814**:Qunt.Chem.&Gp Theo5/4 **815**:Anal.Chem5/4	---	----	---	---	LEAP	
816:**Org. lab Tech-I4/2** **817**:**Inorg.QuantAna&Prep4/2** nar & Report2/--						
819:Org.RecMech&Hetero 5/4 **820**:MainGp&Nucl. Chem.4/4 **821**: Molecular Spec.5/4 **822**:**Org.lab Tech – II4/3** **823**:**Inorg.Se.mic.Qual.Anal4/3** **824**: Gen Trend in ApplChem (Seminar & Report)2/2	CH-**2955**:Bio Org.Chem (or) CH-**2956**: Med.Chem. (or) CH-**2957**:Catalysis 4/3	----	---	2h inside 2h outside* 2+2*/(2)	LEAP ----/(3)	**30** +
Summer Training Programme(3 To 4 Weeks)---/ (1)						
813: Coordn. Chem5/4 814:Therm& Chem. Kintics5/5 815: Sci. Res. Meth. 4/3 816: **Instr.methds of Anal. 4/3** nar& Report 2/--	CH-3951: Appl. Org.Chem (or) CH-3952:Chem.Nanomater (or) CH- 3953:Inorg PhotoChem 4/3	CH-3876:Mat Sci. 6/5	CH-..... One SSP paper (Outside Class Hours) ---/(2)	---	---	**3**
813: Org.Syn& Photo Chem5/4 4814: Electrochem. 6/5 **815: Project 17/13** 4816:Rec Trends in Chem (Seminar & Report) 2/2	---	---	---	---	---	
104/77	8/6	6/5	----/(2)	2+2*/(2+1)	---/(3)	**1**

Department of Chemistry

RESTRUCTURED SYLLABUS

M.Sc. (Chemistry)

(Effective from 2012-2013)

I-SEMESTER

CH-1812: ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY

Semester: I	No. of credits: 4
Category: Major Core (**MC**)	No. of hours: (5h/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 h)

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 (15h)

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. (15h)

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 h)

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 (20h)

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 disubstitutedcyclohexanes; 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 ed., 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*, 3rdedn, 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 ed., Pearson Education Asia, 1975
3. I. L. Finar, *Organic chemistry*, *Vol-1*, 6th ed., Pearson Education Asia, 2004
4. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part-A and B*, 4 thEdn, Kluwer Academic / Plenum Publishers. 2000.
5. S. H. Pine, *Organic Chemistry*, *5th ed.*, McGraw Hill International Ed., 1987.
6. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000.
7. D. Nasipuri, *Stereochemistry of Organic Compounds*, *2nd ed*,, New Age Publishers, 2005.

CH-1813: CONCEPTS IN INORGANIC CHEMISTRY

Semester: I — No. of credits: 4

Category: Major Core (**MC**) — No. of hours: (5 h/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 (12h)

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 (20h)

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-Landeequation, 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 hypotheticalcompounds from thermochemical calculations.

Unit-3: Covalent Bond (20h)

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 (12h)

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 (11h)

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 *Nonaqueous 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 GROUPTHEORY

Semester: I — No. of credits: 4

Category: Major Core (**MC**) — No. of hours:(5h/wk)

Objectives

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

Unit-1:Mathematics for Quantum Mechanicsand Postulates of Quantum Mechanics(12h)

1.1 *Coordinate systems*: Cartesian, spherical polar, cylindrical and elliptical coordinate systems

1.2 *Functions*: Real,complex, odd, even, orthogonal and normalized functions.

1.3. *Differential equations*: Order and degree. Solutions to typical differential equations.

1.4 *Operators*: linear, differential, Hermitian and Hamiltonian operators. Eigen functions and Eigen values

1.5 *Failure of classical mechanics*: Black body radiation, photo electric effect and Compton effect. The need for quantum mechanics.

1.6 Postulates of Quantum Mechanics and Schrodinger wave equation

Unit-2:Some Quantum mechanical models and their applications (15h)

2.1 *Particle in a box* (1Dand 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 QuantumMechanicsto Hydrogen and poly electron atoms (20h)

3.1 *Hydrogen atom and Hydrogen like ions*: Wave equation& solution to hydrogen andhydrogen likesystems .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-Trialwave functions. Variation 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.

Unit4: Molecular Quantum Mechanics and Chemical bonding (12h)

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 applications. (16h)

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

5.2 Matrix representations of symmetry operations. Reducible and irreducible representations.Classes of operations.

5.3 The *Great orthogonality theorem*:Reduction formula.Constructionof character tablefor C_{2v} and C_{3v} point groups.

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

Text books

1. N.Levine, *Quantum Chemistry*, 4thed., 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*. 2nded.,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*, 7thed., Oxford University Press,2002.
5. J. M. Hollas, *Symmetry in Molecules*, Chapman and Hall, London,1972.
6. H. Eyring, J. Walter and E. Kimball, *Quantum Chemistry*, Wiley International Ed, 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 — No. of credits: 4

Category: Major core (**MC**) — No. of hours: (5h/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 chemical analysis.*
3. *To know the principle and instrumentation of different analytical techniques.*

Unit-1: Data analysis (12h)

1.1 *Errors*: Precision and accuracy, Classification of errors, minimization 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 ofresults-students t-test, F-test

and linear regression for deriving calibration plots.Self Study: Normal error curve and its importance.

Unit-2: Chromatography (15h)

Principle and instrumentation of

2.1 Gas chromatography: carrier gas, columns, detectors- hot-wire detector, flame ionization detector, photo ionization 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 (15h)

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 non-aqueous solvents: Principle, Properties – acidic and basic properties, auto-protolysis constant of solvents, dielectric constant and its effect on solvent behaviour. Detection of equivalence point – titrations in ethylene diamine, glacial acetic acid, methanol and ethanol.

Unit-4: Thermal and electroanalytical methods **(**18h)

4.1 *Thermogravimetry*: Principle, factors affecting thermogram, instrumentation andthermal 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 andcobalt, 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+} (ii) Fe^{2+}/ Fe^{3+}- MnO_4^-,H^+/Mn^{2+} systems. 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 h)

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 ofalkali 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, *Analytical Chemistry*,Prentice-Hall of India, 2001.
3. H. Kaur, *Instrumental methods of chemical analysis*, PragatiPrakashan , 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*, SaundersCollege 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 BookCompany, 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 No. of credits: 2

Category: Major core (**MC**) No. of hours: (4 h/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

Reference

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

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CH-1817: INORGANIC QUANTITATIVE ANALYSIS AND PREPARATIONS

Semester: I | No. of credits: 2

Category: Major core (**MC**) | No. of hours: (4 h/wk)

Objectives

1. *To impart the skill in estimation of metal ions by colorimetric and complexometric methods.*
2. *To identify the methodology to estimate a metal ion in the presence of another metal ion.*
3. *To impart 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 books

1. G.H.Jeffery, J.Bassett, J.Mendham and R.C.Denney, *Vogel's Textbook of QuantitativeChemical Analysis*; 5th ed., ELBS, 1989.
2. J.D. Woollins, *Inorganic Experiments*; VCH: Weinheim, 1994

References

3. G.Pass, and H.Sutcliffe, *Practical Inorganic Chemistry*; Chapman Hall, 1965.
4. W.G.Palmer, Experimental *Inorganic Chemistry*; Cambridge University Press, 1954.

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II-SEMESTER

CH-2819: ORGANIC REACTION MECHANISMS AND HETEROCYCLICS

Semester: II | No. of credits: 4

Category: Major core (**MC**) | No. of hours: (5h/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 (20h)

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-enoltautomerism. b) Halogen electrophiles: Halogenation of aldehydes and ketones; carboxylic acidsc) 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 h)

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 (12h)

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 (16h)

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 (12h)

5.1 Nomenclature, reactivity, aromaticity, spectral properties.

5.2 Synthesis and reactions of indole, isoindoleoxazole, 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 ed., 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 ed., Kluwer Academic/Plenum Publishers, 2000.

References

1. S. H. Pine, *Organic Chemistry*, 5th edn, McGraw Hill International Editionn, 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 ed., John-Wiley, 2010.

LOYOLA COLLEGE (AUTONOMOUS)
CHENNAI - 600 034.

CH-2820: MAIN GROUP ELEMENTS AND NUCLEAR CHEMSITRY

Semester: II No. of credits: 4

Category: Major Core (**MC**) No. of hours: (4 h/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 h)

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: *Synthesis and uses of polyanions and cations. Natural and synthetic zeolites and application of zeolites as catalysts.*

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

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 (harshs); SF_4, SbF_3, and SbF_5 (moderate) and organometal reagents-Grignard reagents, organolithium, diorganomercury, and diorganomagnesium.

Self-study: Special techniques for the synthesis of inorganic compounds: the chemical vacuum line, plasmas, photochemical apparatus, and electrolysis.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 h)

3.1 Halogen oxides and oxo compounds: Dichlorine monoxide, chlorine dioxide, dibromine monoxide, and iodine pentoxide-preparation and properties; halogen oxyfluoridestrioxohalofluorides) 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, dinitrogendifluoride, haloamines, oxohalides, and nitrogen trifluoride oxide.

3.4 Sulfur fluorides: Synthesis and reactivity of disulfurdifluoride, sulfur tetrafluoride, substituted sulfur fluorides.

Self study:*Structure of halogen oxides and halogen oxo compounds with the aid of VSEPR model.Reactivity of the halides of N, S, and Xe and applications.*

Unit-4: Radiochemistry (10h)

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, GMcounters, scintillation counters.

Self-study: *Types of nuclei-isotopes, isotones, isobars, nuclear isomers. Radioactive isotopes and radioactive decay series. Half life period, lifetime, decay constant -relationship between them.*

Unit-5: Nuclear Reactions (10h)

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 extractionand 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: *Isotopes used in nuclear fission reactions.Radioisotopes used in noninvasive imaging techniques in nuclear medicine.*

Text books

1. F.A.Cotton, G. Wilkinson,C.A. Murillo andM.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,andP.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.

LOYOLA COLLEGE (AUTONOMOUS)
CHENNAI - 600 034.

CH- 2821: MOLECULAR SPECTROSCOPY

Semester: II | No. of credits: 4

Category: Major Core (**MC**) | No. of hours: (5 h/wk)

Objectives

1. *To learn 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 (20h)

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 (12h)

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 (8h)

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) (25h)

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 Hetero-COSY. ^{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 quadrupole nucleii. 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 (10h)

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 haloorganiccompounds 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*, 6thed., 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.W. 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*, McGraw Hill, London, 1973.

CH-2822: ORGANIC LABORATORY TECHNIQUES -II

Semester: II	No. of credits: 3
Category: Major Core (**MC**)	No. ofhours: 4(h/wk)

Objectives

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

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)

2: Extraction and estimation

a) Caeffine from coffee

b) Nicotine from tobacco leaves

c) Citric acid from citrus fruits

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 — No. of credits: 3

Category: Major Core (**MC**) — No. of hours: 4(h/wk)

Objectives

1. *To study the principle of distribution of common and rare metal ions in different groups.*
2. *To know 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-2824: GENERALTRENDSIN APPLIED CHEMISTRY (Seminar and Report)

Semester: II — No. of Credits:2

Course: Major Core(**MC**) — No. of hours:2 (h/wk)

Objectives:

To make the student to understand publications in journals and present a researchtopic, under the guidance of a professor, in the subject related to Applied Chemistry and his/her broad field of project work in the class room.

Testing:

Each student, during, semester-I or II, will give a one hour seminar on a **Title**of recent trends in applied chemistry taken from current publications in reputed journals.

Titles

Bio-organic and inorganic chemistry, Nano-technology, Supramolecular assemblies, Bio-catalysis, Bio fuels, Solar energy conversions, Nuclear technology, MRI imaging, Sonochemistry, Sensors,

The student will be tested both in subject matter and mode of presentation of the seminar as follows:

Subject matter-50 Marks

Standard of subject and plan
Preparation and mastery
Originality and logical development
Answers to questions
Summary and references

Mode of presentation-50 Marks

Economy of time
Voice as a tool of communication
Blackboard use and teaching aids
Language and diction
Relating to the audience

The student will submit a report of his/her seminar and attend such similar seminars given by others in the class and to keep a record of all. The report and the record maintained will also form a part of the evaluation.

CH-2955: BIO-ORGANIC CHEMISTRY

Semester: II | No. of credits: 3

Category:Elective Subject (**ES**) | No. of hours: (4 h/wk)

Objective

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 **(**15h)

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 **(**15H)

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 **(**12H)

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 (10h)

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 **(**8h)

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, 5th ed., Pearson* Education Asia, 1975.

References

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

CH-2956: MEDICINAL CHEMISTRY

Semester: II | No. of credits: 3

Category: ElectiveSubject (**ES**) | No. of hours: (4 h/wk)

Objectives

1. *Tounderstandthemedicinalpropertiesofvariousfunctionalgroups.*
2. *Tolearnthedifferenttypesofdrugsandtheirmodesofaction.*
3. *Tolearndrugdesignandstructureactivityrelationshipintermsofphysico-chemicalproperties.*

Unit-1: Introduction to Drugs (10 h)

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 **(15h)**

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 (10h)

3.1 Physicochemical properties evolved in the design, preparation of dosage forms. Solubilityand partition coefficients – cut-off point, Meyer Overton theory, Ferguson principle, bio-activities, Hammett sigma values – steric factors partition coefficients π values – surfaceactivity.

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: Bio-availability of Drugs (15 h)

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 Abzymeprodrug 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

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

Unit-5: Screening and testing of drugs (10h)

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 ed, 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.

LOYOLA COLLEGE (AUTONOMOUS)
CHENNAI - 600 034.

CH- 2957: CATALYSIS

Semester: II No. of credits: 3

Category: Elective Subject (**ES**) No. of hours: (4h/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 (11h)

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.Chemisorption of gases on metals and oxides

Unit -2:Homogeneous and Heterogeneous Catalysis (15h)

2.1 Acid-base catalytic reactions, protolytic and protropic mechanisms, activation energy of theprocesses, catalytic activity and acid-base strength, acidity functions: Hammett-Zuckertreatments, 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-Tropschsynthesis, 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 sulfonatedphsphines for hydroformylation reactions.

Unit - 3:PhotocatalysisandElectrocatalysis (15h)

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 degradationof dyes)

3.3 Solar energy conversion, electrochemical cells, photoelectrolysis of water and photocatalyticreactions

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 (9h)

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 h)

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.

SUMMER TRAINING PROGRAM (One Month)

The students will do summer training in reputed industries or research institutes for a period of 3 to 4 weeks and submit a report of it to the Department

III-SEMESTER

CH-3813: COORDINATION CHEMISTRY

Semester: III | No. of credits: 4

Category: Major Core (**MC**) | No. of hours: (5 h/wk)

Objectives

1 *To know the nature of metal-ligand bonding in coordination compounds and bonding parameters.*
2 *To know the chemical and photochemical behavior of coordination compounds.*
3 *To know the mechanisms of reactions of coordination compounds.*
4 *To understand the importance of coordination compounds in the emerging field of supramolecular chemistry and nanotechnology.*

5 To know the application of coordination compounds in catalysis and biology.

Unit-1: Theories of Coordination Compounds (20 h)

1.1 Crystal Field Theory: crystal field splitting in T_d and O_h fields, HS versus LS complexes, spin crossover.

1.2 Jahn Teller Theorem: Jahn Teller effect and static-dynamic Jahn Teller effect.

1.3 Tetragonal distortions from O_h symmetry and crystal field splitting in tetragonally distorted octahedral and square planar geometries.

1.4 Molecular Orbital Theory: Evidences of metal-ligand covalency, TASO-MO concepts of O_h and T_d complexes, MO energy level diagrams of σ- and π-bonding in O_h complexes, nature of metal-ligand π-bonds, evidences for π-back bonding, spectochemical series, and π-acceptor series.

1.5 Angular Overlap Model: Principles, quantification of metal-ligand orbital interactions (e_σ and e_π parameters), angular overlap and geometry, angular scaling factors for e_σ and e_π parameters, computation of Δ_o and Δ_t and their relationship.

Self-study

(a)Structural features of complexes of coordination numbers 2 to 6 and higher coordination numbers.

(b)Computation of CFSE in tetrahedral geometry and LS and HS octahedral geometries, factors which determine 10Dq values, spectrochemical series.

(c)Evidences of crystal field splitting.

Unit-2:Electronic Structure and Geometry of Coordination Compounds (15h)

2.1 Molecular magnetism: diamagnetic and paramagnetic susceptibilities, temperature dependent paramagnetism, the Curie law, ferromagnetic and antiferromagnetic interactions.

2.2 IR spectroscopy: differentiation of linkage isomers-cyano- and isocyano-, nitro- and nitrito-, thiocyanato- and isothiocyanato complexes, IR spectra of terminal and bridging carbonyls.

2.3 Electronic absorption spectroscopy: derivation of term symbols, electronic states and spectra of O_h and T_d complexes of d^nmetal ions, Orgel and Tanabe-Sugano diagrams.

2.4 ESR spectroscopy: isotropic and anisotropic g-values and structure, hyperfine and zero field effects on spectrum, nuclear quadrupole interaction.

Self-study

(a)Methods of determining magnetic susceptibility: Gouy and Faraday balances, vibrating samole magnetometer (VSM) and SQID..

(b)Van Vleck equation and magnetic moments of free metal ions.

Unit-3: Organometallic Compounds and Reaction Mechanisms (15h)

3.1 Classification of reaction types: reactions involving (a) change in the composition and (b) change in the position of ligand in the coordination sphere, (c) electron transfer reactions.

3.2 *Trans*-effect and synthesis of square planar complexes; mechanism of replacement of coordinated water in O_h complexes: *D, A,* I_a and I_d mechanisms; hydrolysis of O_h complexes.

3.3 Electron transfer reactions: mechanisms of inner-sphere and outer-sphere electron transfer.

3.4 Nomenclature of chiral complexes, study of absolute configurations of chiral complexes- ORD and CD, the hapto nomenclature in organometallic chemistry.

3.5 Structure and bonding in metal alkenes, metal-alkynes, and organometallic compounds of cyclic- and open chain π-donors, metallocenes, metal-aryls, double- and triple decker sandwich complexes.

3.6 Catalysis involving coordination compounds: (a) alkene isomerization and metathesis, (b) Ziegler-Natta catalysts and alkene polymerization, (c) alkene hydrogenation (Wilkinson catalyst), (d) carbonylation, (e) hydroformylation, (f) hydrocarboxylation, (g) Fischer-Troph synthesis (d) the Wacker process.

Self-study

(a)Metal carbonyls and metal nitrosyls: synthesis and structure.

(b)Coordinative unsaturation, oxidative addition, insertion reactions.

Unit-4: Supramolecular Chemistry and Photochemistry (12h)

4.1 Crystal field and charge transfer (MLCT, CTTM) photochemistry:photosubstitution and photoisomerization reactions.

4.2 Molecular recognition: molecular receptors, recognition of neutral molecules and anions and cations.

4.3 Supramolecular assemblies and architectures: nature of supramolecular interactions, supramolecular assemblies formed by templates and self assembly.

Unit-5: Bioinorganic Chemistry (13 h)

5.1 Metalloproteins and enzymes- General introduction and properties

5.2 Heme proteins: hemoglobin and myoglobin-structure, mechanism oxygen transport; cytochromes-biological roles and structural features.

5.3 Copper proteins: structure and funciuons of type-I, type-II and type-III copper.

5.4 Photosynthesis:chlorophyll, photosystem-I and photosystem-II, photosynthetic reaction center.

5.5 Enzymes: superoxide dismutase, carboxypeptidase *A*-structure and functions.

Self-study

(a)Essential and trace elements in biology.

(b)Synthetic oxygen carriers.

Text Books

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

2 F. A.Cotton, G.Wilkinson.;C. A.Murillo; M..Bochmann, *Advanced Inorganic Chemistry*, 6th ed.; Wiley Inter-science: New York, 1988

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

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

5. K.K..Rohatgi Mukherjee, *Fundamentals of photochemistry (Revised edition)*, Wiley Eastern Ltd., 1996

References

1. K..Nakamoto,*Infrared and Raman Spectra of Inorganic and coordination Compounds*, Part B: 5th ed.; John Wiley& Sons Inc.: New York, 1997.

2. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd ed.; Elsevier: Amsterdam, 1984.

3. M. L.Tobe and J.Burgess, *Inorganic Reaction Mechanisms*; Longman: New York, 1999.

4. J. A.Weil, J. R.Bolton and J. E.Wertz, *Electron Paramagnetic Resonance*; Wiley Interscience: 1994.

5. O. Kahn, *Molecular Magnetism*, VCH: Weinheim, 1993.

6. J. W.Steed and J. L.Atwood ,*Supramolecular Chemistry*, John Wiley & Sons Ltd.: New York, 2000.
7. J. M. Lehn, *Supramolecular Chemistry, Concepts and Prespectives*, VCH: Weinheim, 1995.
8. S.J. Lippard, and Berg, J.M. *Principles of Bioinorganic Chemistry*, University Science Books, New York, 1994.

CH-3814: THERMODYNAMICS AND CHEMICAL KINETICS

Semester:III | No. of credits : 5

Category: Major Core (**MC**) | No. ofhours:5 (hr/wk)

Objectives:

1. *To know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.*
2. *To understand the inter linking of quantum chemistry and statistical thermodynamics that leads to classical thermodynamics.*
3. *To apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.*

Unit 1:Classical Thermodynamics **(15**h)

1.1. Thermodynamic systems of variable composition: Partial molal quantities - Chemical potential. Gibbs-Duhem equation.Determination of partial molal quantities.Ellingham diagram and its significances.

1.2. Thermodynamics of real gases and real solutions:

Fugacity: Methods of determination. Dependence on temperature, pressure and composition.

Activity and activity coefficient: Standard states, determination of activity and activity coefficient of non-electrolytes and electrolytes

1.3 Ternary systems involving three liquids. Solubility of ionic solids in water-Solubility curves. Ternary system involving water and two soluble ionic solids.Formation of double salts.

Self-study: *Derivation of Kirchoff's equation and calculation of enthalpy of a reaction at different temperatures.Chemical equilibrium: Reactions involving gases and solutions - Temperature dependence of equilibrium constants. Kirchoff's equation and calculation of equilibrium constant.*

.Unit2: Irreversible Thermodynamics (12 h)

2.1. Near equilibrium process: General theory- Conservation of mass and energy- Entropy production in open system by (i) heat (ii) matter and (iii) current flow.

2.2. Onsager theory: Validity and verification.

2.3. Thermoelectricity-Electro kinetic and thermo mechanical effects

2.4. Application of irreversible thermodynamics to biological and non-linear systems.

Unit 3: Statistical Concepts Of Thermodynamics (20h)

3.1. Macro and micro states: Distribution of particles in different energy levels. Maxwel-Boltzmann statistics. Distribution of molecular velocities

3.2. Partition functions:Canonical and molecular partition functions. Separation of partition functions. Translational, rotational, vibrational and electronic partition functions. Interpretation of partition function.

3.3 Statistical approach to Thermodynamic properties: Internal energy, entropy, enthalpy, Helmholtz function, pressure, Gibbs function, residual entropy, equilibrium constant, average energies and equipartition principle.Heat capacity of mono and diatomic gases. Ortho- and parahydrogen Heat capacity of solids- Einstein and Debye models

3.4. Quantum Statistics Bose-Einstein statistics-Theory of paramagnetism. Statistics of a photon gas and liquid helium.Fermi-Dirac statistics-Thermonic emission-Electron gas (metals)

3.5. Statistical approach to equilibrium constants – Free energy function

Self-study:*Results of particle in a box (1D, 2D and 3D); rigid rotor; and harmonic oscillator and third law of thermodynamics*

Unit4: Kinetics of reactions in gas phase and in solutions and Catalysis (13h)

4.1. Kinetic theory of collisions; ARRT, derivation of rate equations; application of ARRT to reactions between (i) atoms (ii) molecules (iii) atoms and molecules - timeand true order

4.2. Unimolecular reactions, Lindemann - Christiansen hypothesis; bimolecular reactions in gas phase (involving atoms and free radicals) potential energy surface

4.3. Factors determining reaction rates in solution; primary and secondary salt effects - influence of ionic strength and dielectric constant on reactions involving (i) ions (ii) dipoles (iii) ion and dipole. Electrostriction; influence of hydrostatic pressure; volume of activation. Linear free energy relationship, Hammett and Taft equations

4.4. General catalytic mechanisms. Equilibrium and steady state treatments.Enzyme catalysis; Michalis-Menten kinetics Mechanism of enzyme inhibition.Mechanisms of reactions on surfaces(Langmuir, Rideal and Langmuir-Hinshelwood mechanisms)

Self-study*: Chemisorption and Physisorption; Langmuir's adsorption isotherm; competitive adsorption*

Unit5: Kinetics of Complex Reactions and Kinetic Methods of Analysis (15h)

5.1. Rate expressions for opposing, parallel and consecutive reactions; Chain reactionsGas phase auto oxidation; explosion and explosion limits.

5.2. Flow techniques - relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis

5.3. Stoichiometry, order, rate law, influence of ionic strength and dielectric constant thermodynamic parameters

5.4. Effect of radical trapper and pH of the medium Isotope effect- interpretation of the data and visualization of reaction mechanisms (with the help suitable examples from literature).

Text Books

1. J. Rajaram and J.C. Kuriacose, *Thermodynamics For Students of Chemistry*, 2 nd ed., S.L.N. Chand and Co., Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, *Chemical thermodynamics*, 6th ed., W.A.Benjamin Publishers, California, 1972.
3. M.C. Gupta, *Statistical Thermodynamics*, New Age International, Pvt. Ltd., New Delhi, 1995.
4. K.J. Laidler, " *Chemical Kinetics*", 3rd ed., Harper and Row Publishers, New York,1987
5. J. Rajaram and J.C. Kuriokose, " *Kinetics and Mechanisms of chemical transformation*, Macmillan India Ltd, Delhi ,1993.

References

1. D.A. McQurrie and J.D. Simon, *Physical Chemistry - A Molecular Approach*, Viva Books Pvt. Ltd., New Delhi, 1999.
2. R.P. Rastogi and R.R. Misra, *Classical Thermodynamics*, Vikas Publishing, Pvt. Ltd., New Delhi, 1990.
3. S.H. Maron and J.B. Lando, *Fundamentals of Physical chemistry*, MacMillan Publishers, New York, 1974

4. K.B. Ytsiimiriski, " *Kinetic Methods of Analysis*", Pergamom press,1996.
5. K.K.Rohatgi Mukherjee, "*Fundamentals of Photochemistry*", Revised edition, New Age International Publishers, New Delhi,1978.
6. D. A.McQuarrie and J. D.Simon, "*A Molecular Approach Physical Chemistry*" ,Viva Books Private Limited, New Delhi,1998.

CH-3815: Scientific Research Methodology

Semester-III | No. of credits: 3

Category: Major Core (**MC**) | No. of hours: (4 h/wk)

Objectives

1. *To introduce the purpose and importance of research for future development.*
2. *To know the various indexes and abstracts in science and technology.*
3. *To learn literature search for current awareness and for retrospective survey.*
4. *To know the classical and comprehensive reference works and general treatises in chemistry.*
5. *To know the methodology of writing thesis and journal articles.*

Unit 1:Meaning of Research (10h)

1.1 The search for knowledge, purpose of research, nature of scientific knowledge, scientific method, role of theory, characteristics of research.

1.2 Types of research: fundamental or pure research, applied research, action research, historical research, experimental research.

1.3 Assessment and evualation-purpose and general methodology.

Unit 2:The Chemical Literature (20h)

2.1 Sources of chemical information: primary, secondary and tertiary sources.

2.2 Indexes and abstracts in science and technology: applied science and technology index, biological abstracts, chemical abstracts, chemical titles, current chemical reactions, current contents, engineering index, index chemicus, index medicus, physics abstracts, science citation index.

2.3 Classical and comprehensive reference works in chemistry: Beilstein's Handbook of Organic Chemistry, Dictionary of Organic Compounds, Merck Index, Handbook of

Chemistry and physics, Lange's Handbook of Chemistry, Atlas of Spectral Data and Physical Constants for Organic Compounds

2.4 General Treatises: Organic Syntheses, Reagents for Organic Synthesis, Compendium of Organic Synthetic Methods, Organic Reactions, Theilheimer's Synthetic Methods of organic Chemistry.

2.5 Reviews: Annual and quarterly reviews, general reviews.

Self-study

(a) *Selected list of compilation of data such as Dictionary of Organic Compounds, Merck Index, CRC Handbook of Chemistry and Physics, Lange's Handbook of Chemistry.*

(b) Selected list of synthetic methods and techniques and general treatises: Organic Synthesis, Reagents for Organic Synthesis, Comprehensive Organic Chemistry, Encyclopedia of Reagents for Organic Synthesis.

Unit 3:The Chemical Abstracts (15h)

3.1 Current awareness searching: CA weekly issues, CA issue indexes.

3.2 Retrospective searching: CA volume indexes-general subject index, chemical substance index, formula index, index of ring systems, author index, patent index.

3.3 CA Collective indexes: Collective index (CI), decennial index (DI).

3.4 Access points for searching CA indexes: index guide, general subject terms, chemical substance names, molecular formula, ring systems, author names, patent numbers.

3.5 Locating the reference: finding the abstract, finding the original document, chemical abstract service source index.

Self-study

(a) The lay out and description of chemical abstracts.

(b) A brief literature survey from Chemical Abstracts for locating relevant journal articles.

Unit 4:The Scientific Writing **(**15h)

4.1 Scientific writings: research reports, thesis, and journal articles.

4.2 Requirement of technical communications: eliminating wordiness and jargon-tautology, redundancy, imprecise words, superfluous phrases.

4.3 Steps to publishing scientific articles in journals: types of publications-communications, articles, reviews; where to publish, specific format required for submission, organization of the material.

4.4 Documenting: abstracts-indicative or descriptive abstract, informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations (CASSI), abbreviations used in scientific writing.

Self-study

(a) Journals which publish only communications in chemistry.

(b) Journals which publish only reviews.

(c) Standard journal abbreviations of select journals in chemistry.

Unit 5:Computer Searches of Literature (5 h)

5.1 ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect, STN International. Google scholar, Scopus.

5.2 Journal home pages.

Text Books

1. B. E. Cain, *The Basis of Technical Communicating*, ACS.,Washington, D.C., 1988.
2. J. W.Best, *Research in Education*, 4th ed. Prentice Hall of India, New Delhi, 1981.
3. H. F. Ebel, C. Bliefert and W.E. Russey, *The Art of Scientific Writing*, VCH, Weinheim, 1988.
4. J. Gibaldi, and W.S. Achtert, *Handbook for writers of Research Papers*; 2nd ed.; Wiley Eastern, 1987.
5. A. Joseph, .*Methodology for Research*; Theological Publications, Bangalore, 1986

References

1. R. L. Dominoswki, *Research Methods*, Prentice Hall, 1981.
2. H. M. Kanare, *Writing the Laboratory Notebook*; American Chemical Society: Washington, DC, 1985.
3. J. S. Dodd, Ed., *The ACS Style Guide: A Manual for Authors and Editors*; American Chemical Society: Washington, DC, 1985.

CH-3816:INSTRUMENTAL METHODS OF ANALYSIS

Semester: III No. of credits : 3

Category:Major Core (**MC**) No. of hours: 4 (h/wk)

Objectives:*The students should be able to*

1. Learn sample handling in different experimental techniques.

2. Learn the operations of instrumentals techniques for quantitativeestimation.

3. Analyze IR spectrum of chemical compounds

Experiments:

1. Determination of functional groups using FT-IR spectrometer.
2. Estimation of concentration of a compound using UV-visible spectrophotometer.
3. Determination of metal to ligand ratio of complexes by Job's method using UV-visible spectrophotometer
4. Estimation of concentration of glucose using Abbe's refractometer.
5. Kinetics of inversion of cane sugar-determination of the pseudo first order rate constants & comparison of acid strength using polarimeter.
6. Verification of Freundlich adsorption isotherm
7. Kinetics of persulphate-iodide reaction, verification of Bronsted-Bjerrum equation (effect of ionic strength)
8. Estimation of Na/K/Ca using flame photometer.
9. Separation and estimation of compounds using column chromatography.
10. Estimation of iron by redox method using potentiometer.
11. Estimation of concentration of halides using potentiometer.
12. Determination of pK_{a1} and pK_{a2} of a weak dibasic acid using potentiometer.
13. Determination of solubility product of inorganic compounds using conductometer.
14. Determination of K_a and K_b of a weak acid or a weak base by conductometry method.
15. Analysis of a mixture of two metal ions by polarography.
16. Determination of ΔEp of a red-ox system by Cyclic voltammetry.

Text Books

01. B. Viswanathan and P.S.Raghavan, *Practical Physical Chemistry*, Viva Books, New Delhi,2009.
02. K. Sundaram, *Practical Chemistry* , S. Viswanathan Co. Pvt., 1996.

References

03. J.N. Gurthu and R. Kapoor,*Advanced Experimental Chemistry*, S. Chand and Co., 1987.
04. David P. Shoemaker, Carl W. Garland and Joseph W. Nibler, *Experiments in Physical Chemistry*, 5th ed., McGraw- Hill , 1989.

CH-3876: MATERIAL SCIENCE

Semester : III — No. of credits: 5

Category:Inter Disciplinary (**ID**) — No. of hours: 6(h/wk)

Objectives:

1.To introduce and give an insight into the fascinating area of solid state physics, solid

state chemistry and material science.

2.This will enable the students in pursuing higher studies and go for research.

Unit 1: Symmetry and diffraction in crystals (20h)

1.1 Crystal planes and directions – Miller indices. Unit cells, Two and Three dimensional space lattices, Operators - proper and improper axis, Mirror planes, Glide planes, Screw axis, Space groups, Crystal Systems,

1.2 Crystal structure by Powder X-ray diffract ions and by Single Crystal analysis. Reciprocal lattices – Fourier Transforms, Fourier Synthesis of Crystal Structures, Single Crystal Analysis and its Applications. Electron Charge Density Maps, Neutron diffraction – Method and Applications.

Unit 2: Experimental techniques & mechanical properties (20h)

2.1 Single crystal growth – Low and High temperature, solution growth technique – Gel and sol-gel methods. Melt growth - Bridgeman-Stockbarger method, Czochralski method. Flux technique, Physical and Chemical Vapour Transport methods (PVT and CVT). Characterization – TG/DTA/DSC methods, SEM/TEM Analysis. Determination of Hardness, Applications of Single Crystals.

2.2 Mechanical properties: Elastic behaviour – Atomic model of elastic behaviour. Modulus as parameter in design, Rubber like elasticity. Plastic deformation – Tensile stress – strain curve. Deformation by slip. Work hardening and dynamic recovery – Effect of grain size and dislocation motion.

Unit 3: Semiconductors and Superconductors (15h)

3.1 Semiconductors, Types of semiconductors – intrinsic and extrinsic, direct and indirect band gap, Elemental and compound semiconductors. Variation of Fermi level and carrier concentration with temperature for n- and p-type semiconductors. Defect semiconductors – stoichiometric and non-stoichiometric defects.

3.2 Applications : p-n junction, photo voltaic cell and for solar conversion. Photo galvanic and photoelctrolytic Cell - Photo electrocatalytic splitting of water using TiO_2, $SrTiO_3$, ZnO, $TiO_{2-x}F_x$ and $WO_{3-x}F_x$.Significance of photocatalysts.

3.3 Superconductivity: Meissner effect, Critical Temperature and Critical Magnetic Field, Type I and Type II Superconductors, BCS Theory of Superconductivity - Cooper Pair Electrons.Josephson Effect.Applications of Superconductor.

Unit4: Modern Materials (15h)

4.1 Soft and hard magnets - Domain theory – Hysteresis Loop - Applications. Magneto resistance and GMR materials. Ferromagnetic and Antiferromagnetic materials -Examples and Applications.Magnetic parameters for recording applications.

4.2 Ferro electric, Piezo elecric, pyroelectric materials and their properties. Shape memory Alloys – characteristics and applications.Non- linear optics - Second Harmonic Generators (SHG) - Mixing of Laser wave lengths by Quartz, Ruby and $LiNbO_3$.

4.3 Liquid crystals: nematic, cholesteric and smectic types and applications.

4.4 Dielectrics : polarisation - electronic, ionic, orientation, and space-charge polarisation. Effect of temperature on dielectric constant.Dielectric loss.Types of dielectric breakdown – intrinsic, thermal, discharge, electrochemical and defect breakdown.

Unit 5: Nanomaterials

(20h)

5.1 Nanomaterials – synthesis of metals – chemical reduction, cirate route, Brust reduction, sonolysis. Oxides – aqueous and non-aqueous route. Microemulsion based methods for nanomaterials and synthesis using supports.

5.2 Characterization of nanostructures – SEM, TEM and STM

5.3 Nanomachines and Nanodevices: MEMS and NEMS –fabrication.

5.4 Nanomaterials for environmental remediation – nanomaterials as sorbents – carbon nanomaterials, nanofiltration, nanoreactors and Nanoscale biopolymers for remediation.

Text Books:

1. P.K. Palanisamy, Materials Science, Scitech Publications, India, 2002.
2. T. Balachandran, Materials Science, Charulatha Publications, India, 2003.
3. Charles P. Poole, Jr., Frank J. Owens, Introduction to nanotechnology,Wiley-India, 2009.
4. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill Publishing Company Limited, 2007.

References:

1. M.G. Arora, Solid State Chemistry, Anmol Publications, New Delhi, 2001.
2. S. O. Pillai, Solid State Physics, Newage Int. (P) Ltd., 1995.
3. R.K. Puri and V. K. Babbar, Solid State Physics, Schad and Company Ltd, 2001.
4. C. Kittel, Solid State Physics, John-Wiley and sons, NY, 1966.

5. H.P. Meyers, Introductory Solid State Physics, Viva Books Private Limited, 1998.

6. A.R. West, solid State Chemistry and Applications, John-Wiley and sons, 1987.

7. T. Pradeep, A Text book of nanoscience and nanotechnology, Tata Mc-Graw-Hill, New Delhi, 2012.

CH-3951: APPLIED ORGANIC CHEMISTRY

Semester:III | No. of credits: 3

Category:Elective Subject (**ES**) | No. of hours: 4(h/wk)

Objectives

1. *To understand the elements of chemical engineering in organic synthesis*
2. *To understand the techniques involved in modern organic synthesis*
3. *To apply the knowledge of chemical reactions in solvent free organic synthesis*

Unit 1: Organic Chemical Technology (15 h)

1.1 Unit operations in chemical engineering: Fluid flow: Reynold's number; Bernoullis' equation, Turbulent flow.Heat transfer: Heat transfer coefficient, Corrosion and scale formation in heat exchangers and condensers. Mass transfer: Distillation - two and three component systems. Leaching & extraction; Stirrers and driers.

1.2 Energy balance over a flow system, heat of reaction, Chemical equilibrium, entropy changes, vapour phase and liquid phase catalytic reactions.

1.3 Factors affecting chemical process kinetics, scaling up of reactions from laboratory to pilot plant to main plant; Materials of construction; Study of industrial scale nitration, sulphonation, halogenations reactions; Preparation of a dye and a drug.

1.4 Quality control, R & D, standardization.

Unit 2: Organometallic Compounds (10 h)

2.1 Synthesis and reactions involving organolithium (n-BuLi, PhLi}, organocadmium, organomagnesium, organoselenium, organo aluminium, and organocopper.

2.2 Reactions promoted by samarium diiodide and dicyclopentadienyl samarium – Barbier type reaction, ketyl-alkene coupling reactions, pinacolic coupling reactions, acyl anion reactions and McMurray olefination.

Unit3: Green Chemistry (10 h)

3.1 The need for green chemistry and eco-efficiency, challenges and green chemistry, Challenges and green methods, green products, recycling waste.

3.2 Twelve principles of green chemistry, inception of green chemistry, awards for green chemistry and international organizations promoting green chemistry

3.3 Designing green synthesis-choice of starting materials, choice of reagents, choice of catalysis-biocatalysts, polymer supported catalysts(examples),choice of solvents.

Unit 4: Microwave Assisted Synthesis and Sonochemistry (15 h)

4.1 Introduction, Importance

4.2 Microwave assisted synthesis: Principle, instrumentation, types, limitations and precautions.

4.3 Applications: Esterification, deprotection of esters and ethers, C- and N-alkylation and condensation of active methylene compounds, rearrangement reactions, synthesis of enamino-ketones and electrophilic alkenes.

4.4 Sonochemistry: Principle, instrumentation, types and precautions.

4.5 Applications: Esterification, hydrolysis, substitution and addition reactions, oxidation and reduction reactions, coupling reactions.

Unit 5: Phase Transfer Catalysts in Organic synthesis (10h)

5.1 Types of PTC, Mechanism and Advantages

5.2 Preparation of quartenary ammonium salts and macrocyclic ethers.

5.3 Application: Substitution, esterification, addition, condensation and polymerization reactions.

Text books

1. W.L. McCabe, J.C. Smith and P. Harriott, *Unit Operations of Chemical Engineering*, 7^{th} *Edn.*, McGraw-Hill, New Delhi,2005.
2. J. M. Swan and D. St. C. Black, *Organometallics in Organic Synthesis*, Chapman Hall, 1974.
3. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, Narosa Publishing House, New Delhi, 2001.
4. K. Tanaka, *Solvent Free Organic Synthesis*, Wiley VCH, Weinheim, 2003.

References

1. P. H. Groggins, *Unit Processes in Organic Synthesis*, 5^{th}*Edn.*, Tata McGraw Hill, New York, 1995.,
2. C. E. Dridens, *Outlines of Chemical Technology*, Affiliated East-West Press Pvt.Ltd, 2001.

3. C. A. Clausen and G. Matson, *Principles of Industrial Chemistry*, John Willey & Sons, New York, 1978.
4. M.Larhed, and K.Olofsson, *Topics in current chemistry*, Springer,*266*,2006
5. R.Sanghi and M.M. Srivastava, *Green chemistry, Environment Friendly Alternatives*, Narosa Publishing House, 2007.
6. V. K. Ahluwalia, Green Chemistry, Ane Books Pvt. Ltd., 2006.
7. B. Michael Smith, *Organic synthesis*, McGraw Hill International Edition 1994.
8. *Methods and Reagents in Green Chemistry*, Edited by P. Tundo, A. Perosa and F. Zacchini, Wiley-Interscience, 2007.

CH-3952: CHEMISTRY OF NANOMATERIALS

Semester : IIINo. of credits: 3

Category: Elective Subject (**ES**)No. of hours : 4(h/wk)

Objectives:

1. *To introduce the concepts and importance of nanomaterials*
2. *To understand the various techniques of preparation, properties and applications of nanomaterials.*

Unit 1:Preparation& Fabricationof nanomaterials

(15h)

1.1 Synthesis by physical methods – inert gas condensation, arc discharge, laser ablation.

1.2 Synthesis by chemical methods – chemical reduction, sol-gel method, spin coating method, solvothermal and hydrothermal method, chemical vapor deposition – reaction types, different kinds of CVD techniques – metalloorganic CVD (MOCVD), plasma enhanced CVD (PECVD) , low pressure CVD (LPCVD).

1.3 Nanofabrication - moulding, embossing, and printing: hard pattern transfer elements-nanoimprint lithography; soft pattern transfer elements-replica molding, solvent-assisted micromolding.

1.4 Self-assemblyfor nanofabrication: Process, self-assembly of nanoparticles using organic molecules and biological templates, nontemplated self-assembly, templated self- assembly, preparation of SAMs, mechanisms of assembly, SAMs as surface layers.

Unit 2: Properties of Nanomaterials (15h)

2.1Electronic properties – energy bands and gaps in semiconductors, Fermi surfaces, donors, acceptors, deep traps, excitons, size dependent effects.

2.2 Optical properties – photonic crystals, optical properties of semiconductors, band edge energy, dependence on nanocrystalline size, optical transitions, absorption and interband transitions.

2.3 Luminescence properties – fluorescence/luminescence, photoluminescence/fluorescence, electroluminescence, photofragmentation, luminescent quantum dots for biological labeling.

2.4 Magnetic properties –ferromagnetic resonance and relaxation, magnetic properties of bulk nanostructures, magnetic clusters, nanopore containment of magnetic particles, nanocarbon ferromagnets.

Unit 3: Classification of nano systems

(10h)

3.1 Carbon nanotubes – Single and multiwalled carbon nanotubes – synthesis and purification, advantages and disadvantages, mechanism of growth, electron structure. Properties of carbon nanotubes – transport, mechanical and physical properties.

3.2 Nanoparticles and nanocomposites – types of nanoparticles, Pure metals – gold and silver. Metal Oxides – silica, iron oxide and alumina.Synthesis and Properties.Core-shell nanoparticles – types, synthesis, and properties.Nanocomposites- metal-matrix, ceramic-matrix and polymer-matrix composites – examples and applications.

3.3 Semiconductor Quantum dots – Electron structure, optical and electrical properties, NLO properties, photon up conversion and anti-stokes processes, electron-phonon relaxation, ZnO, TiO_2– pure and doped quantum dots.

3.4 Supramolecular assembly - Nature of supramolecular interactions, homo-and heteropolymetallic polypyridyl systems, supramolecular host-guest compounds. Dendrimers and metallodendrimers: Synthetic methodology-divergent and convergent methodology, types of metallodendrimers.

Unit 4: Nanomaterials – Analytical Techniques (10h)

4.1 Structural characterization – XRD, particle size determination.

4.2Surface characterization – SEM, TEM, AFM and STM.

Unit 5: Applications of Nanomaterials (10h)

5.1Nanomaterials in energy storage – solar cells (photovoltaics), rechargeable batteries, supercapacitors, hydrogen production, conversion and storage, photoelectrochemical decomposition of water.

5.2 Nanofluids for cooling technology: Challenges in cooling technology, Preparation of nanofluids- physical and chemical dispersion method, Advantages and applications of nanofluids.

5.3 Nanoparticles for catalysis: Oxidation - hydrocarbons and glucose, coupling reactions – Heck and Suzuki reactions, Hydrogenation – unsaturated aldehydes and conjugated dienes. Size and shape dependent catalysis.

5.4 Nanomaterials in medicine: magnetic nanoparticles in cancer therapy, gold nanoparticles – in vivo cancer detection and therapy. Dendrimers as drug carriers – encapsulation and conjugation of drugs.

Text Books:

1. Charles P. Poole, Jr., Frank J. Owens, Introduction to Nanotechnology, Wiley India (P) Ltd., New Delhi, 2006.
2. T. Pradeep, Nano: The Essentials, Tata Mc-Graw-Hill, New Delhi, 2007.

References

1. T. Pradeep, A Text book of nanoscience and nanotechnology, Tata Mc-Graw-Hill, New Delhi, 2012.
2. S.M. Lindsay, Introduction to Nanoscience, OxfordUniversity Press, New York, 2010.
3. John Mongillo, Nanotechnology 101, Pentagon Press, New Delhi, 2009.
4. Laura Costlow, April Peter, Nanomaterials and Nanostructures, Dominant Publishers, New Delhi, 2007.
5. B. Viswanathan, Nanomaterials, Narosa Publishing House Pvt. Ltd., New Delhi, 2009.
6. Subbiah Balaji, Nanobiotechnology, MJP Publishers, Chennai, 2010.
7. Sulabha K. Kulkarni, Nanotechnology - Principles and Practices, Capital Publishing Company, New Delhi, 2007.
8. A. K. Bandyopadhyay, Nanomaterials, Second Edition, New Age International Publishers Ltd., New Delhi, 2007.
9. S. Shanmugam, Nanotechnology, MJP Publishers, Chennai, 2010.

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CH-3953: INORGANIC PHOTOCHEMISTRY

Semester : III | No. of credits: 3

Category:Elective Subject(**ES**) | No. of hours: 4(h/wk)

***Objective*:**

To familiarize the applications of photochemistry in metal complexes

Unit1: Principles of photochemistry of metal complexes (15h)

1.1 Consequences of light absorption-Jablonski diagram and various photophysical processes. Photochemical reactions – primary and secondary processes. Energy transfer in photochemical reactions- photo sensitization and quenching.

1.2 Laws of photochemistry - Grotthus – Draper law, Stark Einstein law of photochemical equivalence. Laws of absorption: Beer Lambert's law

1.3 Quantum yield

Self-study:

Charge transfer reactions-types of charge transfer transitions, MLCT (MnO_4^-, TcO_4^-, ReO_4^-, CrO_4^{2-}, WO_4^{2-})

Unit2: Experimental techniques in inorganic photochemistry (10 h)

2.1 Steady photolysis: Principle- construction of cells for photolysis. Types of lamps, Light filters- Chemical & physical.

2.2 Actinometry. Classification of actinometers- Chemical & Physical. Examples for chemical actinometers. Characteristics of a good chemical actinometer.

2.3 Flash photolysis: Principle- interpretation of results- determination of half-life and life time of shortlived species. Laser Flash photolysis – advantages.

Unit3: Photochemistry of transition metal complexes (10h)

3.1 Adamson's Model, Photoreactions - photoaquation, substitution reactions, photoracemisation reaction of Cr(III), Co(III) and Cu (II) complexes

3.2 Manganese based photo systems for water-splitting.

Self-study:

Complexes of Rh, Ru, Pd, Pt –photochemical generation of hydrogen from alcohol, photocarbonylation of hydrocarbon, photocatalytic hydrogenationof alkene, photochemical reaction of water.

Unit4: Photoinduced electron transfer (15h)

4.1 Electron transfer (ET) – photoinduced ET in chromophore –quencher, MLCT- ET schemes for type 1 and type2 metal organic dyads.

4.2Thermodynamics of photoinduced electron transfer: electron transfer theory, experimental determination of rates of photo induced intramolecular electron transfer, $[Ru(bpy)_3]^{2+}$, Marcus free energy relationship.

4.3Electrochemistry and photo-physics of monoquat (N-methyl-4,4'-bipyridine) to $[Ru(bpy)]^{2+}$ chromophore. Innersphere acceptors and donors of bpy ligands, aromatic amine, electro donors, driving force dependence for ET, phenothiazine electron donor, pyrazole and polypyridine.

Self-study

Photochemical activation and spiltting of water, CO_2 and N_2 of spiltting.

Unit5:Semiconductor nanoparticlesas photocatalysts (10h)

5.1 Photocatalysis : Principles of photo catalysis, kinetics, visible light induced photo catalysis and design of active photocatalyst.

5.2 Nanoclusters; direct band gap exciton, TiO_2 – Photocatalyst for the decomposition of nitroaromatics, nitrophenols.

5.3 Photochemistry on semiconductor surfaces- principle of photo sensitization – mechanistic and kinetic aspects, -Humic acid as sensitizers. Degradation of Textile Dyes and other coloured compounds by photolysis, Methods to improve the efficiency of photocatalytic processes.

Text Books

1. R. Eldik and G. Stochel. Inorganic Photochemistry. II edition, Academic Press, 2003.
2. G.J. Ferraudi Elements of inorganic photochemistry, I edition, wiley InterScience, 1988.
3. K.K.Rohatgi Mukherjee, *Fundamentals of photochemistry (Revised edition)*, Wiley Eastern Ltd., 1996

References

1. V. Ramamurthy and K.S. Schanze. Organic and inorganic photochemistry, New York, Marcel Dekker, 1998.
2. D. C. Neckers, G. V. Bunav, W. S. Jenks, Advances in Photochemistry, vol. 27, John Wiley & sons, 2002.

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CH----: SELF STUDY PAPER

Semester: III Credits: 2

IV-SEMESTER

CH - 4813: ORGANIC SYNTHESISAND PHOTOCHEMISTRY

Semester: IV No. of credits: 4

Category: Major Core (**MC**) No. of hours: 5(h/wk)

Objectives:

The course should prepare the students to

1. *understand the molecular complexity of carbon skeletons and the presence of functional groups and their relative positions.*
2. *Apply disconnection approach and identifying suitable synthons.*
3. *Identify suitable reaction sequences to achieve the synthesis of target molecules.*
4. *Study various synthetically important reactions with a view to appreciate their scope, limitations and potential use in synthetic sequences.*
5. *The concepts of pericyclic reaction mechanisms.*
6. *Learn thephotochemical organic reactions.*

Unit 1: Organic Synthetic Methodology (15h)

1.1 Retrosynthetic analysis; Alternate synthetic routes. Synthesis of organic mono and bifunctional compounds via disconnection approach. Key intermediates, available starting materials and resulting yields of alternative methods.

1.2 Convergent synthesis, Synthesis based on umpolung concepts of seebach. Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups.Illustration of protection and deprotection in synthesis.

1.3 Control elements: Regiospecific control elements. Use of protective groups, activating groups, and bridging elements. Stereospecific control elements. Functional group alterations and transposition.

Unit 2: Reagents and Catalysts for Organic Synthesis (15h)

2.1 Reagents in organic synthesis for functional group transformations: Lithium diisopropylamide (LDA), Gilmann reagent, dicyclohexyl carbodimide (DCC), dichlorodicyanoquinone (DDQ), *Silane reagents*-trialkylsilyl halides, trimethylsilyl cyanide, trimethyl silane, TBDMS,

2.2 Catalysts: *phase transfer catalyst*, crown ethers, cyclodextrins, Ziegler-Natta catalyst, diazomethane, Stark enamine reaction, *phosphorous ylides* - Wittig and related reactions, *sulphur ylides* – reactions with aldehydes and ketones, 1,3-dithiane anions, Peterson reaction.

Unit 3: Modern Synthetic Reactions (20h)

3.1 Oxidation Reactions: Chromium and manganese reagents (CrO_3, $K_2Cr_2O_7$, PCC, PDC, Sarret reagent, Jones reagent, MnO_2, $KMnO_4$),

3.2 Oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetraacetate, periodic acid.

3.3 OsO_4, SeO_2, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Fenton's reagent, Sharpless epoxidation.

3.4 Reductions: Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Rh-C, Ni, Ru),

3.5 Wilkinson catalyst, $LiAlH_4$, $NaBH_4$, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination)

3.6 Diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, Wolff-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride, Bakers yeast.

3.7 Suzuki coupling, Heck reaction, Negishi reaction.

3.8 Electroorganic synthesis.

Unit 4: Pericyclic Reactions (10h)

4.1 Woodward Hoffmann rules; The Mobius and Huckle concept, FMO method and correlation diagrams

4.2 Cycloaddition and Cheletropic reactions; [2+2] and [2+4]-cycloadditions

4.3 Electrocyclization reactions of conjugated dienes and trienes.

4.4 Sigmatropic rearrangements: (1,3), (1,5), (3,3) and (5,5)-carbon migrations, degenerate sigmatropic rearrangements.

4.5 Group transfer reactions.

Self-study:*1,3-Dipolar cycloadditions, cationic and anionic cycloaddition reactions, specific examples on all types of pericyclic reactions*.

Unit 5: Organic Photochemistry (15h)

5.1 Photochemical excitation: Experimental techniques; electronic transitions; Jablonskii diagrams; intersystem crossings; energy transfer processes; Stern Volmer equations.

5.2 Reactions of electronically excited ketones; $\pi \rightarrow \pi^*$ and $r \rightarrow \pi^*$ triplets; Norrish type-I and type-II cleavage reactions; photo reductions; Paterno-Buchi reactions; photochemistry of α,β-unsaturated ketones; cis-trans isomerisation.

5.3 Photon energy transfer reactions:

5.4 Photocycloadditions: Photochemistry of aromatic compounds; photochemical rearrangements; photostationery state; di-π-methane rearrangement; Reaction of conjugated cyclohexadienone to 3,4-diphenyl phenols; Barton's reactions; Low temperature photochemistry, Flash photolysis.

Self-study:*Modified Jablonskii diagram, luminescence, lifetimes, quantum yield, Zimmerman approach to photochemical rearrangements, pivot mechanism.*

Text Books

1. Francis A.Carey and Sundberg, *Advanced Organic Chemistry, 5thed*, Tata McGraw-Hill, New York, 2003.

2.J. March and M Smith, *Advanced Organic Chemistry*, 5thed., John-Wiley and sons, 2001.

3. Ian Fleming, *Pericyclic Reactions*, Oxford Science Publications, Cambridge, 1999

4. Ireland R.E, *Organic synthesis*, Prentice Hall India, Goel publishing house, 1990

5. Smith, M.B, *Organic synthesis*, McGraw Hill International Edition 1994

6. House H.O. *Modern Synthetic reactions*, W.A. Benjamin Inc, 1972

References

1. Gill and Wills, *Pericyclic Reactions*, Chapman Hall, London, 1974

2. Carruthers W, *Modern methods of organic synthesis*, Cambridge University Press, 1993.

3. Norman R.O.C., *Organic synthesis*, Chapman Hall, London, 1980.

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Semester :IV	No. of credits : 5
Category : Major Core (**MC**)	No. of hours : 6(h/wk)

Objectives:

The student should be able to

i. understand the behavior of electrolytes in solution

ii. know the structure of the electrode surface

iii. differentiate electrode kinetics from other types of kinetics.

iv. know the applications of electrode process

Unit1: Ionics (24h)

1.1 Ions in solution:

Deviation from ideal behavior.Ionic activity, ion-solvent and ion-ion interactions.Expression for free energy.Debye-Huckel-Bjerrum model.Expressions for the mean activity coefficient. Applications of Debye-Huckel limiting law -Diverse ion effect – Extent of dissociation of a weak electrolyte in the presence of an inert electrolyte. Arrhenius theory.Limitations, van't Hoff factor and its relation to colligative properties.Debye-Huckel theory of strong electrolytes. Debye Huckel length and potential around a central ion, its interpretation

1.2 Transport of ions in Solution:

Electrolytic conduction- Debye-Huckel-Onsager treatment of the conductance of strong electrolyte-Experimental verification and limitations. Evidence for the existence of ionic atmosphere.Ion association and triple ion formations.Anomalous conductance of non-aqueous electrolytic solution.Abnormal mobility of hydrogen and hydroxyl ions.

Self-study: *Evaluation of thermodynamic quantities. Calculation of* K_a,K_b, K_{sp}, K_w, *and stability constants using emf data*.

Unit2: Electrical Double Layer (15h)

2.1. Introduction to electrical double layer

Evidences for electrical double layer.Electrocapillary phenomena-Electro capillary curves, surfactants –Lipmann's equation, interpretation and electro-kinetic phenomena. Zeta potential and its applications.

2.2. Structure of electrical double layer

Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer-Applications and limitations.

Self-study:*Faraday's laws of electrolysis. Significance and numerical problems.Role of applied potential and current.*

Unit3:Electrodics of Elementary Electrode Reactions (18h)

3.1. Behavior of electrodes:

Standard electrodes and electrodes at equilibrium.Ohmic and non-Ohmic behaviors .Study of electrode reaction.The model of three electrode system. Sign conventions. Rates of electro chemical reactions.Over potential and chemical & electro chemical conditions for the discharge of ions.

3.2. Rates of simple electrode reactions

Elementary electron electrode process.Butler-Volmer equation-Exchange current density and symmetry factor-Experimental determinations-Electrode rectification.Nernst equation as a special case of Butler -Volmer equation – Reaction resistance- Polarisable& non-polarisable electrodes-Low and high field approximations-Tafel equations.

Self-study: *Construction of current vs applied potential diagrams for different magnitudes of exchange current density and symmetry factors*.

Unit 4: Electrodics of multistep multi electron system (18h)

4.1. Rates of multi-step electrode reactions

Examples of multi electron reactions.Butler -Volmer equation for a multi-step reaction. The concept of rate determining step of an electrode reaction. Transfer coefficients and stoichiometric number

4.2. Electro-chemical reaction mechanisms

Proposal of electro-chemical reaction mechanisms- Electrochemical reaction order. Surface coverage-Rate expressions. Reduction of (i) I_3^- and (ii) Fe^{2+}. Dissolution of iron to iron(II). Over voltage and evolution of (i) oxygen and (ii) hydrogen at different pH. Symmetry factors vs transfer coefficients.

Self-study:*Dissolution of iron to iron(III) and rusting of iron –Pourbiax diagram*.

Unit5: Concentration Polarisation (15h)

5.1. Transport of the electro active species to electrode

Different types of over voltages-Chemical and electro chemical over potentials. Phase, activation and concentration over potentials.Diffusion, migration and hydrodynamic modes of transports. The role of supporting electrolyte Theory of diffusion over potential. Polarography- Ilkovic equation Limiting current density and its importance.

5.2. Electro organic reactions at the electrodes

Electrochemical reduction of alkyl halides, carbonyl, nitrocompounds, alkenes, anthracene, pyrene.

Self-study:*Electro chemical dimerisations-Synthesis of bipyridines.*

Text Books

1. J.O.M.Bockris and A.K.N.Reddy, "*Morden Electro chemistry*" vol.1 & 2B, Springer, Plenum Press, New York, 2008.
2. J.O.M.Bockris, A.K.N.Reddy and M.G. Aldeco "*Morden Electro chemistry*" vol. 2A, Springer, Plenum Press , New York, 2008
3. S.Glasstone, "*Electro chemistry*", Affiliated East-West Press, Pvt., Ltd., New Delhi, 1974.

References

1. D.A.McQurrie and J.D.Simon, "*Physical Chemistry*", A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
2. J.Rajaram and J.C. Kuriakose, "*Kinetics and Mechanism of Electrochemical Transformations*", Macmillan IndiaLtd., New Delhi, 1993.
3. Philip H. Rieger, "*Electrochemistry"*2nded., Springer, New york, 2010.
4. B. Viswanathan, S.Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, "*Electrochemistry-Principles and applications*" S. Viswanathan Printers, Chennai,2000.
5. R. A. Alberty& R.J. Silbey,*Physical Chemistry, 2nded.*, Wiley Eastern Ltd., New York 1997.

CH -4815: PROJECTAND REPORT

Semester-IV | No. of Credits: 13

Course: Major Core(**MC**) | No. of hours : 17(h/wk)

Objectives:

To make the student to understand and present a research finding on a topic in the subject related to Chemistry under the guidance of a Department Staff .

Testing:

The student will be tested both in subject matter of the report and the mode of presentation inthe viva-voce examination.

The viva-voce examination, on the project work done, will be conducted by two examiners(Project guide & an external examiner appointed by the Controller of examination)

Project report:75 Marks

Standard of subject and plan

Preparation and mastery

Originality and logical development

Summary and references

Viva-voce: 25 Marks

Economy of time

Communication

Blackboard use and teaching aids

Language and diction

Answer to questions

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CH -4816: **RECENT TRENDS IN CHEMISTRY** (Seminar and Report**)**

Semesters:IV | No. of Credits:2

Course: Major Core(**MC**) | No. of hours: 2(h/wk)

Objectives:

To make the student to understand publications in journals and present a researchtopic, under the guidance of a professor, in the subject related to Chemistryandto his/her project work.

Testing:

Each student, during, semester-III or IV, will give a one hour seminar on a **Title**ofrecent trends in chemistry taken from current publications in reputed journals relevant to his/her project work,.

Titles

Bio-organic and inorganic chemistry, Nano-technology, Supramolecular assemblies, Bio-catalysis, Bio fuels, Solar energy conversions, Nuclear technology, MRI imaging, Sonochemistry, Sensors,

The student will be tested both in subject matter and mode of presentation of the seminar as follows:

Subject matter-50 Marks

Standard of subject and plan

Preparation and mastery

Originality and logical development

Answers to questions

Summary and references

Mode of presentation-50 Marks

Economy of time

Voice as a tool of communication

Blackboard use and teaching aids

Language and diction

Relating to the audience

The student will submit a report of his/her seminar and attend such similar seminars given by others in the class and to keep a record of all. The report and the record maintained will also form a part of the evaluation.