DEPARTMENT OF CHEMISTRY

M.Sc (Chemistry)-SYLLABUS

Effective from the Academic Year 2008-2009

Loyola College *(Autonomous)*

Chennai - 34

CONTENTS

	SUBJECT	Page
	Syllabus Template	4
	List of Courses	5
I.	**SEMESTER-I** (Major Core-**MC**)	
	CH-1806 ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY	6
	CH-1807 CONCEPTS IN INORGANIC CHEMISTRY	8
	CH-1808 QUANTUM CHEMISTRY AND GROUP THEORY	10
	CH-1809 ANALYTICAL CHEMISTRY	12
	CH-1810 ORGANIC LABORATORY TECHNIQUES-I	14
	CH-1811 INORGANIC QUANTITATIVE ANALYSIS AND SYNTHESIS	15
II.	**SEMESTER-II** (Major Core-**MC**)	
	CH-2813 SEMINAR & REPORT	17
	CH-2814 ORGANIC SUBSTITUTION, ADDITION AND ELIMINATION REACTIONS	17
	CH-2815 CHEMISTRY OF MAIN GROUP ELEMENTS	19
	CH-2816 THERMODYNAMICS AND STATISTICAL MECHANICS	22
	CH-2817 LABORATORY TECHNIQUES IN ORGANIC CHEMISTRY-II	24
	CH-2818 INORGANIC QUALITATIVE ANALYSIS	25
	SUBJECT ELECTIVE (SE) : Any one	
	CH-2953 HETEROCYCLICS AND NATURAL PRODUCTS	26
	CH-2954 NUCLEAR AND RADIO CHEMISTRY	27

III. SEMESTER-III (Major Core-**MC**)

CH-3808 PHOTOCHEMISTRY AND ORG SYNTHESIS 30
CH-3809 COORDINATION CHEMISTRY 32
CH-3810 MOLECULAR SPECTROSCOPY 34
CH-3811 INSTRUMENTAL METHODS OF ANALYSIS 37
CH-3812 CHEMICAL KINETICS 38

INTER DISCIPLINARY (ID)

CH-3875 MATERIAL SCIENCE 40

IV. SEMESTER-IV (Major Core-MC)

CH-4808 ELECTROCHEMISTRY 42
CH-4809 APPLICATIONS OF SPECTROSCOPY 44
CH-4810 SCIENTIFIC RESEARCH METHODOLOGY 47
CH -4811 SEMINAR & REPORT 49
CH 4812 PROJECT WORK AND DESSERTATION 49

SUBJECT ELECTIVE (ES): Any one

CH-4955 ORGANIC CHEMICAL TECHNOLOGY 49
CH-4956 ADVANCED COORDINATION CHEMISTRY 51

EXTRA DISCIPLINARY(ED): For Other Depts

CH-2901/ CH-3901 INSTRU METHODS OF CHEM ANALYSIS FOR BIOLOGISTS 54

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SEM	Major Core (MC) Hrs/Cr	Subject Elective (SE) Hrs/Cr	Extra Disciplinary (ED) Hrs/Cr	Inter Disciplinary (ID) Hrs/Cr	Total Hours	Total Credits
I	CH-1806: Org. Reac. Mech. and Ster 5/4 CH-1807: Concepts in Inorg.Chem. 5/4 CH-1808: Quantum Chem. 5/4 CH-1809: Analytical Chem. 5/4 **CH-1810: Org. Pract – I 4/3** **CH-1811: Inorg. Quantitive Ana. and Syn 4/3** Seminar 2/0	--	--	--	30	**22**
II	CH-2814: Org.subs. add.and elim eaction 5/4 CH-2815: Chem of Maingroup Elements 5/4 CH-2816: Thermo. and Stat. Mechanics 5/4 **CH-2817: Org. Lab. Pract – II 4/3** **CH-2818: Inorg. Semi micro Quali.Anal. 5/3** **CH-CH-2813: Seminar 2/1**	CH-2953: Hetero.& Nat Prod. 4/4 **OR** CH-2954:Nuclear & Radiochem. 4/4	--	--	30	**23**
III	CH-3808: Photochem. and Org.Syn. 4/4 CH-3809: Coord. Chem. 5/4 CH-3810: Molecular Spectr. **CH-3811: Instru. Methods of anal Pract 4/3** CH-3812: Chemical Kinetics 4/4 Seminar 2/0	--	**CA-3900:Comp Appl 3/1**	**CH-3875:Mat Sci. 3/2**	30	**22**
IV	CH-4808: Electrochemistry 5/4 CH-4809: Appl. of Spectro. 5/4 CH-4810: Sci Res Method 2/1 **CH-4811: Seminar and Report 2/1** **CH-4812: Project Work 12/10**	CH-4955: Organic Chem.Tech., 4/3 **OR** CH-4956:Adv.Coor. Chem. `4/3	--	--	30	**23**
Total	106 Hrs/80 Cr	8 Hrs/7 Cr	11 Hrs/7 Cr	3 Hrs/2 Cr	120	**90**

LIST OF COURSES

SEM	CODE	PAPER	CRE	SUB	LT	CAT
I	CH-1806	Organic Reaction Mechanisms and Stereochemistry	4	MC	T	Both
	CH-1807	Concepts in Inorganic Chemistry	4	MC	T	Both
	CH-1808	Quantum Chemistry and Group Theory	4	MC	T	Both
	CH-1809	Analytical Chemistry	4	MC	T	Both
	CH-1810	**Organic Laboratory Techniques-I**	**3**	**MC**	**L**	**Both**
	CH-1811	**Inorganic Quantitative Analysis and Synthesis**	**3**	**MC**	**L**	**Both**
II	CH-2814	Organic Substitution, addition and Elimination Reactions	4	MC	T	Both
	CH-2815	Chemistry of Main Group Elements	4	MC	T	Both
	CH-2816	Thermodynamics and Statistical Mechanics	4	MC	T	Both
	CH-2817	**Organic Laboratory Techniques -II**	**3**	**MC**	**L**	**Both**
	CH-2818	**Inorganic Semimicro Qualitative Analysis**	**3**	**MC**	**L**	**Both**
	CH-2953	Chemistry of Heterocyclics and Natural Products	4	SE	T	Both
		OR				
	CH-2954	Nuclear and Radiochemistry	4	SE	T	Both
	CH-2813	Seminar and Report	1	MC	L	C.A.
	CH-2901 / CH-3901:	Instrumental Methods of Chemical Analysis	3	ED	T	Both
III	CH-3808	Photochemistry and Organic Synthesis	4	MC	T	Both
	CH-3809	Coordination Chemistry	4	MC	T	Both
	CH-3810	Molecular Spectroscopy	4	MC	T	Both
	CH-3811	**Instrumental methods of analysis (lab)**	**3**	**MC**	**L**	**Both**
	CH-3812	Chemical Kinetics	4	MC	T	Both
	CH-3875	Material Science	2	ID	T	Both
		(Offered by both chemistry & physics departments)				
	CA-3900	Computer Application (Offered byComp Dept to chemistry Students)				
IV	CH-4808	Electrochemistry	4	MC	T	Both
	CH-4809	Applications of Spectroscopy	4	MC	T	Both
	CH-4810	Scientific Research Methodology	1	MC	L	C.A.
	CH-4811	Seminar and Report	1	MC	L	C.A.
	CH-4812	**Project Work and Dissertation**	**10**	**MC**	**P**	**C.A.**
	CH-4955	Organic Chemical Technology	3	SE	T	Both
		OR				
	CH-4956	Advanced Coordination Chemistry	3	SE	T	Both

COURSES OFFERED TO OTHER DEPARTMENT STUDENTS:

CH-2901/3901: Instrumental methods of Chemical Analysis for Biologists 4/3

SEMESTER:I

CH-1806 ORGANIC REACTION MECHANISMS AND STEREOCHEMISTRY

SEMESTER : I **CREDIT: 4**
CATEGORY : MC **NO. OF HOURS / WEEK : 5**

Objectives:

1. *To understand the mechanism of a chemical reaction, the path and the feasibility of a reaction.*
2. *To suggest synthetic route for simple organic compounds with 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 make the students understand and appreciate the concept of stereochemistry and reaction mechanism.*

Unit - 1 : Mechanisms and Methods (10h)

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- determination of rate law and rate constants; 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 (10h)

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

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

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

Self study:

Longer nucleophilic rearrangements, Carbene rearrangements, dienone -phenol rearrangements.

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

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

3.2 Oxidation Reactions: Aromatization of six membered rings; dihydro elimination; oxidation of alcohols and dehydrogenation of amines; Reactions involving cleavage of C-C bonds; ozonolysis; cleavage of double bonds; oxidative decarboxylation.

3.3 Reduction Reactions involving replacement of oxygen by hydrogen:- Wolff Kishner and Clemmenson reductions; Removal of Oxygen from substrate; Reduction with cleavage; Reductive coupling.

Self study:

Oxidative coupling, oxidation of amines and thiols.

Unit - 4 : Stereochemistry-I

4.1 Optical isomerism due to asymmetric carbon atoms

4.2 Racemic modifications; racemisation; thermal, anion, cation, reversible formation

4.3 Epimerisation; mutarotation; I and II order asymmetric transformations

4.4 Resolution of racemic modifications; asymmetric transformations; asymmetric synthesis destruction; Cram's and Prelog's rules; absolute asymmetric synthesis

4.5 Criteria for optical purity; D, L, R, S-notations; Cahn-Ingold-Prelog rules, absolute and relative configuration; configurations of allenes, spiranes, and biphenyls

Unit-5 :Stereochemistry-II (15h)

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

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

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

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

5.5 Stereoselective synthesis: Synthesis of yohimbine, reserpine

Self study:

Molecular dissymmetry; specific and molar rotations; polarimetry; Fischer, Newmann and Sawhorse notations; Geometrical isomerism; E,Z notations; optical isomerism of lactic and tartaric acids.

REFERENCES

1. J. March and M. Smith, Advanced Organic Chemistry, 5th edn, John-Wiley and Sons. 2001.
2. E.S. Gould, Mechanism and Structure in Organic Chemistry Holt, Rinehart and Winston Inc., 1959.
3. E.L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, (2000)
4. P.S. Kalsi, Stereochemistry, 3rd edn, New Age International Publishers, 1995.

5. I.L. Finar, Organic chemistry. Vol-2, 5th edition, Pearson Education Asia. 1975
6. I.L. Finar, Organic chemistry, Vol-1, 6th edition, Pearson Education Asia. 2004
7. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part-A and B, 4th edn, Kluwer Academic/Plenum Publishers. 2000.
8. S.H. Pine, Organic Chemistry, 5th edn, McGraw Hill International Edition. 1987.
9. L.F. Fieser and M. Fieser, Organic Chemistry, Asia Publishing House, Bombay, 2000.
10. Nasipuri, Stereochemistry, Alhed Publishers, 2003.

CH-1807 CONCEPTS IN INORGANIC CHEMISTRY

SEMESTER : I **CREDIT : 4**
CATEGORY : MC **NO. OF HOURS / WEEK : 5**

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 special types of compounds through weak chemical forces.*
5. *To identify relevant inorganic compounds for specific applications.*

Unit - 1 : Atomic Structure and Periodic Table

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 Effective nuclear charge- Slater rule and their uses: computation of and radii of atoms and ions.

1. 3 Modern periodic table: periodic properties, trends and the underlying reasons.

Self study:

(a) Periodicity - the trend in the atomic and ionic radii, ionization potential, and electron affinity along the period..
(b) Electronic configuration: the exchange energy and Aufbau principle.

Unit - 2 : Ionic and Covalent Compounds

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

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

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

2.4 Born-Haber cycle: thermochemical calculations, radii of nonspherical ions, solubility and thermal properties of ionic compounds as a function of U_0 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-, interstitial-, and electron deficient compounds.

Self study:

(a) Layer lattices, applications, and properties of crystal defect structures.
(b) Thermodynamic parameters affecting lattice energy and factors affecting ionic radii.
(c) Predicting the existence of certain ionic compounds and the nonexistence of hypothetical compounds from thermochemical calculations.

Unit - 3 : Covalent Bond

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 HCI).

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

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

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 acids and bases, classification, HSAB principle, levelling effect, symbiosis, proton sponges.

5.2 Nonaqueous solvents: classification-protic 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) Strength of protonic acids: binary acids, oxo acids, pure acids and relative acidities, properties of perchloric acid, fluorosulfuric acid, trifluoromethanesulfonic acid.

Unit - 6 : Crystallography

6.1 Principles: Miller indices, crystal lattices, and unit cells.

6.2 X-ray diffraction: Bragg's law, powder method, single crystal diffraction, structure factor, and Fourier synthesis.

6.3 Structure of sodium chloride, cesium chloride, flourite, antifluorite, zinc blende, wurtzite, rutile, spinels, inverse spinels, and perovskite.

6.4 Electron and neutron diffraction: basic principles and typical applications.

Self Study:

(a) Comparison of X-ray, electron-, and neutron diffraction methods.
(b) Unit cell diagrams of the different types of crystal lattices.

REFERENCES

1. Huheey, J. E.; Keiter, E. A. Keiter, R. L. Inorganic Chemistry; 4th ed.; Harper and Row: NewYork, 1983.
2. Cotton, F. A.; Wilkinson, G.; Murillo, C. A.; Bochmann, M. Advanced Inorganic Chemistry; 6th ed.; Wiley Interscience: New York, 1988.
3. Purcell, K. F.; Kotz, J. C. Inorganic Chemistry; Saunders: Philadelphia, 1976.
4. Moeller, T. Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.
5. Shriver, D. F.; Atkins, P. W.; Langford, C. H. Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.
6. Stout, G. H.; Jenson, L. H. X-Ray Structure Determination, 2nd ed.; John Wiley & Sons: New York, 1989.
7. West, A. R. Solid State Chemistry and its Applications, John Wiley & Sons: New York, 1989.
8. Rhodes, G. Crystallography Made crystal Clear; Academic Press, Inc.: New York, 1993.
9. Hammond, C. The Basics of Crystallography and Diffraction; Oxford University Press; 1997.
10. Smart, L.; Moore, E. Solid State Chemistry An Introduction; 2nd ed.; Nelson Thomes Ltd.: Cheltenham, 1996.

CH 1808 QUANTUM CHEMISTRY AND GROUP THEORY

SEMESTER : I **CREDIT : 4**
CATEGORY : MC **NO. OF HOURS / WEEK : 5**

Objectives:

1. *To have a good foundation in understanding the physical and mathematical aspects of quantum mechanics.*
2. *To become familiar with the required mathematics for solving quantum mechanical problems.*
3. *To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.*

Unit -1 : Mathematics for quantum Mechanics (QM) and QM Postulates

1. 1 Coordinate systems

1.2 Complex numbers

1.3 Functions (odd & even, orthogonality and normalization)

1.4 Differential equations

1.5 Operators: linear, differential, and Hermitian and Hamiltonian operators

1.6 Eigen functions and eigen values

1.7 Failure of Classical Mechanics and the need for QM

1.8 Postulates of QM

1.9 The time-dependent and time-independent Schrodinger wave equations

Unit - 2 : Some QM Models and their Application's

2.1 Particle in a box (1 D, 2D & 3D), degeneracy and its application to linear conjugated molecular systems, free particle. Bohr's correspondence principle. QM tunneling

2.2 Rigid Rotor: wave equation and solution calculation of rotational constants and bond length

2.3 Harmonic Oscillator: wave equation and solution, anharmonicity force constant and its significance

Unit - 3 : Application of OM to H-atom and Multi-Electron Atoms

3.1 The Hydrogen atom and H-like ions: Solution to H and H-like wave equation, radial and angular functions, quantum numbers n, l and m and their importance. the radial distribution functions and H-like orbitals and their representation.

3.2 Approximation Methods: The variation method - trial variation function and variational integral (examples of variational calculations from particle in a box)

3.3 Quantum mechanical treatment of angular momentum - simultaneous measurement of several properties: evaluation of commutators such as [x, px), (x, px^2), (Lx, Ly] and (Lx2, Lx] and their significance.

3.4 He atom: The electron spin, Pauli exclusion principle and Slater determinant for He atom.

3.5 Atomic term symbols: LS and JJ coupling

Unit - 4 : Molecular QM and Chemical Bonding

4.1 Hydrogen molecule ion - the use of linear variation function, the LCAO method

4.2 Hydrogen molecule: Molecular orbital theory and Heitler-London treatment.

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

Unit - 5 : Group Theory and its Applications

5.1 Symmetry elements and operations

5.2 Point groups, groups and classes of symmetry operations

5.3 Non-degenerate representations, character table. reduction formula, character of matrices

5.4 Degenerate representations

5.6 Applications to molecular vibrations (IR and Raman activity) and chemical bonding

TEXT BOOKS

1. Levine, Quantum Chemistry, IV edition. Allyn & Bacon Inc.. 1983.
2. Alan Vincent- Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications. John and Willy & Sons Ltd. 1977.

REFERENCE BOOKS

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. Donald A. McQuaric & John D. Simon. Physical chemistry - A Molecular Approach, Viva Books Pvt. Ltd.. New Delhi. 1998.
4. Donald A. McQuarie, Quantum Chemistry. Viva Books PW. Ltd.. New Delhi. 2003. R.L. Flurry. Jr. Symmetry Groups. Theory and Chemical Applications. Prentice Hall. Inc.. 1980.
6. F. Albert Cotton, Chemical Applications of Group Theory. 2°'' ed.. John Wiley & Sons, 1971.
7. P.W. Atkins and Julio de Paula. Atkins' Physical Chemistry, VII ed. Oxford University Press. 2002.

CH-1809 ANALYTICAL CHEMISTRY

SEMESTER : I **CREDIT: 4**
CATEGORY : MC **NO. OF HOURS / WEEK : 5**

Objectives:

a. To help students develop the habits of accurate manipulation and an attitude of critical thinking.
b. Learn the basic analytical methods and have a sound knowledge of chemistry involved in an analysis.

UNIT - 1 : STATISTICS: INTRODUCTION TO CHEMOMETRICS

1.1 Errors: Classification of errors, minimisation or elimination of errors.

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

UNIT-2: CHROMATOGRAPHY

2.1 Electrophoresis: Principle, instrumentation - capillary electrophoresis and detector.

2.2 Gas chromatography: Principle, instrumentation, nature of carrier gas, columns, detectors, hot-wire detector, flame ionisation detector, photo ionisation detector and ECD.

2.3 HPLC: Principle, instrumentation, ultra-violet detectors and separation of artificial colourants in confectionery. Advantages of HPLC.

UNIT-3 : TITRIMETRIC METHODS OF ANALYSIS

3.1 Introduction to Titrimetric Analysis: Principle, reactions used for titrations, concentration systems, and stoichiometric calculations involving acid base and redox systems.

3.2 Neutralisation Titrations: Neutralisation curves for strong acid-strong base, weak acid-strong base titrations, indicators, determining the colour change range of an indicator,

choice of indicator, feasibility of acid base titrations, factors affecting pH at the equivalence point. Titration curves of a weak dibasic acid versus strong base.

3.3 Complexation Titrations: Stability of complexes - stepwise formation constants, titration curves, feasibility of complexation titration, equilibria involved in EDTA titration, effect of pH on the concentration of completely dissociated form of EDTA, absolute and conditional stability constant for metal-EDTA complex. Factors affecting the equivalence point, metallochrome indicators - determination of percentage composition in alloys or mixtures using masking and demasking agents.

3.4 Precipitation Titrations: Solubility equilibria, titration curves and feasibility of titration. Theory of indicators. Mohr method and Fajans method of estimation of halides.

UNIT - 4 : THERMOANALYTICAL & ELECTROANALYTICAL METHODS

4.1 Thermogravimetry: Principle, factors affecting thermogram, instrumentation and thermal decomposition of $CaC_20_4H_20$ and $CuSO_4.5H_20$

4.2 Differential techniques: Instrumentation , experimental, instrumental factors of DTA and DSC. Thermal studies of $CuSO_4.5H_20$ by DTA and determination of purity of pharmaceuticals and phase transition studies by DSC - evaluation of thermodynamic parameters.

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

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

4.5 Potentiometry: Principle, potentiometric titration, equivalence point potential for (i)Fe^{2+} - Ce^{4+} system (ii) Fe^{2+} - MnO_4^-/H^+ system, determination of concentration of the species at the equivalence point. Ion selective electrodes, solid state ion selective detectors, Biochemical electrodes.

4.6 Voltammetry: D.C polarography, principle, Ilkovich equation, instrumentation, role of supporting electrolyte, polarographic maximum, - cyclic voltammetry, anodic and cathodic stripping voltammetry. Estimation of ascorbic acid in fruit juices.

UNIT - 5 : SPECTROMETRY

5.1 Atomic Absorption Spectroscopy: Principle, instrumentation, the nebuliser - burner system, graphite tube furnace, resonance line source, monochromators, detectors, and spectral and chemical interferences - determination of calcium and magnesium in water and determination of tin in canned fruit juices.

5.2 Flame Spectrometry: Principle, instrumentation and interferences determination of alkali metals.

5.3 Spectophotometry: Beer Lambert's law - significance of molar extinction coefficient, photoelectric photometer, spectophotometric titration, determination of Fe (III) with EDTA and determination of Fe (III) in the presence of aluminium.

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, instrumentation - determination of quinine in tonic water and determination of codeine and morphine in a mixture.

REFERENCES:

I. Douglas A. Skoog, Donald M. West and F.James Holler, Fundamentals of analytical Chemistry, Harcourt Asia Pte. Ltd., 2001.
2. Douglas A.Skoog, Donald M.West and F.James Holler, Analytical Chemistry An Introduction. Saunders College Publishers, 1990.
3. R.A.Day, Jr. and A.L.Underwood, Prentice-Hall of India, 2001.
4. J.Mendham, R.C.Denney, J.D.Barnes and M.Thomas, Vogel's Text book of quantitative Chemical Analysis, Pearson Education Pvt..Ltd.. 2004.
5. G.H.Jeffery, J.Bassett, J.Mendham and R.C.Denney, Vogel'.s Textbook of Quantitative Chemical Analysis, Longman Scientific and Technical, 1989,

CH-1810 ORGANIC LABORATORY TECHNIQUES-I

SEMESTER : I **CREDIT: 3**
CATEGORY : MC **NO. OF HOURS / WEEK : 4**

Objectives:

1. *To enable the student to develop analytical skill in organic qualitative analysis and to develop preparative skills in organic preparations involving two or three stages .*
2. *To enable the students to understand better the concepts of organic analysis and appreciate better the applications of organic chemistry towards chemical, industrial and biological systems.*
3. *To enable to students to understand the mechanism involved in the name reactions and conditions of the reactions involving the preparations.*
4. *At the end of the course the student should be able to plan experimental projects and execute them.*

1. Analysis of two component and three component mixtures; separation and characterization of compounds.

2. Preparations involving two or three stages comprising of the following processes.

   a) Nitration
   b) Halogenation
   c) Diazotization
   d) Rearrangement
   e) Hydrolysis
   f) Reduction
   g) Alkylation
   h) Oxidation

3. Preparations illustrating the following:

   a) Benzoin condensation
   b) Cannizaro reaction
   c) Perkin reaction

d) Fries rearrangement

e) Reimer-Teimann reaction

f) Sandmeyer reaction

g) Skraup synthesis

REFERENCE 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(Organic), S. Chand and Co., 1987.
3. Vogel's Textbook of Practical organic chemistry, 401 edition, ELBS/Longman, England, 1984.

CH-1811 INORGANIC QUANTITATIVE ANALYSIS AND SYNTHESIS

SEMESTER :I **CREDIT :3**
CATEGORY :MC **NO. OF HOURS/WEEK :4**

Objectives:

1. *To improve the skill in quantitative estimation of metal ions by colorimetry.*
2. *To improve the skill in quantitative estimation of metal ions by complexometric titration.*
3. *To identify the methodology to quantitatively separate and estimate mixture of metal ions.*
4. *To identify the methodology to estimate a metal ion in the presence of another metal ion.*
5. *To improve the skill in synthesis of inorganic compounds.*

Unit - 1 : Colorimetry

1.1 Beer-Lambert's law and spectrophotometric method of estimation, principle and methods of visual colorimetry.

1.2 Estimation of iron and nickel by visual colorimetry.

Unit - 2 : Comptexometric Titration

2.1 Types of complexometric titrations-theories of direct titration, back titration, and substitution titrations.

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

2 3 Estimation of mixture of metal ions-pH control, masking, and demasking agents.

2.4 Determination of calcium and lead in a mixture (pH control), determination of magnesium, manganese, and zinc in a mixture using demasking agent.

2.5 Determination of manganese in the presence of iron, and nickel in the presence of iron.

Unit - 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 complexometric titration in a mixture.

Unit - 4: Synthesis

Synthesis of potassium tris(oxalato)ferrate(III), hexaamminenickel(II) tetrafluoroborate, potassium tetrachlorocuprate(II), and tris(thiourea)(sulfato)zinc(II).

REFERENCES

1. Jeffery, G. H.; Bassett, J.; Mendham, J.; Denney, R. C. Vogel's 's Textbook of Quantitative Chemical Analysis; 5th ed., ELBS" 1989.
2. Woollins, J. D. Ed., Inorganic Experiments; VCH: Weinheim, 1994.
3. Pass, G.; Sutcliffe, H. Practical Inorganic Chemistry; Chapman Hall, 1965.
4. Palmer, W. G. Experimental Inorganic Chemistry; Cambridge University Press, 1954.

SEMESTER: II

CH - 2813 : SEMINAR & REPORT

SEMESTER : I & II **CREDIT : 1**
CATEGORY :MC **NO. OF HOURS / WEEK : 2**

Seminar is offered in all the four semesters and the credit is given at the end of the fourth semester.

Objectives :

To make the student to understand and present the topics in the subject related to Chemistry in a class room.

Testing :

The student will be tested both in subject matter and the mode of presentation.

The components in the subject matter include

1) Standard of subject and plan
2) Preparation and mastery
3) Originality and logical development
4) Answers to questions
5) Summary and references

The components in the mode of presentation include

1) Economy of time
2) Voice as a tool of communication
3) Blackboard use and teaching aids
4) Language and diction
5) Relating to the audience

CH- 2814: ORGANIC SUBSTITUTION, ADDITION AND ELIMINATION REACTIONS

SEMESTER :II **CREDIT :4**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

Objectives:

1. *To understand the mechanism of a chemical reaction.*
2. *To understand the techniques involved in the substitution, addition and elimination reactions.*
3. *To appreciate the concept of substitution, addition and elimination reactions and their reaction mechanism.*

UNIT - 1 : AROMATIC AND ALIPHATIC ELECTROPHILIC SUBSTITUTION (12h)

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

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

Self study:

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

UNIT - 2 : AROMATIC AND ALIPHATIC NUCLEOPHILIC SUBSTITUTION (13h)

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

2.2 Typical 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 - Ambient 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 REACTIONS (7h)

3.1 E2, E1, E1cB and E2C mechanisms. - Syn Eliminations - E1-E2-E1cB spectrum

Orientation of the double bond: Hoffmann and Saytzeff rules

3.2 Reactivity: Effect of substrate, attacking bases, leaving group and medium. - Mechanisms and orientation in pyrolitic eliminations.

Self study:

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

UNIT - 4 : FREE RADICAL REACTIONS (6h)

4.1 Long Lived and short lived radicals - Detection of radicals and characteristics of free radical reactions. - N-group participation and free radical rearrangements, Mechanisms in aromatic substrates.

4.2 Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

Self study:

Wohl-Ziegler bromination, oxidation of aldehydes into carboxylic acids, Reed, Eglinton, Gomberg and Sandmeyer reactions.

UNIT - 5 : ADDITION TO CARBON-CARBON MULTIPLE BONDS (10h)

5.1 Mechanism: Electrophilic, nucleophilic, free radical addition.

5.2 Orientation and Reactivity: Stereochemical orientation, addition to cyclopropane rings.

5.3 Reactions: Addition of hydro-hydro; -halo; -hydroxy; -alkoxy; -acyloxy; -alkylthio; -amino; -amido; -alkyl; -acyl; -carboxy; -carbonyl; -allyl groups to double bonds. Addition of dihydro-oxo; dialkyl groups to triple bonds. Addition of boranes. Addition of halogen-oxygen; dihydroxy addition; oxyamination; diamination.

Self study:

Stork-Eschenmoser hypothesis, Nazarov cyclization, Michael and Koch reactions.

TEXT BOOKS

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

REFERENCE BOOKS

5. S. H. Pine, Organic Chemistry, 5th edn, McGraw Hill International Edn, 1987.
6. L. F. Fieser and M. Fieser, Organic Chemistry, Asia Publishing House, Bombay, 2000.
7. E.S. Gould, Mechanism and structure in organic chemistry, Holt, Rinehart and Winston Inc., 1959.

CH-2815: CHEMISTRY OF MAIN GROUP ELEMENTS

SEMESTER :II **CREDIT :4**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

Objectives:

1. *To know the different kinds of compounds of the main group elements.*
2. *To know the structure and bonding in inorganic chains, rings, and cages.*
3. *To identify ligands of main group elements and complexing agents for main group metals.*
4. *To know the synthetic techniques in inorganic chemistry.*
5. *To identify specific reagents of main group elements and to synthesize important classes of nonmetal compounds.*

UNIT - 1 : NATURE OF BONDING OF MAIN GROUP ELEMENTS (10h)

1.1 Types of compounds and E-H, E-X, E-O, and E-N bond types for B, C, N, Si, P, and S.

1.2 Element-element and multiple bonding.

1.3 Catenation and heterocatenation: polysilanes and polyphosphazenes.

1.4 Alkali and alkaline earth metal complexes: ligands-alkylamines, alkoxides, β-diketones, crown ethers, cryptands, and calixeranes

1.5 Electron deficient, electron precise, and electron rich compounds of main group elements.

1.6 Allotropes of carbon: graphite, diamond, fullerenes-types and structures, carbon nanotubes.

1.7 Biological significance: chlorophyll, Na^+/K^+ ion pump, biological roles of alkali and alkaline earth metal ions and ionophores.

Self study:

(a) Small chain and polymer of silicons-preparation and uses.

(b) A comparative study of electron deficient, electron precise, and electron rich compounds of main group elements and their reactivity.

(c) Si and P compounds with element-element and double bonds.

UNIT - 2 : INORGANIC CHAINS, RINGS, AND CAGES(16h)

2.1 Chemistry of simple boranes, silanes, phosphanes and sulphanes.

2.2 Boranes: 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.

2.3 Carboranes: synthesis and polyhedral geometries, metalloboranes, and metallocarboranes.

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

2.5 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 and cyclopolysilanes.

2.6 Isopoly and heteropoly acids and salts: isopolymolybdates and isopolytungstates; heteropolyanions-structure and reactivity; heteropoly blues.

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

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

Self study:

(a) Borazine as inorganic analogue of benzene, its reactivity, and derivatives.

(b) Synthesis and uses of polyanions and cations.

(c) Natural and synthetic zeolites and application of zeolites as molecular sieves.

UNIT-3: NITROGEN AND PHOSPHORUS LIGANDS AND MAIN GROUP ORGANOMETALLICS (7h)

3.1 Nitrogen ligands: macrocyclic amines, imines, polyimines, phthalocyanines, porphyrins, and polypyrazolyl borate ligands.

3.2 Phosphorus ligands: phosphine, monophosphines, diphosphines, polydentate phosphines, and macrocyclic phosphines.

3.3 Organometals of Li, Be, and Mg: synthesis and applications.

3.4 Organometals of Si and Al: silsesquioxanes, aryl- and alkyl silicon halides, aluminium alkyls.

Self study:

(a) Illustrative examples of transition metal complexes of different kinds of N and P ligands.

(b) Organometallic compounds of alkali- and alkaline earth metals in synthesis.

UNIT - 4 : HALOGEN AND NOBLE GAS CHEMISTRY (7H)

4.1 Halogen oxides and oxo compounds: dichlorine monooxide, chlorine dioxide, dibromine monooxide, and iodine pentaoxide-preparation and properties; halogen oxyfluorides (trioxohalofluorides) and ionic oxyhalogen species.

4.2 Xenon oxides and fluorides: xenon trioxide, xenon difluoride, xenon tetrafluoride, xenon oxofluoride.

4.3 Halogen compounds of nitrogen: nitrogen trifluoride, tetrafluorohydrazine, dinitrogen difluoride, haloamines, oxohalides, and nitrogen trifluoride oxide.

4.4 Sulfur fluorides: Synthesis and reactivity of disulfur difluoride, sulfur tetrafluoride, substituted sulfur fluorides.

Self study

(a) Structure of halogen oxides and halogen oxo compounds with the aid of VSEPR model.

(b) Reactivity of the halides of N, S, and Xe and applications.

UNIT - 5 : SYNTHESIS AND TECHNIQUES IN MAIN GROUP CHEMISTRY (8h)

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

5.2 Solvolysis of nonmetal halides, synthesis of chains, rings, and polyhedra of B, N, and P.

5.2 Synthesis of important classes of nonmetal compounds: catenation by coupling (cyclic silicon and phosphorus compounds); hydrometalation-hydroboration and hydroalumination; substitution by hydrogen and organics (hydrogenation and alkylation/arylation).

5.4 Reactivity of boranes: hydroboration reaction as precursor for metalloborane and heteroborane clusters.

Self study:

*(*a) Special techniques for the synthesis of inorganic compounds: the chemical vacuum line, plasmas, photochemical apparatus, and electrolysis.

(b) Synthetic importance of diborane, boranes, PCl_3, and silylating agents.

TEXT BOOKS

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th ed.; Wiley Interscience: New York, 1988.
2. J. E. Huheey, E. A. Keiter, and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: New York, 1983.
3. K. F. Purcell, and J. C. Kotz, Inorganic Chemistry; Saunders: Philadelphia, 1976.

REFERENCE BOOKS

4. D. F. Shriver, P. W. Atkins, and C. H. Langford, Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.
5. T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn, McGraw-Hill International Edition, 1991.
7. G. S. Girolami, T. B. Rauchfuss, and R. J. Angelici, Synthesis and Technique in Inorganic Chemistry, 3rd ed., University Science Books, Sausalito, 1999.
8. W. L. Jolly, The Synthesis and Characterisation of Inorganic Compounds, Prentice Hall, New Jercy, 1970.

CH-2816: THERMODYNAMICS AND STATISTICAL MECHANICS

SEMESTER :II **CREDIT :4**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

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 (8h)

Self study: Zeroth, first, second and third laws of thermodynamics and thermodynamic properties that emerge out these laws.

1.1. Thermodynamic systems of variable composition: Partial molar quantities - Chemical potential. Gibbs-Duhem equation. Determination of partial molar quantities. Thermodynamic aspects of extraction of metals- Reduction of oxides and sulphides - 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

UNIT - 2 : EQUILIBRIA (8h)

Self study: Derivation of Kirchoff's equation and calculation of enthalpy of a reaction at different temperatures.

2.1. Chemical equilibrium: Reactions involving gases and solutions-Temperature dependence of equilibrium constants. Kirchoff's equation and calculation of equilibrium constant.

Self study: Thermodynamic derivation of phase rule and its application to one and two component systems.

2.2. Phase equilibria: Applications to binary liquid systems-Separation of two miscible liquids – Fractional distillation, formation azeotropic mixture.

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.

UNIT-3 : IRREVERSIBLE THERMODYNAMICS (8h)

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

3.2. Onsager theory: Validity and verification.

3.3. Thermoelectricity-Electro kinetic and thermo mechanical effects

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

UNIT-4 : STATISTICAL CONCEPTS OF THERMODYNAMICS (16H)

Self study: Results of particle in a box (1D, 2D and 3D); rigid rotor; and harmonic oscillator.

4.1. Macro and micro states: Distribution of particles in different energy levels. Most probable distribution. Maxwel-Boltzmann statistics. Distribution of molecular velocities- Most probable, average and RMS velocities.

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

4.3. 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 para hydrogen and mixture of the two viz., o-H_2 and p-H_2.

Heat capacity of solids- Einstein and Debye models – thermodynamic properties of solids

UNIT-5 : APPLICATIONS OF STATISTICAL THERMODYNAMICS (10h)

5.1. Quantum Statistics

Bose-Einstein statistics-Theory of paramagnetism. Statistics of a photon gas and liquid helium

Fermi-Dirac statistics-Thermonic emission-Electron gas (metals)

5.2. Equilibrium theory of chemical reaction rates

Rate of association and dissociation. Effect of rotation on the latter. ARRT - Calculation of rate constant and temperature coefficient of rate constant.

TEXT BOOKS

1. K. Rajaram and J.C. Kuriacose, Thermodynamics For Students of Chemistry, 2nd Edition, S.L.N. Chand and Co, Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A.Benjamin Publishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt., Ltd., New Delhi, 1995.

REFERENCES BOOKS

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

CH- 2817: LABORATORY TECHNIQUES IN ORGANIC CHEMISTRY-II

SEMESTER :II **CREDIT :3**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

Objectives:

1. *To enable the student to develop analytical skill in organic quantitative analysis*
2. *To understand the techniques involved in the preparation of standard solutions, standardization and calculations in the estimations of compounds.*
3. *To appreciate and apply the techniques involved in the estimation of substances.*

Unit - 1 : Estimation of the following organic compounds

a) Phenols

b) Ketones (ethyl methyl ketone)

c) Sugars (Glucose)

d) Ascorbic acid (Vitamin-C tablets)

e) Amino groups (aromatic amines)

f) Nitro groups (aromatic nitro compounds)

g) Amino acids (Glycine)

Unit - 2 :Extraction and estimation of

a) Caeffine from coffee

b) Nicotine from tobacco leaves

c) Citric acid from citrus fruits

Unit - 3 : Separation of components of a mixture using

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 BOOKS

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

CH-2818: INORGANIC SEMIMICRO QUALITATIVE ANALYSIS

SEMESTER :II **CREDIT :3**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

Objectives:

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

Unit - 1 : Theoretical Principles

1.1 Classification of cations into groups, group reagents

1.2 Intergroup and intragroup separations

1.3 Confirmatory test for cations-the reactions and the products

Unit - 2 : Analysis of Mixture of Cations

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

Common cations: Group I: Pb and Hg; Group II: Hg, Cu, Cd, Bi, Sb, As, and Sn; Group III: Al, Fe, and Cr; Group IV: Mn, Zn, Co, and Ni; Group V: Ca, Sr, and Ba; Group VI: Mg, K, and NH_4^+.

Rare cations: Group I: W and Tl; Group IA: Se and Te; Group II: Mo; Group III: Be, Tl, Ce, Ti, Th, Zr, V, and U; Group VI: Li

TEXT BOOK

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rd ed., The National Publishing Company, Chennai, 1974.

REFERENCE BOOK

2. Vogel's Text book of Inorganic Qualitative Analysis, 4th Ed, ELBS, London, 1974.

CH- 2953: HETEROCYCLICS AND NATURAL PRODUCTS

SEMESTER :II **CREDIT :4**
CATEGORY :SUBJECT ELECTIVE(SE) **NO. OF HOURS / WEEK :4**

Objectives:

1. *To enable the student to understand and appreciate the importance of heterocyclic compounds*
2. *To understand the techniques involved in the extraction and methods of determination of structure of alkaloids and terpenes.*
3. *To understand and appreciate the steroid chemistry and its importance in the living systems.*

UNIT - 1 : HETEROCYCLIC CHEMISTRY: (15h)

1.1 Nomenclature – reactivity – aromaticity – spectral properties.

1.2 Elementary study of the following systems only – indole, isoindole – oxazole, imidazole, thiazole, pyridines, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid, xanthiones and flavonoids.

Self study:

Synthesis and reactions of 5 membered (pyrrole, thiophene, furan) and 6 membered heterocyclic compounds (pyridine), fused rings (quinoline and isoquinoline)

UNIT - 2 : ALKALOIDS (10h)

2.1 General methods of structural elucidation of alkaloids -a general survey.

2.2 The structural elucidation of Belladine, Papaverine, Cocaine, Atropine, Heptaphylline, Peepuloidin, Morphine.

Self study:

Occurrence, isolation, classification, functions and general properties of alkaloids.

UNIT - 3 : TERPENES (6h)

3.1 General methods of determination of structure.

3.2 Structural elucidation of Camphor, Cadinene, Vitamin A, Abietic acid, Gibberelic acid, Zinziberine and Squalene

Self study:

Occurrence, isolation, classification, functions and general properties of terpenes.

UNIT 4 : STEROIDS (6h)

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

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

4.3 Synthesis of cholestrol, androgens, oestrone, progesterone and cortisone. (questions on complete synthesis is not included for examination)

Self study:

Nomenclature and classification of steroids, steroidal alkaloids

UNIT - 5 : ANTHOCYANINS (8h)

5.1 General nature of anthocyanins – structure of the anthocyanidins

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 – depsides – tannins.

Self study:

Synthesis of delphinidin chloride, peonidin chloride, malvidin chloride, and quercetin.

TEXT BOOKS

1. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 1, Goel Publishing House, Meerut, 1997.
2. O. P. Agarwal, Chemistry of Organic Natural Products, Vol. 2, Goel Publishing House, Meerut, 1997.
3. I. L. Finar, Organic Chemistry Vol-2, 5th edn, Pearson Education Asia, 1975.

REFERENCE BOOKS

4. T.L. Gilchrist, Heterocyclic Chemistry, Longman Scientific and Tech, 1985
5. I. L. Finar, Organic Chemistry Vol-1, 6th edn, Pearson Education Asia, 2004.
6. Pelletier, Chemistry of alkaloids, Van Nostrand Reinhold Co, 2000.
7. Shoppe, Chemistry of the steroids, Butterworthes, 1994.

CH -2954 : NUCLEAR AND RADIO CHEMISTRY

SEMESTER :II **CREDIT :4**
CATEGORY :SUBJECT ELECTIVE(SE) **NO. OF HOURS / WEEK :4**

Objectives:

01. To make the students knowledgeable in nuclear chemistry.
02. To familiarize the students with nuclear and radioisotopes techniques.
03. To equip the students for their future career in nuclear industry.

UNIT - 1 : THE NUCLEUS (10h)

1.1 Radius of atomic nuclei: binding energy of nuclei, force between nucleons.

1.2 Nuclear moment: nuclear angular momentum, nuclear magnetic dipole moment, electric quadrupole moment - NQR

1.3 Nuclear models: liquid drop model, nuclear shell model, fermi gas model.

Self Study:

The subatomic particles: electron, proton, neutron, antiproton, positron, meson, quacks. Mass of nuclei: isotopes, isobars, mass spectrometry-identification of isotopes.

UNIT - 2 : RADIOCHEMISTRY (15H)

2.1 Alpha decay: theory of emission, alpha-ray energy spectra.

2.2 Beta-decay: decay theory, electron capture, double beta decay.

2.3 Gamma ray: theory of emission, internal conversion, the Auger effect, nuclear resonance absorption. Principles of Mossbauer spectroscopy.

2.4 Counters: Geiger counters, scintillation counters, proportional counters, semiconductor detectors.

Self Study:

Radioactive series decay: radioactive series growth and decay, determination of half-lives.

UNIT - 3 : NUCLEAR REACTION (10H)

3.1 Types of nuclear reactions: reaction cross section-compound nucleus theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear reactions.

3.2 Source of nuclear bombarding particles: Charged particle accelerators, gamma ray, X-ray and neutron sources.

3.3 Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor - nuclear reactors in India. Fusion reactions-hydrogen bomb and energy of sun.

3.4 Transuranium elements: Synthesis, separation and properties of transuranium elements. Reprocessing of spent fuels. Solvent Extraction - Specific sequestering agents for transuranium elements.

Self Study:

Nuclear reactions – one example of each category.

UNIT - 4 : RADIATION CHEMISTRY (5H)

4.1 Interaction of radiation with matter: range of alpha, beta and gamma radiations, neutron through matter, radiation dosimetry.

4.2 Radiolysis of water: Mechanism-hydrated electron.

4.3 Radiation safety precaution: Safety standards and safe-working methods.

UNIT - 5 : ANALYTICAL METHOD IN NUCLEAR CHEMISTRY (10H)

5.1 Radio isotopes: Co-precipitation, ion-exchange, solvent extraction - as a tracer, Synthesis of labeled compounds (any two), isotopic dilution and radiopharmaceuticals.

5.2 Neutron activation analysis, positron annihilation and autoradiography.

Self Study:

Dating of objects and mechanistic study.

TEXT BOOKS

1. H. J. Arnikar, "Essentials of Nuclear Chemistry", Wiley Eastern Ltd., New Delhi (1982)
2. A.K. Srivatsava and P. Jain, "Essential of nuclear Chemistry", S.Chand, N.Delhi, 1989
3. G.R. Choppin, "Radiochemistry and Nuclear chemistry", 2002.

REFERENCE BOOKS

4. G. Friedlander, J. W. Kennedy, and J. M. Miller, "Nuclear and Radiochemistry", John Wiley and Sons Inc., Japan Second Edition (1964)
5. S. Glasstone, "Source book on Atomic Energy", Van Nostrand Co. Inc., New Jersey, Second Edition (1958)
6. R. Gopalan, "Elements of nuclear chemistry", Sultan Chand, Delhi, 2000.

SEMESTER-III

CH - 3808 : PHOTOCHEMISTRY AND ORGANIC SYNTHESIS

SEMESTER :III **CREDIT :4**
CATEGORY :MC **NO. OF HOURS / WEEK :4**

Objectives:

1. *To understand the nature of carbon-hetero atom multiple bond additions*
2. *To know the nature of addition in pericyclic reactions*
3. *To understand the chemical and photochemical organic reactions*
4. *To know the methods of synthetic strategies and applications*
5. *To apply the knowledge of chemical reactions in organic synthesis*

UNIT - 1 : Addition to carbon-hetero atom multiple bonds (6h)

1.1 Hydroboration, hydroxylation, Michael addition and 1,3-dipolar additions.

1.2 Carbenes and their addition to double bonds-Simon Smith reaction, Mannich, Stobbe, Darzens, Wittig, Wittig-Horner and benzoin reactions.

1.3 Stereochemical aspects of each reaction.

Self study:

Mechanistic study with specific examples, factors influencing addition reaction.

UNIT - 2 : Organic Synthetic Methodology (6h)

4.1 Preliminary planning; Knowns and unknowns of the synthetic system studied.

4.2 Analysis of the complex and interrelated carbon framework into simple rational precursors.

4.3 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. Convergent synthesis.

4.4 Synthesis based on umpolung concepts of seebach.

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

Self study:

Examples on retrosynthetic approach, calculation of yield, advantages of convergent synthesis.

UNIT - 5 : Modern Synthetic Reactions (13h)

5.1 Reductions: Hydrogenation and dehydrogenation: Catalytic hydrogenation: reactions

5.2 Metal hydride reductions: Typical reactions and conditions used. LAH reductions. $NaBH_4$ reductions. Hydroboration.

5.3 Dissolving metal reductions: Birch reduction. Clemmenson reduction. Electroorganic synthesis.

5.4 Reduction with hydrazine derivatives: Wolf Kishner reduction.

5.5 Oxidation with Cr and Mn compounds: Oxidation by Cr(VI) and $KMnO_4$.

5.6 Oxidation by peracids and peroxides: Oxidations using lead tetraacetate, mercuric acetate and SeO_2.

5.7 Alkylation of active methylene compounds; Aldol condensation and related reactions: Claisen-Schmidt and Knoevenagel reactions. Perkin, Stobbe and Darzens reactions. Reformatsky reaction, Wittig reaction.

5.8 Synthesis: Cubane, Prostaglandin, longifolene and norethisterone.

Self study:

Mechanism for each reactions, synthesis of organometallic compounds and reactions.

UNIT - 4 : Pericyclic Reactions (8h)

2.1 Woodward Hoffmann rules; use of FMO method and correlation diagrams; Electrocyclic reactions of 1,3,5-hexatrienes.

2.2 Cycloaddition; 2+2 and 2+4 cycloadditions; The Mobius Huckle concept.

2.3 Sigmatropic rearrangements: (1,3), (1,5) and (3,3) carbon migration.

2.4 Cheletropic reaction (use of FMO method and correlation diagrams)

Self study:

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

UNIT - 5 : Organic Photochemistry (12h)

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

3.2 Reactions of electronically excited ketones; $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ triplets; alpha cleavage or Norrish type I cleavage. Gamma hydrogen transfer or Norrish type II cleavage; photo reductions; Paterno-Buchi reactions; photochemistry of an α,β-unsaturated ketones; cis-trans isomerisation.

3.3 Photocycloadditions: Photochemistry of aromatic compounds; photochemical rearrangements; photostationery state; 1,3,5-trimethylbenzene to 1,2,4-trimethylbenzene; di-π-methane rearrangement; Reaction of conjugated cyclohexadienone to 3,4-diphenyl phenols; Barton's reactions; α-tropolone methyl ether to 4-oxo-2-cyclopentyl acetate; Low temperature photochemistry.

Self study:

Modified Jablonskii diagram, luminescence, lifetimes, quantum yield, Zimmerman approach of photochemical rearrangements, pivot mechanism.

TEXT BOOKS

1. Francis A.Carey and Sundberg, Advanced Organic Chemistry, 5th edition, Tata McGraw-Hill, New York, 2003.
2. Jerry March, Advanced Organic Chemistry,
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

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1. Gill and Wills, Pericyclic Reactions, Chapman Hall, London, 1974
2. Carruthers W, Modern methods of organic synthesis, Cambriudge Uni.Press, 1993.
3. Norman R.O.C., Organic synthesis, Chapman Hall, London, 1980

CH- 3809 : COORDINATION CHEMISTRY

SEMESTER :III **CREDIT :4**
CATEGORY :MC **NO. OF HOURS / WEEK :5**

Objectives:

1 To know the nature of metal-ligand bonding in coordination compounds and quantification of the bonding parameters.
2 To know the chemical and photochemical behavior of coordination compounds.
3 To understand the importance of coordination compounds in the emerging field of supramolecular chemistry and nanotechnology.
4 To know the application potential of coordination compounds in catalysis and in biology.

UNIT - 1 : Theories of Coordination Compounds (10h)

1.1 Crystal Field Theory: crystal field splitting in T_d and O_h fields, HS vs 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_τ and their relationship.

Self study:

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

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

(c) Evidences of crystal field splitting.

UNIT - 2 : Electronic Structure and Geometry of Coordination Compounds (6h)

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^n metal 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.

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

UNIT - 3 : Organometallic Compounds and Reaction Mechanisms (10h)

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) alkene polymerization (Ziegler-Natta polymerization), (c) alkene hydrogenation (Wilkinson catalyst), (d) carbonylation, (e) hydroformylation, (f) hydrocarboxylation, (g) 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 (6h)

4.1 Crystal field and charge transfer photochemistry: photosubstitution and photoisomerization.

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

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

UNIT - 5 : Bioinorganic Chemistry (8h)

5.1 Heme proteins: hemoglobin and myoglobin-structure, mechanism oxygen transport.

5.2 Copper proteins: type-I, type-II, and type-III copper.

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

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

Self study:

(a) Essential and trace elements in biology.

(b) Synthetic oxygen carriers.

REFERENCE BOOKS

1 Huheey, J. E., Keiter, E. A.; Keiter, R. L. Inorganic Chemistry, 4th ed.; Harper and Row: New York, 1983.
2 Cotton, F. A.; Wilkinson. G.; Murillo, C. A.; Bochmann, M. Advanced Inorganic Chemistry, 6th ed.; Wiley Inter-science: New York, 1988
3 Purcell, K. F.; Kotz, J. C. Inorganic Chemistry; Saunders: Philadelphia, 1976.
4 Lever. A. B. P. Inorganic Electronic Spectroscopy, 2nd ed.; Elsevier: Amsterdam, 1984.
5 Nakamoto. K. Infrared and Raman Spectra of Inorganic and coordination Compounds, Part B: 5th ed.; John Wiley & Sons Inc.: New York, 1997.
6 Drago, R. S. Physical Methods in Chemistry; Saunders: Philadelphia, 1977.
7 Tobe, M. L.; Burgess, J. Inorganic Reaction Mechanisms; Longman: New York, 1999.
8 Weil, J. A.; Bolton, J. R.; Wertz, J. E. Electron Paramagnetic Resonance; Wiley Interscience: 1994.
9 Kahn, O. Molecular Magnetism, VCH: Weinheim, 1993.
10 Steed J. W., Atwood J. L., Supramolecular Chemistry, John Wiley & Sons Ltd.: New York, 2000.
11 Lehn J. M., Supramolecular Chemistry, Concepts and Prespectives, VCH: Weinheim, 1995.

CH - 3810 : MOLECULAR SPECTROSCOPY

SEMESTER : III CREDIT : 4
CATEGORY : MC NO. OF HOURS / WEEK : 5

Objectives:

1. *To know quantization of energy and the interaction of electromagnetic radiation with matter.*
2. *To learn the fundamentals of molecular spectroscopy.*
3. *To understand the mathematical foundations of different branches of spectroscopy.*
4. *To know the application of spectroscopy to study the structure of molecules.*

UNIT - 1 : Introduction to Spectroscopy (5h)

1.1 Electromagnetic radiation: quantization of energy; rotational, vibrational, and electronic energy levels and transitions in molecules; regions and representation of spectra.

1.2 Resolution and intensity of spectral transition: signal-to-noise ratio; width of spectral lines-collision broadening, Doppler broadening, Heisenberg uncertainty principle; intensity of spectral lines-selection rules and transition probability, transition moment integral, Einstein absorption and emission coefficients, Boltzmann distribution.

1.3 Enhancing sensitivity of spectral lines: Fourier transform (FT) and computer averaging techniques (CAT).

Self study:

Techniques and instrumentation of microwave, IR and UV-Visible spectrometers.

UNIT - 2 : Rotational and Vibrational Spectroscopy (13h)

2.1 Diatomic molecules as rigid rotors: rotational energy levels, intensity of spectral lines, selection rules, effect of isotopic substitution.

2.2 Diatomic molecules as non-rigid rotors: rotational transitions, centrifugal distortion constant; rotational spectra of linear and symmetric top polyatomic molecules.

2.3 Vibrating diatomic molecule: energy of diatomic molecules as simple harmonic oscillator- energy levels, vibrational transitions, selection rules; anharmonic oscillator-energy levels, selection rules, vibrational transitions.

2.4 Diatomic vibrating rotator: Born-Oppenheimer approximation, vibration-rotation spectra, selection rules, P, Q, R branches.

2.5 Vibrations of polyatomic molecules: symmetry and fundamental vibrations, normal modes of vibration, overtones, combination, difference bands; influence of rotations on the spectra of polyatomic molecules-parallel and perpendicular vibrations in linear and symmetric top molecules.

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

2.7 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; rotation-vibration Raman spectra of diatomic molecules.

2.8 Applications of IR and Raman spectroscopy: skeletal and group vibrations, fingerprinting and absorption frequencies of functional groups for inorganic and organic compounds.

Self study:

(a) Schematic representations of fundamental vibrations of linear and nonlinear molecules.

(b) Characteristic group absorptions of organic molecules.

UNIT - 3 : Electronic Spectroscopy (10h)

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

3.2 Chemical analysis by electronic spectroscopy: assignment of electronic transitions, application to the study of organic compounds.

3.3 Emission spectroscopy: fate of electronically excited molecules-dissociation, reemission, fluorescence, phosphorescence; emission spectra of molecules.

3.4 Lasers: nature of stimulated emission-coherence and monochromaticity, population inversion, cavity and mode characteristics, Q-switching, mode locking; types of lasers-solid-state, gas, chemical, and dye lasers.

3.5 Photoelectron spectroscopy (PES): principle and technique of PES, ultraviolet PES, X-ray PES.

Self study:

(a) Woodward-Fieser rules to the structural studies of conjugated diones and unsaturated ketones.

(b) Photoactive inorganic and organic compounds.

UNIT - 4 : Magnetic Resonance Spectroscopy (NMR and EPR) (12h)

4.1 Theory of NMR spectroscopy: nuclear spin and magnetic nuclei, nuclear magnetic moment, behavior of a bar magnet in a magnetic field, the NMR transition, the Bloch equations, relaxation mechanisms.

4.2 Parameters of NMR: measuring the chemical shift, shielding and deshielding of magnetic nucleus, chemical shifts in aliphatic and aromatic compounds, factors affecting chemical shift-inductive effect, anisotropy of chemical bonds, hydrogen-bond, temperature, solvent.

4.3 Spin-spin splitting: effect of spin-spin splitting on the spectrum, mechanism of spin-spin splitting, chemical exchange, coupling constants; application of spin-spin splitting to structure determination-geminal-, vicinal-, long-range coupling; factors influencing geminal and vicinal coupling.

4.4 FT and two dimensional NMR spectroscopy: principle of FT NMR-FIDs, Fourier transformation; ^{13}C, ^{19}F, ^{31}P NMR-range of chemical shift values, spectra of typical examples; 2D NMR spectra-introduction and types of 2D techniques.

4.5 Electron paramagnetic resonance spectroscopy: theory of epr spectroscopy, 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, epr spectra of triplet states and zero field splitting.

Self study:

(a) Survey of proton chemical shift values in different classes of organic compounds.

(b) Solvents and standards used in ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR.

UNIT - 5 : NQR and Mossbauer Spectroscopy and Mass Spectrometry (10h)

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

5.2 NQR spectra: effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure.

5.3 Principles of Mössbauer spectroscopy: Doppler shift, recoil energy, experimental technique- sources, absorber, calibration.

5.4 Mössbauer spectra: isomer shift, quadrupole splitting, magnetic hyperfine interaction, chemical applications-isomer shift and quadrupole splitting in iron complexes.

5.5 Mass spectrometry: ion production-electron impact and chemical ionization, field desorption, FAB, electrospray ionization, MALDI; ion analysis-magnetic field reflections, quadrupole mass spectrometry, time of flight, tandem mass spectrometry, FT-ICR.

5.6 Determination of molecular formula: molecular ion and isotope peaks, fragmentation, rearrangements; mass spectra of different classes of organic compounds.

Self study:

Nature of compounds and ionization modes in mass spectrometry.

REFERENCE BOOKS

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, New Delhi, 2000.
2. K. V. Raman, R. Gopalan and P. S. Raghavan, Molecular Spectroscopy, Thomson and Vijay Nicole, Singapore, 2004.
3. P. Atkins and J. de Paula, Physical Chemistry, 7th ed., Oxford University Press, Oxford, 2002.
4. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons, New York, 1974.
5. A. Rahman, Nuclear Magnetic Resonance-Basic Principles, Springer-Verlag, New York, 1986.
6. D. L. Andrews, Lasers in Chemistry, 3rd ed., Springer-Verlag, London, 1997.
7. K. Nakamoto, Infrared and Raman Spectra of Inorganic and coordination Compounds, Part B: 5th ed., John Wiley & Sons Inc., New York, 1997.
8. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1977.
9. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience: 1994.
10 D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 4th ed., Tata McGraw-Hill Publishing Company, New Delhi, 1988.
11. R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th ed., John Wiley & Sons, New York, 2003.

CH - 3811: INSTRUMENTAL METHODS OF ANALYSIS

SEMESTER :III **CREDIT : 3**
CATEGORY :MC **NO. OF HOURS / WEEK : 4**

Objectives:.

2. To learn the sample handlin
1. To learn the operations of instruments g techniques and data processing
3. To analyse and estimate quantitative parameters in some instrumental technique.
4. To analyse qualitatively the spectrum of certain chemical compounds.

Experiments:

1. Determination of functional groups using FTIR 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. Estimation of Na/K/Ca using flame photometer.
7. Separation and estimation of compounds using column chromatography.
8. Estimation of iron by redox method using potentiometer.
9. Estimation of concentration of halides using potentiometer.
10. Determination of pK_{a1} and pK_{a2} of a weak dibasic acid using potentiometer.
11. Determination of solubility product of inorganic compounds using conductometer.
12. Determination of Ka and Kb of a weak acid or a weak base by conductometry method.
13. Analysis of a mixture of two metal ions by polarography.
14. Determination of DEp of a redox system by Cyclic voltammetry.

CH - 3812 : CHEMICAL KINETICS

SEMESTER :III **CREDIT : 4**
CATEGORY :MC **NO. OF HOURS / WEEK : 4**

Objectives:

To elucidate the use of chemical kinetics in understanding reaction mechanisms and to apply the theories and concepts of it for homogenous and heterogeneous catalysed reactions.

UNIT - 1 : Theories of reaction rate (9h)

1.1 Scope, laws of chemical kinetics, stoichiometry; time and true order; determination of order of reaction.

1.2 Influence of temperature on reaction rate; potential energy surface, contour diagrams.

1.3 Kinetic theory of collisions; ARRT, derivation of rate equations; application of ARRT to reactions between (i) atoms (ii) molecules (iii) atoms and molecules.

Self study:

Factors affecting rate of chemical reactions, Collisions theory

UNIT - 2 : Elementary reactions in gas phase and in solution: (9h)

2.1 Unimolecular reactions, Lindemann - Christiansen hypothesis; bimolecular reactions in gas phase (involving atoms and free radicals)

2.2 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.

2.3 Electrostriction; influence of hydrostatic pressure; volume of activation. Linear free energy relationship, Hammett and Taft equations

Self study:

Comparison between order and molecularity of a chemical reaction.

UNIT - 3 : Homogeneous and Heterogeneous Catalysis(9h)

3.1 General catalytic mechanisms. Equilibrium and steady state treatments Enzyme catalysis; Michalis-Menten kinetics; activation energies of enzyme-catalyzed reaction Acid - base catalysis - protolytic and prototropic mechanisms. Acidity functions - Kinetic methods of analysis

3.2 Chemisorption and Physisorption; Langmuir's adsorption isotherm; competitive adsorption-Mechanisms of reactions on surfaces (Langmuir, Rideal and Langmuir-Hinshelwood mechanisms);

3.3 Activation energies Non- ideal adsorption; multiplayer adsorption; capillary condensation; measurement of surface area, BET equation

Self study:

Factors affecting enzyme catalysed reactions, effect of pH on enzymes

UNIT - 4 : Complex reactions: (9h)

4.1 Rate expressions for opposing, parallel and consecutive reactions; Chain reactions - Thermal and photochemical reactions; steady-state approximations; Stern-Volmer equation;

4,2 Reactions between hydrogen and halogens - Gas phase auto oxidation; explosion and explosion limits.

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

UNIT - 5 : Kinetic data to reaction mechanisms (9h)

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

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

Self study:

Units of rate constants for different orders of the reactions.

TEXT BOOKS:

1. K.J. Laidler, " Chemical Kinetics", 3rd edn. 1987, Harper and Row Publishers. New York
2. J. Rajaram and J.C. Kuriokose, " Kinetics and Mechanisms of chemical transformation, 1st edn 1993, Macmillan India Ltd, Delhi

REFERENCES:

1. A.A. Frost and R.G. Pearson, " Kinetics and Mechanism",(2nd edn), 1963, John Wiley and sons INC
2. K.B. Ytsiimiriski, " Kinetic Methods of Analysis" 1996, Pergamom press.

3. K.K.Rohatgi Mukherjee, "Fundamentals of Photochemistry", Revised edition 1978, New Age International Publishers, New Delhi.
4. Donald A.McQuarrie and John D.Simon, "Physical Chemistry-A Molecular Approach" 1st Edition 1998, Viva Books Private Limited, New Delhi.

CH - 3875 : MATERIAL SCIENCE

M.Sc. Chemistry(Offered by both Chemistry & Physics departments)

SEMESTER :III **CREDIT : 2**
CATEGORY :ID **NO. OF HOURS / WEEK : 3**

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 - I : Symmetry and diffraction in crystals (10h)

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 diffractions 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 - II : 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 - III : Metallics Compounds. (5h)

3.1 One, two and three dimensional compounds – Preparation and examples. One Dimensional conducting solids, Na_xWO_3, Tetracyanoplatinates, $(SN)_x$.

3.2 Two dimensional conducting solids – Graphite, Graphite interclation compounds, Li^+ Interclated with TiS_2, TaS_2 and Mo_6S_8 Cheverel phases

UNIT - IV : Semiconductors and Superconductors. (15h)

4.1 Semiconductors, its infulence on doping on band gap. Defect semiconductors – Metal oxides and halides and sulphides. Control Valence semiconductors.

4.2 Applications : p-n junction, photo voltaic cell and for solar conversion. Photo galvonic and photoelctrolytic Cell, Photo electro catalytic splitting of water using TiO_2, $SrTiO_3$, $TiO_{2-x}F_x$ and $WO_{3-x}F_x$. Hydron as the future Fuel.

4.3 Superconductivity: Meissner effect, Critical Temperature and Critical Magnetic Field – Type I and Type II Superconductors, Ternary Oxides – Structure of 123 Oxides (Y-Ba-Cu-O). Cheveral phases ($PbxMo_6S_8$). BCS Theory of Superconductivity –Cooper Pair Electrons. Josephson Effect. Applications of Super-conducting compounds.

Unit - V : Materials (10h)

5.1 Soft and hard magnets – Domain theory – Hysterisis Loop - Applications. Magnato resistance and GMR materials. Ferromagnetic and Antiferromagnetic materials – Examples and Applications.

5.2 Ferro electric, Piezo elecric, pyroelectric matrials and their properties. Solid state electrolytes – Na^+ in b -Alumina and YSZ. Shape memory Alloys. Non-linear optics – Second Harmonic Generators (SHG) – Mixing of Laser wave lengths by Quartz, Ruby and $LiNbO_3$

REFERENCE BOOKS:

1. V. Raghavan, Mateiral Science and Engineering, Prutice Hall of India, New Delhi, 1991.
2. S. O. Pillai, Solid State Physics, Newage Int. (P) Ltd., 1995.
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4. C.Kittel, Solidstate Physics, John-Wiley and sons, NY,1966
5. W.L.Jolly, Modern Inorganic Chemistry, Mc Graw Hill Book Company, NY,1989
6. H.P.Meyers, Introductroy Solid State Physics, Viva Books Private Limited,1998
7. A.R.West, solid State Chemistry and Applications, John-Wiley and sons, 1987
8. D.F.Shriver and P.W.Atkins, Inorganic Chemistry, Oxfort university press,1990

SEMESTER-IV

CH - 4808 : ELECTROCHEMISTRY

SEMESTER :IV **CREDIT : 4**
CATEGORY :MC **NO. OF HOURS / WEEK :5**

Objectives:

After this course the student should be able

i. To understand the behavior of electrolytes in solution
ii. To know the structure of the electrode surface
iii. To differentiate electrode kinetics from other types kinetic studies
iv. To know the applications electrode process

UNIT - 1 : Ionics

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. Expression 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.

UNIT - 2 : Electrical Double Layer

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:

Faradays laws of electrolysis. Significance and numerical problems. Role of applied potential and current.

UNIT - 3 : Electrodics of elementary electrode reactions

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

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.

UNIT - 5 : Concentration Polarisation

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 supporting electrolyte Theory of diffusion over potential. Polarography- Limiting current density and its importance:

5.2. Electro organic reactions at the electrodes.

Reduction of aldehydes to alcohols, nitrobenzene to aniline, acetone to isopropyl alcohol or pinacol , quinone to hydroquinone.

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 & 2, Plenum Press , New York ,1970.
2. S.Glasstone, "Electro chemistry", Affiliated East-West Press, Pvt., Ltd., New Delhi, 1974.
3. L.Antropov , "Theoretical Electro Chemistry", Mir Publications , Moscow , 1977.

REFERENCE BOOKS

4. D.A.McQurrie and J.D.Simon, "Physical Chemistry", A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
5. J.Rajaram and J.C. Kuriakose, "Kinetics and Mechanism of Electrochemical Transformations", Ch-13, Macmillan India Ltd., New Delhi, 1993.

CH-4809 : APPLICATIONS OF SPECTROSCOPY

SEMESTER :IV **CREDIT : 4**
CATEGORY :MC **NO. OF HOURS / WEEK : 5**

Objectives:

1. *To learn the applications of spectroscopy for the study and structural elucidation of molecules.*
2. *To apply the principles of mass, UV-Visible, IR, NMR, ESR, NQR spectroscopy through simple problems.*
3. *To interpret given spectra to elucidate the structures of molecules.*

UNIT - 1 : Mass Spectrometry (5h)

1.1 Determination of molecular formula: molecular ion, nitrogen rule, isotope peak, metastable ions.

1.2 Fragmentation: basic fragmentation types and rules, factors influencing fragmentation, fragmentation patterns of hydrocarbons, hydroxyl compounds, alcohols, ethers, ketones, aldehydes, carboxylic acids, amines, nitro compounds, alicyclic and heterocyclic compounds.

1.3 Applications of FAB, MALDI-TOF, ESI and ICP mass spectrometry: characterization of metal complexes, supramolecules, nanostructures, biopolymers (proteins and nuclei acids).

Self study:

(a) Nature of compounds and ionization methods employed in mass spectrometry.

(b) Common rearrangements of ions in mass spectrometry.

UNIT - 2 : UV and Visible Spectroscopy (5h)

2.1 Differentiating isomers: geometrical isomers-cis- and trans-isomers of organic and coordination compounds.

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 Electronic spectra of inorganic and coordination compounds: intensity of d-d transitions, electronic spectra of transition metal halides and oxo compounds, spin allowed crystal field transitions in octahedral and tetrahedral complexes-Orgel diagrams.

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

Self study:

Solvents used to record electronic spectrum, solvent corrections, and solvent cut off regions.

UNIT - 3 : IR Spectroscopy (8h)

3.1 Quantitative studies: calculation of force constants of IR vibrations, hydrogen bonding-intra- and intermolecular hydrogen bonding.

3.2 Conformational studies: cyclic 1,2-diols and 1,3-diols, cyclohexanes.

3.3 Characteristic group absorptions of organic compounds: carbon skleton vibrations, alcohols, phenols, ethers, peroxides, ketones, aldehydes, carboxylic acids, esters, lactones, amines, amino acids; groups absorbing in the fingerprinting region, aromatic overtones and combination bands.

3.4 Study of isomerism: linkage isomerism in coordination compounds-cyano and isocyano-, thiocyanato- and isothiocyanato complexes, geometrical isomers of organic compounds.

3.5 Interpretation of typical IR spectra of organic compounds:

3.6 Changes in the IR spectra of donor molecules upon coordination: changes in the spectra accompanying changes in symmetry upon coordination, differentiation of coordinated water and lattice water and bridging and terminal carbonyls.

3.7 IR spectra of gases: diatomic molecules, linear polyatomic molecules, nonlinear polyatomic molecules.

Self study:

(a) The absorption range of CH stretching and bending modes of vibrations in different types of organic compounds.

(b) IR spectra of organic halogen compounds, phosphorus, and silicon compounds.

UNIT - 4 : NMR Spectroscopy (12h)

4.1 Chemical shifts: region of proton chemical shift in organic molecules; chemical shift equivalence- interchange through symmetry operations, tagging, restricted rotations, magnetic equivalence.

4.2 NMR spectra of protons bonded to O, N, S: chemical exchange, hydrogen bonding, decoupling by quadrupole moment-alcohols, phenols, enols, carboxylic acids, amines, amides, carbamates.

4.3 Conformational analysis by H-H, H-C coupling constant: geminal coupling ($^2J_{H-H}$)-influence of adjacent s-bonds and electronegative substituents; vicinal coupling ($^3J_{H-H}$)-influence of dihedral angle, presence of electronegative substituent, angle strain, bond length; long-range coupling; trans-coupling, aromatic coupling, virtual coupling.

4.4 Interpretation of proton NMR spectra of different classes of organic compounds involving 2d correlations.

4.5 Coupling protons to ^{19}F, ^{31}P, ^{13}C: proton NMR spectra of typical examples.

Self study:

(a) Methods of simplifying complex NMR spectra-NMR shift reagents and high field NMR.

UNIT - 5 : ESR, NQR, and Mossbauer Spectroscopy (10h)

5.1 Hyperfine splitting: hyperfine splitting in isotropic systems involving one nucleus and more than one nucleus, hyperfine splitting caused by quadrupole nucleii.

5.2 Anisotropic systems: anisotropy in g-value, factors causing anisotropy.

5.3 EPR spectra of systems with more than one unpaired electrons: zero-field splitting, causes of ZFS, ZFS and epr transitions, epr spectrum of triplet naphthalene and high-spin Mn(II) complexes.

5.4 Applications of NQR spectroscopy: the quadrupole coupling constant e^2qQ and the asymmetry parameter interpretation of NQR spectra, structural information from NQR spectra, NQR spectra of haloorganic compounds and complexes.

5.5 Applications of Mossbauer spectroscopy: isomer shift, quadrupole splitting, magnetic interactions; magnetic and quadrupole splitting in ferromagnetic ^{57}Fe compounds, Mossbauer spectra of high- and low-spin Fe(II) and Fe(III) compounds; site symmetry of metal centers in iron complexes; differentiation of nonequivalent metal centers in polynuclear complexes; discovering oxidation states-Sn, Sn(II), Sn(IV) compounds.

5.6 Structural elucidation of compounds involving UV,IR, NMR and Mass spectra.

REFERENCE BOOKS

1. R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th ed., John Wiley & Sons, New York, 2003.
2. W. Kemp, Applications of Spectroscopy, English Language Book Society, 1987.
3. J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds.
4. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 4th ed., Tata McGraw-Hill Publishing Company, New Delhi, 1988.
5. K. Srivastava, K., Jain, P. C. Chemical Analysis, An Instrumental Approach, 3rd ed., S. Chand and Co., New Delhi, 1997.

6. K. Nakamoto, Infrared and Raman Spectra of Inorganic and coordination Compounds, Part B: 5th ed., John Wiley & Sons Inc., New York, 1997.
7. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1977.
8. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience: 1994.

CH - 4810 : SCIENTIFIC RESEARCH METHODOLOGY

SEMESTER : III CREDIT : 1
CATEGORY : MC NO. OF HOURS / WEEK : 2

The credit of this paper will be given along with the project work in IV semester.

Objectives:

1. *To introduce the purpose and importance of research for future development and sustinence.*
2. *To know the various indexes and abstracts in science and technology as a source of information in chemistry.*
3. *To learn the ways of carrying out literature search for current awareness and for retrospective survey.*
4. *To know the methodology of writing thesis and journal articles.*

UNIT - 1 : Meaning of Research (4h)

1.1 The search for knowledge, purpose of research, 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.

UNIT - 2 : Chemical Literature (4h)

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, compilations of data, synthetic methods and techniques, treatises, 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 : Chemical Abstracts (10h)

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 formulas, 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 : Scientific Writing (5h)

4.1 Scientific writings: research reports, theses, journal articles, and books.

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

4.3 Steps to publishing a scientific article in a journal: types of publications-communications, articles, reviews; when to publish, 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 (2h)

5.1 ASAP Alerts, CA Alerts, SciFinder, ChemPort, ScienceDirect, STN International.

5.2 Journal home pages.

REFERENCE BOOKS

1. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
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. B. E. Cain, The Basis of Technical Communicating, ACS., Washington, D.C., 1988.
5. H. M. Kanare, Writing the Laboratory Notebook; American Chemical Society: Washington, DC, 1985.
6. J. S. Dodd, Ed., The ACS Style Guide: A Manual for Authors and Editors; American Chemical Society: Washington, DC, 1985.
7. Gibaldi, J. Achtert, W. S. Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
8. Joseph, A. Methodology for Research; Theological Publications: Bangalore, 1986.

CH - 4811 : SEMINAR & REPORT

SEMESTER : III & IV **CREDIT : 1**
CATEGORY :MC **NO. OF HOURS / WEEK : 2**

Seminar is offered in all the four semesters and the credit is given at the end of the fourth semester.

Objectives :

To make the student to understand and present the topics in the subject related to Chemistry in a class room.

Testing :

The student will be tested both in subject matter and the mode of presentation.

The components in the subject matter include

1) Standard of subject and plan
2) Preparation and mastery
3) Originality and logical development
4) Answers to questions
5) Summary and references

The components in the mode of presentation include

1) Economy of time
2) Voice as a tool of communication
3) Blackboard use and teaching aids
4) Language and diction
5) Relating to the audience

CH 4812 : PROJECT WORK AND DESSERTATION

SEMESTER :IV **CREDIT :10**
CATEGORY :MC

CH-4955 : ORGANIC CHEMICAL TECHNOLOGY

SEMESTER :IV **CREDIT : 3**
CATEGORY :SE **NO. OF HOURS / WEEK : 4**

Objectives:

1. *To understand the elements of chemical engineering in organic synthesis*
2. *To know the unit processes in organic chemical technology*
3. *To understand the techniques involved in typical organic synthesis*
4. *To know the thermodynamics in organic unit processes*
5. *To apply the knowledge of chemical reactions in organic synthesis*

UNIT - 1 : Elements of Chemical Engineering (25h)

1.1 Unit operations in chemical engineering: Fluid flow: Reynold's number; Laminar and turbulent flow. Bernoullis' equation, head loss in piping. Calculation of head as an aid in selecting pumps. Turbulent flow and its relevance in heat transfer. Agitation and mixing of liquids.

1.2 Heat transfer: Heat transfer coefficient, Importance of heat transfer in chemical process. Special provisions for heat transfer in highly exothermic reactions. Corrosion and scale formation in heat exchangers and condensers. Preliminary data to aid design of heat transfer equipment.

1.3 Mass transfer: Distillation- two and three component systems. Ideal and non-ideal systems, various types of fractioning columns. Calculation of HETP from distillation curves. Leaching and extraction based on process parameters.

1.4 Filtration and Drying: Selection of proper equipment for above operations.

Self study:

Case study of each processes, examples on two or three component systems. Various methods of filtration and drying.

UNIT - 2 : Applications of Thermodynamics in Organic Unit Processes (6h)

2.1 Energy balance over a flow system, heat of reaction, effect of temperature upon heat of reaction

2.2 Chemical equilibrium, calculation of equilibrium conversion, entropy changes, simultaneous reactions, vapour phase and liquid phase catalytic reactions.

Self study:

Some examples of chemical equilibrium and simultaneous reactions.

UNIT - 3 : Organic Chemical Process Kinetics (5h)

3.1 Factors affecting chemical processes

3.2 Type and shape of reactors used, the method of operation, temperature control

3.3 Batch or flow process, batch mixing, fixed or fluidized bed.

Self study:

Examples of factors affecting chemical processes, model study of batch or flow processes.

UNIT - 4 :Unit Process in Industrial Organic Synthesis (12h)

4.1 Study of Organic reactions as they apply to industrial processes. Process parameters of importance in scaling up of these reactions from laboratory to pilot plant to main plant.

4.2 Selection of suitable plant equipment, especially the shape and size of the reactor stirrer, condenser etc. choice of material of construction.

4.3 Study of industrial scale nitration, sulphonation, homogeneous and heterogeneous hydrogenation, oxidation and halogenations reactions.

Self study:

Simple examples of organic reactions, study of various reactions.

UNIT - 5 : Study of Detailed Technologies of Manufacture- a dye, a drug and a pigment (12h)

5.1 Three specific chemicals, one each from the above category will be discussed, illustrating the chemical engineering principles used in proper selection of equipment

5.2 The logic involved in the layout of the plant, the control tests for the process itself and isolation methods of the product and its standardization.

5.3 Importance of quality control and technical service to customers will be pointed out.

Self study:

Study of layout of the plant, quality control parameters.

TEXT BOOKS

1. W.L. McCabe and J.C. Smith, Unit Operations of Chemical Engineering, McGraw-Hill Kogakusha Ltd., Third Edition, 1976.
2. P.H. Groggins, Unit Processes in Organic Synthesis, McGraw-Hill Kogakusha Ltd., Tokyo, Fifth Edition, 1958.

REFERENCE BOOKS

1. Dridens, Outliones of Chemical Technology, Affiliated East-West Press Pvt.Ltd, 2001.
2. BIOS, CIOS and FIAT technical reports on the German chemical industry.
3. Chris A. Clausen and Guy Matson, Principles of Industrial Chemistry, John Willey & Sons, New York, 1978.
4. Gopalarao and Marshall sittig, Outlines of Chemical Technology, Affiliated East-West Press Pvt.Ltd, 2001.

CH – 4956 : ADVANCED COORDINATION CHEMISTRY

SEMESTER :IV **CREDIT : 3**
CATEGORY :SE **NO. OF HOURS / WEEK : 4**

Objectives:

1 To quantify bonding parameters in cubic and distorted geometries from absorption spectra.
2 To identify coordination compounds with noble electrochemical and photochemical properties suitable for the construction of supramolecular assemblies and nanostructures.
3 To envision the importance of inorganic photosensitizers for solar energy conversion.
4 To identify complexes suitable for application in medicinal inorganic chemistry.
5 To set research goals in the highly topical areas of research in coordination chemistry.

UNIT - 1 : Electronic Structure and Geometry of Coordination Compounds (12h)

1.1 Electronic spectroscopy: crystal field spectra of O_h and T_d complexes, effect of distortion on the spectra, structural evidence from electronic spectra, evaluation of Δ_o and Δ_t values in Co(III) and Ni(II) O_h and T_d complexes, quantification of covalency-nephelauxetic ratio.

1.2 Tetragonal distortion in octahedral complexes and evaluation of D_q^{xy} and D_q^{z} in tetragonally distorted octahedral Co(III) complexes.

1.3 Nuclear magnetic resonance spectroscopy: application of spin-spin coupling to inorganic structural determinations, NMR spectra of quadrupolar nuclei, NMR of paramagnetic transition metal complexes: scalar shift and pseudocontact shift, scalar shift and covalency.

1.4 Electron spin resonance spectroscopy: hyperfine and zero field effects on the epr spectra of coordination compounds, ligand field interpretation of the g- and A-tensors, nuclear qudrupole interaction.

1.5 Mossbauer spectroscopy: quadrupole and magnetic interactions, isomer shift and site symmetry of metal ions in coordination compounds, Mossbauer emission spectroscopy and applications.

Self study:

(a) Causes of tetragonal distortion in transition metal complexes and their effect on the electronic spectra.

(b) Effect of quadrupole nuclei on spin-spin splitting and hyperfine splitting.

(c) Causes of anisotropy and anisotropic g-values.

UNIT - 2 : Electrochemical Studies and Photochemistry(8h)

2.1 Applications of AC polarography, cyclic voltammetry, and differential pulse voltammetry to the study of coordination compounds: computation of electrochemical parameters and evaluation of reversibility.

2.2 Spectroelectrochemistry: optically transparent electrodes and cells, chronoabsorptometry.

2.3 Solar and renewable energy: light-to-chemical energy conversion in lamellar solids and thin films, solar energy conversion by dye-sensitized photovoltaic cells and by coordination compounds anchored onto semiconductor surfaces.

2.4 Photochemistry of lanthanide complexes: A-ET-E processes, NIR-to-visible photon upconversion, nonlinear optical behavior, exciton multiplication and relaxation dynamics in quantum dots and applications.

Self study:

(a) Causes of electrochemical irreversibility and coupled chemical reactions.

(b) Ru(II) and Os(II) polypyridyl complexes employed in solar energy conversion.

UNIT - 3 : Supramolecular Assemblies and Devices (12h)

3.1 Supramolecular assemblies: design principles, homo- and heteropolymetallic polypyridyl systems, intercomponent energy and electron transfer, role of bridging ligands.

3.2 Dendrimers and metallodendrimers: synthetic methodology-divergent and convergent methodologies; types of metallodendrimers, dendrimer encapsulated catalysis.

3.3 Molecular devices: supramolecular photochemistry, photo- and electrochemical sensors, molecular electronic devices.

Self study:

(a) Terpyridine and bipyridine-appended spacers, phenazene based spacers.

(b) Different kinds of supramolecular assemblies constructed by covalent-, coordination-, and hydrogen bonding.

UNIT - 4 : Inorganic Biochemistry and Medicinal Inorganic Chemistry (12h)

4.1 Photosynthesis: biological photosynthesis, chemical approaches to artificial photosynthesis-light harvesting dendrimers and multiporphyrin arrays.

4.2 Bioredox agents: rubredoxins and ferredoxins-functions and structural features.

4.3 Contrast enhancing agents for MRI: thoeory of MRI imaging, synthesis of Gd-based contrast agents.

4.4 Metal complexes for radiotherapy: diagnostic radiopharmaceuticals, non-technitium for diagnostic imaging, Tc-labelled small molecules and peptides as diagnostic radiopharmaceuticals.

4.5 Metal complexes as photosensitizers.

Self study:

(a) Antenna effect and funneling of electronic energy in supramolecular assemblies.

(b) Generation of ^{99m}Tc chelates.

UNIT - 5 : Synthesis of Novel Coordination Compounds and Assemblies (6h)

5.1 Synthesis of Schiff base macrocycles and macrocyclic binucleating ligands by coordination template effects.

5.2 Polyazamacrocycles and macrocycles with pendant arms.

5.3 Construction of polynuclear supramolecular assemblies and nanostructures.

Self study:

(a) Design of Robson-type compartmental Schiff base macrocycles derived from 2,6-diformyl-4-methylphenol and 2,6-diformylpyridine.

(b) Methods of appending pendant arm functionalities onto macrocyclic frameworks.

REFERENCES

1 Huheey, J. E.; Keiter, E. A.; Keiter, R. L. Inorganic Chemistry, 4th ed.; Harper and Row: New York; 1983.
2 Cotton, F. A.; Wilkinson. G.; Murillo, C. A.; Bochmann, M. Advanced Inorganic Chemistry, 6th ed.; Wiley Interscience: New York; 1988.
3 Purcell, K. F.; Kotz, J. C. Inorganic Chemistry; Saunders: Philadelphia, 1976.
4 Lever. A. B. P. Inorganic Electronic Spectroscopy, 2nd Ed.; Elsevier Publishing Company: Amsterdam; 1984.
5 Drago, R. S. Physical Methods in Chemistry; Saunders: Philadelphia, 1977.
6 Weil, J. A.; Bolton, J. R.; Wertz, J. E. Electron Paramagnetic Resonance; Wiley Interscience; 1994.
7 Kissinger, P. T.; Heinnan, W. R. Laboratory Techniques in Electroanalytical Chemistry; 2nd ed.; Marcel Dekker Inc.: New York; 1996.
8 Sawyer, D. T.; Sobkowiak, A.; Roberts, Jr., J. L. Electrochemistry for Chemists, 2nd ed.; Wiley Interscience: New York; 1995.
9 J. W. Steed, J. L. Atwood, Supramolecular Chemistry, John Wiley & Sons Ltd.: New York; 2000.
10 J.-M. Lehn, Supramolecular Chemistry, Concepts and Prespectives, VCH: Weinheim; 1995.

11 Izatt, R. M.; Christensen, J. J. Eds. Synthesis of Macrocycles: The Design of Selective Complexing Agents, Progress in Macrocyclic Chemistry, Vol. 3; Wiley-Interscience: NY, 1987.
12 Lindoy, L. F. The Chemistry of Macrocyclic Ligand Complexes; Cambridge University Press: Cambridge; 1989.
13 Caravan, P.; Ellison, J. J.; McMurry, T. J.; Lauffer, R. B. Chem. Rev. 1999, 99, 2293.
14 Merbach, A. E.; Toth, E., Eds.; The Chemistry of Contrast Agents in Medical Magnetic Resonance Imaging; John Wiley & Sons, Ltd.: New York, 2001.
15 Bosman, A. W.; Janssen, H. M.; Meijer, E. W. "About Dendrimers: Structure, Physical Properties, and Applications"; Chem. Rev. 1999, 99, 1665.
16 Newkome, G. R.; He, E.; Moorefield, C. N. "Suprasupermolecules with Novel Properties: Metallodendrimers"; Chem. Rev. 1999, 99, 1689.
17 Jurisson, S. S.; Lydon, J. D. "Potential Technetium Small Molecule Radiopharmaceuticals", Chem. Rev. 1999, 99, 2205-2218.
18 Anderson, C. J.; Welch, M. J. Radiometal Labeled Agents (Non-Technetium) for Diagnostic Imaging", Chem. Rev. 1999, 99, 2219-2234.
19 Ali, H.; van Lier, J. E. "Metal Complexes as Photo- and Radiosensitizers", Chem. Rev. 1999, 99, 2379-2450.
20 Majoral, J.-N.; Caminade, A.-M. "Dendrimers Containing Heteroatoms", Chem. Rev. 1999, 99, 845.
21 Bunzli, J.-C. G; Piguet, C. "Lanthanide-Containing Molecular and Supramolecular Polymetallic Functional Assemblies", Chem. Rev. 2002, 102, 1897-1928.
22 Kuriki, K.; Koike, Y. "Plastic Optical Fiber Lasers and Amplifiers Containing Lanthanide Complexes", Chem. Rev. 2002, 102, 2347-2356.
23 Parker, D.; Dickins, R. S.; Puschmann, H.; Crossland, C.; Howard, J. A. K. "Being Excited by Lanthanide Coordination Complexes: Aqua Species, Chirality, Excited-State Chemistry, and Exchange Dynamics", Chem. Rev. 2002, 102, 1977-2010.

CH-2901/3901: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS FOR BIOLOGISTS

(For M.Sc. Zoology and M.Sc. Biomedical Instrumentation Science)

SEMESTER :II **CREDIT :3**
CATEGORY :ED **NO. OF HOURS / WEEK :4**

Objectives:

1. *To understand the basic principle of analytical chemistry in the preparation of solutions, standardization and preservation.*
2. *To understand the techniques involved in the instrumental analysis.*
3. *To understand and appreciate the techniques involved in the instrumental analysis particularly in optical methods and electro analytical methods.*
4. *To provide a sound knowledge in chromatographic techniques in the separation and identification of components from biological sources.*
5. *To expose the different methods of spectroscopic analysis of biological compounds*

UNIT - 1 : PREPARATION OF SOLUTIONS (3h)

1.1 Preparation of solutions: Percentage by weight, volume and strength. Normality, molarity, ppm and ppb.

1.2 Standard solutions: dilutions to known concentrations.

UNIT - 2 : OPTICAL METHODS (15h)

2.1 Spectrophotocolorimetry: Lambert and Beers Law, verification, deviations-Significances of l_{max} and Molar absorption coefficients. Single beam and double beam spectrophotometers-photocathode, photomultiplier tube-Applications to biological samples.

2.2 Principle of turbidometry – Instrumentation. Determination of sulphate, phosphate

2.3 Spectrofluorimetry: Principles – description of fluorimeter – Analysis of riboflavin thiamine, tetracycline, and benzpyrene in cigarette smoke.

2.4 Atomic absorption: Principle – Instrumentation - Flame sources – Hollow cathode lamp – Analysis of Zn^{2+}, Cu^{2+}, Pb^{2+} and Cd^{2+}. Flameless AAS for Hg^{2+} analysis – Inductively coupled plasma (ICP) method of analysis of Ca^{2+} and Mg^{2+} in water samples.

2.5 Optical rotatory dispersion method, circular dichroism studies – application.

UNIT - 3 : ELECTROANALYTICAL METHODS (7h)

3.1 Determination of pH – use of pH meter, calibration, pH and potentiometric titrations.

3.2 Preparation of buffer solutions – Tris and phosphate

3.3 Ion selective electrode – Fluoride analysis in drinking water.

UNIT - 4 : CHROMATOGRAPHIC METHODS (5h)

4.1 Gas chromatography: Principle and instrumentation – Detectors: Thermal conductivity, flame ionization, electron capture detectors.-Applications

4.2 HPLC: Principle – instrumentation – Detectors.- Applications

UNIT - 5 : SPECTROSCOPY AND DIFFRACTION STUDIES(15h)

5.1 IR spectroscopy – characteristic absorption bands of functional groups - applications.

5.2 ^{1}H NMR : Principle, instrumentation, chemical shift, splitting – Use of ^{13}C and ^{15}N NMR applications.

5.3 EPR: Principle, Instrumentation, detection of free radicals.

5.4 Mass spectrometry: Principle, instrumentation, fragmentation in alkane, alkene, aldehydes, ketones, carboxylic acids and aromatic compounds - Tandem mass spectrometry – Applications.

5.5 X ray methods- Braggs law, calculation of d values, powder diffractogram, single crystal analysis – Significance and applications. Applications of neutron and electron diffraction.

5.6 Isotopic dilution analysis: Principle and applications.

TEXT BOOKS

1. K. Wilson and K. H. Goulding, A Biologists Guide to Principles and Techniques of Practical Biochemistry, ELBS 3rd edition, 1997.
2. B. K. Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House, Meerut, 2001.
3. G.R. Chatwal and S.K. Anand,, Instrumental Methods of Chemical Analysis, Himalaya Publishing House, Delhi,2000 .

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4. D. A. Skoog, D. M. West and F. J. Hoeller, Analytical Chemistry 5th Edn, Sanders Publishers, Philadelphia, 1990.
5. R. A. Day and L. R. Underwood, Quantitative Analysis 5th edn, Prentice Hall of India, New Delhi, 1988.
6. J. R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall of India, New Delhi, 1989.