

M.Sc. - BRANCH - III - CHEMISTRY

SEMESTER SYSTEM

SCHEME OF THE ACADEMIC PROGRAMME

As per guidelines issued by the UGC the effective teaching days per semester must be not less than 90 days (18 weeks per Semester). Based on the assumption that there will be 5 days in a week of 6 hours duration per day. The syllabus has been designed.

COURSE	THEORY	LAB COURSE	TOTAL HOURS
I SEMESTER	18 Hrs./week (324 Hrs./Sem)	12 Hrs./week (216Hrs./Sem)	30 Hrs./week (540 Hrs./Sem.)
II SEMESTER	18 Hrs./week (324 Hrs./Sem)	12 Hrs./week (216Hrs./Sem)	30 Hrs./week (540 Hrs./Sem.)
III SEMESTER	18 Hrs./week (324 Hrs./Sem)	12 Hrs./week (216Hrs./Sem)	30 Hrs./week (540 Hrs./Sem.)
IV SEMESTER	15 Hrs./week (270 Hrs./Sem)	15 Hrs./week (270Hrs./Sem)	30 Hrs./week (540 Hrs./Sem.)

M.Sc. CHEMISTRY
COURSE STRUCTURE

FIRST YEAR

FIRST SEMESTER:

PAPER	COURSE No.	TITLE OF THE PAPER	HOURS
I	CH-401	INORGANIC CHEMISTRY - I	90
II	CH-421	ORGANIC CHEMISTRY - I	90
III	CH-441	PHYSICAL CHEMISTRY - I	90
IV	CH-400	LAB. COURSE - I (Inorganic)	216

SECOND SEMESTER:

PAPER	COURSE No.	TITLE OF THE PAPER	HOURS
V	CH-402	INORGANIC CHEMISTRY - II	90
VI	CH-422	ORGANIC CHEMISTRY - II	90
VII	CH-442	PHYSICAL CHEMISTRY - II	90
VIII	CH-420	LAB. COURSE - II (Organic)	216

SECOND YEAR

THIRD SEMESTER:

PAPER	COURSE No.	TITLE OF THE PAPER	HOURS
IX	CH-501	INORGANIC PHOTOCHEMISTRY & BIOINORGANICS.	90
X	CH-521	ORGANIC SPECTROSCOPY	90
XI	CH-541	PHYSICAL CHEMISTRY - III	90
XII	CH-540	LAB. COURSE - III (Physical)	216

FOURTH SEMESTER:

PAPER	COURSE No.	TITLE OF THE PAPER	HOURS
XIII	CH-572	ADVANCED TOPICS IN CHEMISTRY	90
XIV	CH-582	ELECTIVE PAPER*	90
	CH-582A	ENVIRONMENTAL CHEMISTRY	
	CH-582B	NATURAL PRODUCTS AND HETEROCYCLICS	
	CH-582C	COMPUTATIONAL CHEMISTRY	
	CH-582D	POLYMER CHEMISTRY	
XV	CH-570	PROJECT/ADVANCED LEVEL PRACTICALS/REVIEW WORK	150
XVI	CH-580*	LAB. COURSE - IV (Electives)	120

* FROM THE ELECTIVE PAPERS A TO D STUDENTS ARE REQUIRED TO SELECT ONE PAPER

Note: Seminar, Test, and Library can be allotted one hour each per week

- CH 580 Lab course - IV (electives) shall be designed by the concerned faculty depending on the elective course taken by the student. Details of the Lab course shall be informed to the University well in advance.

M.Sc. CHEMISTRY
EXAMINATION PATTERN

SEMESTER	PAPER	DURATION OF EXAM.	MARKS		TOTAL
			INTERNAL	EXTERNAL	
1	CH-401	3 Hrs.	25	75	100
1	CH-421	3 Hrs.	25	75	100
1	CH-441	3 Hrs.	25	75	100
1	CH-400	6 Hrs.	50	50	100
2	CH-402	3 Hrs.	25	75	100
2	CH-422	3 Hrs.	25	75	100
2	CH-442	3 Hrs.	25	75	100
2	CH-420	6 Hrs.	50	50	100
3	CH-501	3 Hrs.	25	75	100
3	CH-521	3 Hrs.	25	75	100
3	CH-541	3 Hrs.	25	75	100
3	CH-540	6 Hrs.	50	50	100
4	CH-572	3 Hrs.	25	75	100
4	CH-582(A,B,C,D)	3 Hrs.	25	75	100
4	CH-570	6 Hrs.	50	50	100
4	CH-580	6 Hrs.	100	--	100

UNIT - I : COVALENT BONDING AND STRUCTURE

18 Hrs.

Nature of covalent bond - V.B and M.O. Theories - Symmetry and Orbital Overlap - M.O. diagrams for homo and hetero nuclear diatomic and simple polyatomic (NH_3 , SF_6) - Hybridisation, Delocalisation, Ionic character in covalent bond - dipole moment calculations. Bond properties - bond order, bond length, bond energy - correlation. Electron deficient Hydrides - structure of Diborane, tetraborane, dodecaborane, carboranes, metallocarboranes and Borohydrides.

UNIT - II : IONIC BONDING AND SOLID STATE

18 Hrs.

Symmetry elements- proper and improper rotation axes, screw axis, glide plane. Symmetry groups - point and space groups. close packing of atomic spheres. Crystal systems, unit cell, Bravais lattices. Basic principles and applications of X-ray, Neutron and electron diffraction to structural studies. Structures of CsCl, Sphalerite, wurtzite, fluorite and antiferite, rutile, perovskite and spinels. Energetics of ionic bonding - Born-Landé, Born-Mayer and Kapustinskii equations - Born-Haber cycle and energetics of dissolution of ionic compounds.

UNIT - III : THEORY OF SOLIDS

18 Hrs.

Metallic states - free electron and band theories - imperfections in solids - Frankel and Schottky defects, non-stoichiometry defects, line defects, plane defects - defect equilibria.

Introduction to properties of metals - insulators and semiconductors - Hall effect - super conductivity and High TC superconductivity. Inter metallic compounds, Solid solutions, Leves-zintl phases - Hume-Rothery rules.

UNIT - IV : NUCLEAR CHEMISTRY

18 Hrs.

Radioactive decay and equilibrium - Transient and secular equilibria - types of nuclear reactions - counting techniques - G.M., Ionisation and Proportional counters. Radio active techniques, tracer technique - Neutron activation analysis - isotopic dilution analysis - Szilard Chalmer's process.

UNIT - V : INORGANIC CHAIN AND RING COMPOUNDS

18 Hrs.

Polyanions - Isopoly and heteropoly anions of Vanadium, Molybdenum and Tungsten. Inorganic rings - Borazines, Phosphazines, Silicates, Sulphur-Nitrogen compounds [S_2N_2 , S_4N_4 , $(\text{SN})_x$] and Phosphorus sulphides (P_4S_3 , P_4S_4 , P_4S_5 , P_4S_7 , P_4S_{10}). Metal clusters - di, tri, tetra and hexa nuclear clusters.

BOOKS RECOMMENDED:

1. J.E. HUEEY, Inorganic Chemistry - principle, structure and reactivity, Harper and Row - 4th Edition - 1983
2. DOUGLAS, McDaniel AND ALEXANDER - Concepts and models in inorganic chemistry - Wiley - 2nd edition - 1983.
3. P.W. ATKINS, D.K. SHRIVER AND C.H. LANGFORD - Inorganic chemistry - Oxford - 3rd edition - 1999.
4. L.V. AZARAFF, - Introduction to Solids - Tata McGraw Hill - 1987
5. A.F. WELLS, - Structural Inorganic Chemistry - ELBS - 1979
6. N.B. Hannay, Solid State Chemistry, Prentice - Hall - 1976
7. WEST, W.R. - Solid state Chemistry and its applications - John Wiley - 1984
8. ARNIKAR, H.J. - Essentials of Nuclear chemistry - Wiley - Eastern - 2nd edition, 1988
9. GLASSTONE, S. - Source book of atomic energy - Von Honstrand

UNIT - 1: NATURE OF BONDING AND REACTIVE INTERMEDIATES. 18 Hrs.

Delocalised chemical bonding - conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes, tautomerism.

Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckels rule, energy level of π Molecular Orbital, annulenes, ψ - aromaticity, anti aromaticity, homoaromaticity, PMO approach.

Bonds weaker than covalent - addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

Generation, Structure and reactions of carbocations, carbanions, radicals, carbenes and nitrenes.

UNIT - II : STERIOCHEMISTRY AND CONFORMATIONAL ANALYSIS. 18 Hrs.

Configuration : - Fischer projection - Sawhorse and Newman projections - R & S notations, methods of determining configurations, enantioselective and diastereoselective asymmetric synthesis, Cram's rule and Prelog's rule.

Geometrical isomerism of monocyclic and fused ring compounds.

Enantiotopic and diastereotopic atoms, groups and phases, stereospecific and stereoselective reactions.

Conformation and reactivity of cyclohexane, mono and di substituted cyclohexanes and decalins.

UNIT - III : ORGANIC REACTION MECHANISMS : STRUCTURE AND REACTIVITY.

18 Hrs.

Types of reactions, types of mechanisms, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanism, isotopic effects, hard and soft acids and bases.

Effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatment. Hammett equation and linear free energy relationships, substituent and reaction constants, Taft equation.

UNIT - IV : SUBSTITUTION REACTIONS

18 Hrs.

Aliphatic substitution reactions: Neighbouring group mechanism- Anchimeric assistance- classical and non-classical carbocations, phenonium ions, and norbornyl system. S_N1 mechanism - structure and reactivity - Phase transfer catalysis - ambident nucleophile, regioselectivity.

Aromatic substitution reactions:

The arenium ion mechanism - orientation and reactivity, energy profile diagrams. ortho-para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles. diazo coupling, Vilsmeier reaction, Gattermann Koch reaction.

S_NAr , S_Ni , Benzyne and $S_{RN}1$ mechanisms and reactivity - effect of substrate structure, leaving group and attacking nucleophile.

UNIT - V : ADDITION REACTIONS

18 Hrs.

Addition to C-C multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio and chemo selectivity, orientation and reactivity. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.



Addition to Carbon – Hetero multiple bonds: Addition of Grignard reagents, Organo zinc and Organo lithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

BOOKS RECOMMENDED:

1. ADVANCE ORGANIC CHEMISTRY – REACTION MECHANISM AND STRUCTURE – J.March – John Wiley.
2. ADVANCE ORGANIC CHEMISTRY – Part A & B - F.A.Carey and R.J.Sundberg – Plenum press - 2000.
3. UNDERSTANDING ORGANIC REACTION MECHANISM – A.Jacobs, Cambridge University Press – 1997
4. STEREOCHEMISTRY OF CARBON COMPOUNDS – E.L.Eliel – John Wiley – 1997
5. STEREO CHEMISTRY OF ORGANIC COMPOUNDS – D.Nasipuri, New Age International
6. REACTIVE INTERMEDIATES – C.J.Moody and G.H. Whitham – Oxford University press – 1992
7. ORGANIC CHEMISTRY – R.T.Morrison and R.N. Boyd – Printice Hall
8. ORGANIC CHEMISTRY – Stanely H.Pine – McGraw Hill.
9. ORGANIC REACTION MECHANISMS – V.K.Ahluwallia and R.K.Parashar – Narosa publishers – 2002

UNIT I : CLASSICAL THERMODYNAMICS 18 HRS.

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies.

Partial molar properties : Partial molar free energy, partial molar volume and partial molar heat content and their significance . Determination of these quantities. Concept and determination of fugacity.

Non- ideal system: Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficient ; ionic strength.

UNIT II : SURFACE PHENOMENA 18 HRs.

Adsorption at surfaces- Gibbs adsorption isotherm , physical methods of studying surfaces : UVPEs, Electron microscopy LEED, EELS, FEM techniques. Physisorption and chemisorption - desorption . Adsorption isotherms - Langmuir, Freundlich and BET isotherms. Determination of surface area - catalytic activity at surfaces, kinetics of surface adsorption , classification of surface active agents and CMC .

UNIT III : MACROMOLECULES 18 HRS.

Types of Polymer , electrically conducting , fire resistance, liquid crystal polymers, kinetics and mechanism of polymerisation .

Molecular mass: number and mass average molecular mass, determination of molecular mass by Osmometry, Viscometry and Sedimentation method. Chain configuration of macromolecules.

UNIT IV : ELECTROCHEMISTRY - I 18 HRS.

Electrochemistry of solution : Debye - Huckel - Onsager treatment and its extension, ion - solvent interactions, Debye -Huckel - Jerum model. Thermodynamics of electrified interface equations. Derivation of electro- capillarity, Lippmann equations (surface excess) , methods of determination . Structure of electrified interfaces : Helmholtz - Perrn, Guoy-Chapman , Stern , Graham- Devanathan - Mottwatts, Tobin, Bockris, and Devanathan models.

UNIT V : CHEMICAL KINETICS 18 HRS.

Molecularity, order and rate of reactions, Arrhenius theory - complex reactions : reversible, side reactions, consecutive , chain and photochemical , oscillatory reactions - Lindemann's theory of unimolecular reactions - Laser flash photolysis, flow techniques and relaxation methods.

BOOKS RECOMMENDED:

1. CHEMICAL KINETICS - K. J. Laidler, 3rd Edn. , Harper International , 1987.
2. BASIC CHEMICAL KINETICS- G. L. Agarwal , Tata MaGraw Hill, 1990.
3. MODERN ELECTROCHEMISTRY Vol. I & II- Bockris and Reddy, Plenum.
4. INTRODUCTION TO POLYMER SCIENCE - V. R. Gowariker, N.V. Vishwanathan & J. Sridhar, Wiley Eastern.
5. AN INTRODUCTION TO CHEMICAL THERMODYNAMICS - R.P. Rastogi & R.R. Misra,, Vikas Publ. House pvt . Lt.
6. PHYSICAL CHEMISTRY OF SURFACES - Adamson, Wiley.
7. THERMODYNAMICS FOR STUDENTS OF CHEMISTRY - J. Rajaram & J.C. Kuriacose, LCSE Edition.

PAPER - IV
CH - 400 - LABORATORY COURSE - I
INORGANIC CHEMISTRY

216 Hrs.

QUALITATIVE AND QUALITATIVE ANALYSIS

- A. Less common metal ions : Se, Te, W, Ti, Mo, Ce, Th, Zr, V, U, Li. (Two metal ions in cationic/anionic forms - insolubles: oxides, sulphates and halides.)
- B. Separation and determination of two metal ions :
1. Analysis of ores (Dolomite)
 2. Analysis of alloys (Magnesium, brass, stainless steel)
 3. Mixture of Cu and Ni.
- C. Separation of cations and anions by
1. Paper chromatography
 2. Column chromatography - ion exchange

PREPARATION AND ANALYSIS OF INORGANIC COMPOUNDS

Preparation of selected inorganic compounds and their electronic spectral analysis.

1. $\text{VO}(\text{acac})_2$
2. $\text{K}_3[\text{Fe}(\text{Ox})_3]$
3. Prussian blue
4. $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2 \cdot$
5. $\text{Ni}(\text{DMG})_2$
6. $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

UNIT - I : THEORY OF COORDINATION COMPOUNDS 18 Hrs.

Review of Valence bond and Crystal Field theory - Crystal field splitting, application of d-orbital splitting to explain the properties of complexes - Magnetic, low spin and high spin, CFSE, spectrochemical series, thermodynamic aspects of CFT - ionic radii, heats of ligation, lattice energies, site preference energies and chelate effects. Molecular Orbital theory of complexes involving only sigma bond and sigma and pi bond.

UNIT - II : ELECTRONIC SPECTRA AND MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES 18 Hrs.

Spectroscopic ground state - Russell and Saunders for free ions and Mulliken for complexes. Orgal and Tanabe-Sugano diagrams for transition metal complexes (d1 to d9 states), electronic spectra of complexes. The hole formalism - calculation of Dq, B and Beta parameters. Charge transfer spectra in octahedral and tetrahedral complexes. Jahn - Teller distortion and its effect. Cotton effect - CD and ORD and their applications.

UNIT III : CHEMISTRY OF COMPLEXES WITH PI BOND 18 Hrs.

18-electron rule, transition metal carbonyls, structure and bonding, important reactions of metal carbonyls. preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, metallocenes (M.O. theory of bonding), Metal - alkyl and aryl complexes.

UNIT - IV : REACTION MECHANISM OF TRANSITION METAL COMPLEXES

18 Hrs.

Energy profile of the reactions, reactivity of metal complexes, inert and labile complexes, kinetic application of VB and CF Theories, kinetics of octahedral substitutions, Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism. anion reaction, reactions without metal-ligand bond cleavage. substitution reactions in square planar complexes, Trans effect, mechanism of the substitution reaction. redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outersphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

UNIT - V: ORGANO METALLIC REACTIONS AND CATALYSIS 18 Hrs.

Oxidative addition, reductive elimination, insertion reactions. Olefin hydrogenation, hydroformylation, Wacker process, Ziegler - Natta polymerisation, cyclooligomerisation, olefin isomerisation, olefin metathesis. Fischer-Tropsch process.

BOOKS RECOMMENDED:

1. J.E.HUHEEY, Inorganic Chemistry - principle, structure and reactivity, Harper and Row - 4th Edition - 1983
2. DOUGLAS, McDaniel AND ALEXANDER - Concepts and models in inorganic chemistry - Wiley - 2nd edition - 1983.
3. P.W. ATKINS, D.K. SHRIVER AND C.H., LANGFORD - Inorganic chemistry - Oxford - 3rd edition - 1999.
4. F.A.COTTON AND G.WILLKINSON - Advanced inorganic chemistry - John Wiley - 5th edition.
5. J.D.LEE - New concise inorganic chemistry - ELBS - 5th edition- 1999.
6. S.J.LIPPORD - Progress in inorganic chemistry - Vol. 30, John-Wiley - 1983
7. R.S.DRAGO - Physical methods in chemistry - W.B.Saunders - 1987.
8. N.N.GREENWOOD & A.EARNSHAW - Chemistry of the elements - Pergamon press - 1989

9. B.N.FIGGIS - Introduction to ligand fields - John-Wiley - 1956
10. A.W.PARKINS & R.C.POLLER - An introduction to Organometallic chemistry - Oxford university press - 1986
11. R.H.CRABTREE - The organometallic chemistry of the transition metals - John Wiley.
12. J.PCOLLIMER, L.S.HEGSDUS, J.R.NORTON & R.G.FINKE - Principles and applications of Organo transition metal chemistry - University Science books.

UNIT - I : ELIMINATION REACTIONS

18 Hrs.

E1, E2, E1cB mechanism, reactivity - Hoffman & Zaitsev rules, Competition between elimination and substitution, mechanism and orientation in pyrolytic eliminations.

Typical reactions - dehydration, dehydrohalogenation, Chugaev reaction, Hoffman degradation and Cope elimination.

Elimination reactions in Organic synthesis.

UNIT - II : OXIDATION AND REDUCTION REACTIONS.

18 Hrs.

Mechanism and study of the following reactions- oxidation with Chromium, Manganese, Osmium, Lead, Ruthenium and Selenium.

Reductions: catalytic hydrogenation, metal hydride reduction (LAH, NaBH and their derivatives) Metal ammonium reduction, selectivity in reduction.

UNIT - III : CONCERTED REACTIONS.

18 Hrs.

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward-Hoffman correlation diagrams, FMO and PMO approach. Electrocyclic reactions - con and dis rotatory motions, $4n$, $4n+2$ and allyl systems. Cycloadditions - antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, 2+2 addition of ketene, 1,3-dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements.

UNIT - IV : ORGANIC PHOTOCHEMISTRY AND REARRANGEMENT REACTIONS.

18 Hrs.

Introductory theory - Jablonski diagram, study of the photochemical reactions of carbonyl compounds, photoreductions, photocycloadditions and photorearrangements - di-pi methane rearrangement.

Study of the following rearrangement reactions: Favorski, Bayer - Villiger, Wolf and Stevens.

UNIT - V : BIOMOLECULES.

18 Hrs.

Carbohydrates : Cellulose and Starch

Lipids : Phospholipids and Cholesterol

Aminoacids, Peptides and Proteins - Structure and synthesis

Nucleic acids and Nucleotides: Structure and biochemistry.

BOOKS RECOMMENDED:

1. ADVANCE ORGANIC CHEMISTRY - REACTION MECHANISM AND STRUCTURE - J. March - John Wiley.
2. ADVANCE ORGANIC CHEMISTRY - Part A & B - F.A. Carey and R.J. Sundberg - Plenum press - 2000.
3. ORGANIC CHEMISTRY - R.T. Morrison and R.N. Boyd - Printice Hall
4. ORGANIC CHEMISTRY - Stanely H. Pine - McGraw Hill.
5. PERICYCLIC REACTIONS - S.M. Mukerji - Macmillan.
6. REACTION MECHANISMS IN ORGANIC CHEMISTRY - S.M. Mukerji and S.P. Singh - Macmillan
7. PHOTOCHEMISTRY - Cox and Kemp
8. THE CONSERVATION OF ORBITAL SYMMETRY - R.B. Woodward, Hoffman - Academic press.



9. ORGANIC PHOTOCHEMISTRY – J.D.Coyle – Wiley, 1985.
10. PRINCIPLES OF BIOCHEMISTRY – A.L.Lehninger – Worth publishers.
11. BIOCHEMISTRY – E.E.Conn, P.K.Stumpf and Doi – John Wiley.1992

UNIT I: STATISTICAL THERMODYNAMICS

18 HRS.

Concept of distribution, thermodynamic probability and most probable distribution, Microstate and macrostates, different types of ensembles, Maxwell - Boltzmann Statistics, Bose-Einstein statistics and Fermi-Dirac statistics (using Lagrange's methods of undetermined multipliers) and their distribution laws.

Partition functions - translational, rotational and vibrational partition functions. Calculation of thermodynamic properties and equilibrium constant of reaction $A + B = C + D$ in terms of partition functions. Application of partition functions for calculation of thermodynamic parameters of mono atomic and diatomic gases molecules. Einstein theory of heat capacity of solids.

UNIT II: NON EQUILIBRIUM THERMODYNAMICS

18 HRS.

Thermodynamic criteria for non-equilibrium state, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction) transformations of the generalised fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations.

UNIT III: MOLECULAR REACTION DYNAMICS

18 HRS.

Collision and activated complex theory, comparison of results with Eyring and Arrhenius equations-reactive collisions, molecular beam experiments, introduction to potential energy surfaces: treatment of $H_2 + H$ reaction - ionic reactions: salt effect.

UNIT IV: ELECTROCHEMISTRY-II

18 HRS.

Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Polarography theory, Ilkovic equation; half wave potential and its significance.

Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention methods.

UNIT V: QUANTUM CHEMISTRY-I

18 HRS.

Lagrange's and Hamilton's equation of motion, Poisson Brackets, Inadequacy of classical mechanics, Schrodinger's and Heisenberg's formulation of quantum mechanics, postulates of quantum mechanics, need for operators, Linear and Hermitian operators, operator algebra eigen value and eigen functions, commutation relations.

BOOKS RECOMMENDED:

1. THERMODYNAMICS, KINETIC THEORY & STATISTICAL THERMODYNAMICS- F.W. Sears & G.L. Salinger, Narosa, 1986.
2. STATISTICAL THERMODYNAMICS - M.C.Gupta,
3. ADVANCE PHYSICAL CHEMISTRY - D.N. Bajpai,
4. INTRODUCTION TO QUANTUM CHEMISTRY - A.K.Chandra, Tata McGraw Hill, 1988.
5. ELECTROCHEMISTRY - P.H. Reiger, Prentice Hall, 1987.
6. ELECTROCHEMICAL METHODS, FUNDAMENTAL AND APPLICATIONS - A.J. Bard & L.R. Faulker, John Wiley, 1980.
7. CHEMICAL KINETICS & DYNAMICS - J.I. Sheinfeld, J.S. Francisco, W.L. Hasse, Prentice Hall, 1998.

PAPER - VIII
LABORATORY COURSE-II

CH-420 ORGANIC CHEMISTRY PRACTICAL

(216 Hours)

I. QUALITATIVE ANALYSIS

Separation of a mixture of containing three organic components.
Separation, purification and identification of a binary mixture

II. QUANTITATIVE ANALYSIS

1. Estimation of amines/phenols using bromate bromide solution
2. Determination Iodine and Saponification values of an oil sample.
3. Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.

III. ORGANIC SYNTHESIS

Preparations involving two steps for synthesis of organic compounds.

- a) Acetylation and deacetylation
- b) Oxidation and reduction
- c) Hydrolysis
- d) Aldol condensation
- e) Sandmeyer reaction
- f) Aromatic Electrophilic substitutions: Nitration and Halogenation.

IV. EXTRACTION/CHROMATOGRAPHY/SPECTROPHOTOMETRIC ESTIMATION

(A) EXTRACTION OF ORGANIC COMPOUNDS FROM NATURAL SOURCES:

1. Isolation of caffeine from tea leaves.
2. Isolation of lactose/caesin from milk.
3. Isolation of β -Carotene from carrots.
4. Isolation of piperine from black pepper.

or

(B) PAPER CHROMATOGRAPHY

Separation and identification of the sugars present in the given mixture of Glucose, Fructose and Sucrose by paper chromatography and determination of R_f values.

or

(C) SPECTROSCOPY

Identification of Organic compounds by the analysis of their spectral data
(UV, IR, PMR, CMR & MS)

or

(D) SPECTROPHOTOMETRIC (UV/VIS) ESTIMATIONS

Amino acids, Proteins, Carbohydrates, Cholesterol, Ascorbic acid, Aspirin, Caffeine

BOOKS RECOMMENDED:

1. VOGEL'S TEXT BOOK OF PRACTICAL ORGANIC CHEMISTRY- ELBS- London.
2. THE SYSTEMATIC IDENTIFICATION OF ORGANIC COMPOUNDS - R.L. Shriner and D.Y. Curtin
3. ORGANIC ANALYTICAL CHEMISTRY-THEORY AND PRACTISE - Jag Mohan , Narosa Publishing House- 2003.
4. PRACTICAL ORGANIC CHEMISTRY - Mann and Saunders.

UNIT-I : METAL IONS IN BIOLOGICAL PROCESSES

18 Hrs.

Essential and trace elements. Role of metal ions in biological processes - Na⁺/K⁺ pump. DNA polymerisation, glucose storage and metal complexes in transmission of energy. Chlorophyll, photosystem I and photosystem II in cleavage of water. Biological fixation of nitrogen.

UNIT -II : KINETICS OF INORGANIC PHOTOCHEMICAL REACTIONS 18 Hrs.

Photostationary States, rate law - Photolysis, flash photolysis and flow techniques. Thermal effects of photoluminescence - radiative and nonradiative transitions.

Electronically excited states of metal complexes, Charge transfer spectra, Charge transfer excitations, methods for obtaining charge transfer spectra.

UNIT - III : LIGAND FIELD PHOTOCHEMISTRY AND REDOX REACTIONS 18 Hrs.

Photosubstitution, Photooxidation and Photoreduction - lability and selectivity, Zero vibrational levels of ground state and excited state, zero-zero spectroscopic energy.

Energy transfer under conditions of weak and strong interaction - exciplex formation, conditions of the excited states to be useful as redox reactants.

Metal complexes as attractive reactant (2,2'-bipyridine and 1,10-phenanthroline complexes.)

Reducing and oxidising character of Ru²⁺(bipyridyl complex, comparison with Fe(bipy)₃)

UNIT - IV : METALLOENZYMES

18 Hrs.

Zn enzymes- carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzymes-superoxide dismutase. Molybdenum oxotransferase enzymes-xanthine oxidase. Co-enzyme vitamin B-12

UNIT V : DIOXYGEN AND ELECTRON TRANSFER IN BIOLOGY

18 Hrs.

Heme proteins and oxygen uptake. Structure and function of haemoglobin, myoglobin haemocyanins and haemerythrin. Ferredoxin and Rubredoxins. Structure and function of metalloproteins in electron transport processes- cytochromes and iron-sulphur proteins.

BOOKS RECOMMENDED:

1. J.E.HUHEEY, Inorganic Chemistry - principle, structure and reactivity, Harper and Row - 4th Edition - 1983
2. DOUGLAS, McDaniel AND ALEXANDER - Concepts and models in inorganic chemistry - Wiley - 2nd edition - 1983.
3. P.W. ATKINS, D.K. SHRIVER AND C.H. LANGFORD - Inorganic chemistry - Oxford - 3rd edition - 1999.
4. F.A.COTTON AND G.WILLKINSON - Advanced inorganic chemistry - John Wiley - 5th edition.
5. S.J.LIPPARD AND J.M.BERG - Principles of bioinorganic chemistry- University Science books.
6. I.BEERTINI, H.B.GRAY, S.J.LIPPARD AND J.S.VALENMTINE - Bioinorganic chemistry - University science Books
7. G.L.EICHHORN (ED) - Inorganic biochemistry vol. I & II - Elsevier
8. A.W.ADAMSON AND P.D.FLEISCHAUER - Concepts of Inorganic Photochemistry - Wiley.
9. V.BALZARI AND V.CARASSITI - Photochemistry of coordination compounds - Academic press
10. G.J.FERRAUDI - Elements of Photochemistry - Wiley.

PAPER - X
CH 521- ORGANIC SPECTROSCOPY 90 HOURS

UNIT - I : APPLICATIONS OF UV-VISIBLE AND IR SPECTROSCOPY 18 Hrs.

Study of UV-Visible Spectroscopy to organic structure determination - Woodward - Fischer rules, Octant rule and Axial haloketone rule. Applications of ORD - CD to stereochemical assignment.

IR spectroscopy - Basic principles, characteristic frequencies of common functional groups. Effect of Hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance.

UNIT - II : APPLICATIONS OF NMR SPECTROSCOPY. 18 Hrs.

Basic principles, introduction to NMR techniques, - CW and FT NMR techniques.

^1H NMR Spectral paramers - Intensity, Chemical shift, multiplicity, Coupling constant, factors affecting. Analysis of first and second order spectra. Structure determination of organic compounds by ^1H NMR.

UNIT - III : ^{13}C NMR and MULTI DIMENSIONAL NMR SPECTROSCOPY 18 Hrs..

^{13}C NMR - Proton coupled, off resonance decoupled, proton noise decoupled ^{13}C NMR spectra.

Assignment of chemical shifts, additive effect, characteristic chemical shift of common organic compounds and functional groups. DEPT and SEPT spectra (elementary treatment).

2D.NMR Techniques - ^1H - ^1H COSY, ^1H - ^{13}C COSY, HMBC and NOESY

UNIT - IV : APPLICATIONS OF MASS SPECTROMETRY 18 Hrs.

Basic principles, modern techniques of Ionisation, molecular ion, isotope abundance, Nitrogen rule, double bond equivalent, daughter ions, metastable ions, McLafferty rearrangement, common fragmentation pathways. Structure determination of organic compounds by MS data.

UNIT - V : PROBLEM SOLVING EXCERCISES 18 Hrs.

Problems solving exercises involving UV, IR, Mass and NMR data.

BOOKS RECOMMENDED:

1. ORGANIC SPECTROSCOPY - W.Kemp - 3rd Edition - Macmillan- 1994
2. SPECTROMETRIC IDENTIFICATION OF ORGANIC COMPOUNDS - R.M.Silverstein and F.X. Webster - John Wiley - 1997
3. INTRODUCTION TO MULTINUCLEAR NMR - W.Kemp - Macmillan.
4. SPECTROSCOPIC METHODS IN ORGANIC CHEMISTRY - D.H. Willams and Ian Fleming - Tata-McGraw Hill - 1998

UNIT I: SYMMETRY AND GROUP THEORY IN CHEMISTRY 18 HRS.

Symmetry elements and operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup: Conjugacy relation and classes. Point groups and their systematic classification flow chart diagram- multiplication table-representation of groups - reducible and irreducible representations-character table and their construction for C_{2v} , C_{3v} , C_{2h} , D_3 and D_{2h} - Great Orthogonality theorem(without proof) and its consequences. Simple application of character tables to spectroscopy (IR and Raman) and hybrid orbitals.

UNIT II: QUANTUM CHEMISTRY - II 18 HRS.

Solution of Schrodinger's equation for the following system (1) particle in 1D- 2D- and 3D- boxes and applications (2) particle in a ring and sphere, spherical harmonics, angular momentum rigid rotator, (3) simple harmonic oscillator and (4) hydrogen atom, Zeeman effect and electron spin.

UNIT III: QUANTUM CHEMISTRY - III 18 HRS.

Variation and perturbation methods: examples - Variation methods: (1) Hydrogen atom, Hydrogen atom in an electric field, (2) Helium atom.

Perturbation method: (1) perturbed particle in a box, (2) perturbed harmonic oscillator, (3) Hydrogen atom in electric field.

Antisymmetric wave functions of many electron atoms, Slater determinants, Hartree and Hartree - Fock self consistent field model for atoms.

UNIT IV: VIBRATIONAL AND ROTATIONAL SPECTROSCOPY 18 HRS.

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, non-rigid rotor.

Vibrational energies of diatomic molecules, force constant, band strength - selection rules - energy of anharmonic oscillator - selection rules, fundamental, first and 2nd overtones and hot bands. Vibration - rotational spectroscopy - origin of PQR branches, normal mode of vibrations (eg. H_2O & CO_2), Fermi resonance and group frequencies.

Raman spectra: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibration-rotational Raman spectra, selection rules-mutual exclusion principle-Resonance Raman spectroscopy.

Molecular spectroscopy: Energy levels, molecular orbitals, vibronic transition, Franck-Condon principle, Morse potential energy diagram. Concept of molar absorptivity - Oscillator strength - band width - Jablonski diagram for a diatomic molecules, radiative and non radiative decay and internal conversion.

UNIT V: NMR SPECTROSCOPY 18 HRS.

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J' classification (ABC, A_2B_2), spin decoupling, use of NMR in medical diagnostics.

ESR Spectrum: Basic principles, Zero field splitting and Kramer's degeneracy, factors affecting the 'g' value, isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, application to simple free radicals in solutions.

NQR spectroscopy - Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting and applications.



BOOKS RECOMMENDED:

1. CHEMICAL APPLICATIONS OF GROUP THEORY - F.A. Cotton, Wiley Eastern, 1985.
2. GROUP THEORY IN CHEMISTRY - Ramakrishnan & M.S. Gopinathan, Vishal Publ.
3. QUANTUM CHEMISTRY - D.A. McQuarrie, Oxford university press.
4. ELEMENTARY QUANTUM CHEMISTRY - F.L. Pilar, McGraw Hill.
5. ADVANCED ENGINEERING MATHEMATICS - E. Kreyzig.
6. QUANTUM CHEMISTRY THROUGH PROBLEMS AND SOLUTIONS - R.K. Prasad, New Age International, 1997
7. MODERN SPECTROSCOPY - J.N. Hollas, John Wiley.
8. INTRODUCTION TO MAGNETIC RESONANCE - A. Carrington and A.D. MacLachlan, Harper and Row.
9. MOLECULAR SPECTROSCOPY - Graebner, Prentice Hall.
10. MOLECULAR SPECTROSCOPY - Banwell and Emmett, Tata-Mcraw Hill, 1998.
11. NMR, NQR, EPR AND MOSSBAUER SPECTROSCOPY IN INORGANIC CHEMISTRY - R.V. Parish, Ellis Harwood.

1. POLAROGRAPHY

Estimation of Pb^{2+} and Cd^{2+}/Zn^{2+} and Ni^{2+} ions in a mixture of Pb^{2+} and Cd^{2+} and Ni^{2+}

2. SPECTROSCOPY

Determination of pK_a of an indicator in

- i) Aqueous media
- ii) Micellar media
- iii) Determination of stoichiometry and stability constant of inorganic and (eg. ferric-salicylic acid) and organic (e.g. amine-iodine) complexes

3. ELECTROCHEMISTRY

a) Conductivity experiments

- i) Determination of cell constant
- ii) Verification Onsagar equation
- iii) Titration of Strong acid Vs Strong Base
- iv) Titration of Weak acid Vs Strong Base
- v) Titration of Mixture of Acids Vs Strong Base
- vi) Precipitation Titration
- vii) Dissociation Constant of Weak acid

b) Potentiometric experiments

- i) Determination of single electrode potential
- ii) Redox Titration
- iii) Solubility product of Sparingly soluble salt
- iv) Instability Constant of Silver Ammonia Complex
- v) Titration of Weak Acid Vs Strong base
- vi) Titration of Strong acid Vs Strong base
- vii) Mixture of Halides with Silver Nitrate
- viii) Determination of pH of a buffer solution

4. KINETICS

- i) Iodination of Acetone
- ii) Persulphate -Iodide
- iii) Effect of ionic strength on rate of reaction between persulphate and iodide
- iv) Saponification of an ester
- v) Hydrolysis constant of Urea-hydrochloride

5. PHASE EQUILIBRIA

- i) Association factor of benzoic acid
- ii) Ternary system

BOOKS RECOMMENDED:

1. EXPERIMENTAL PHYSICAL CHEMISTRY - D.P.Shoemaker, C.W.Garland and L.W.Niber, McGraw Hill.
2. FINDLAY'S PRACTICAL PHYSICAL CHEMISTRY - revised B.P.Levett, Longman
3. EXPERIMENTS IN PHYSICAL CHEMISTRY - J.C.Ghosh, Bharathi Bavan.

UNIT - 1 : PHYSICAL METHODS IN INORGANIC CHEMISTRY

18 Hrs.

Applications of NMR techniques to Inorganic compounds containing ^1H , ^{15}N , ^{19}F and ^{31}P . Mossebauer spectroscopy - basic principles, instrumentation and applications to Fe^{2+} and Fe^{3+} compounds. Photoelectron spectroscopy - basic principles, photoelectric effect, ionisation process, Koopman's theorem. Auger electron spectroscopy - basic idea.

UNIT - II : ORGANIC SYNTHETIC METHODOLOGY -I

18 Hrs.

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions. the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, Chemoselectivity, reversal of polarity, cyclization reactions, amine synthesis.

Principle of protection of alcohols, amines, carbonyl and carboxyl groups

UNIT - III : ORGANIC SYNTHETIC METHODOLOGY -II

18 Hrs.

One group C-C disconnections - Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis

Two group C-C disconnections - Diel - Alder reaction, Michael addition, and Robinson annelation, Stark - Enamine reaction.

UNIT - IV : SOLID STATE CHEMISTRY

18 Hrs.

Diffusion in solids: diffusion mechanisms, Ficks laws of diffusion, diffusion as a random walk problem. Optical properties: thermionic emission, photovoltaic effect, and optical adsorption of semiconductors. Dielectric properties: dielectric constant and related properties, behaviour of dielectrical materials in ac fields, Clausius - Mosotto equation. Thermoelectric effects: Thomson effects, Peltier effect, Seebeck effect, thermocouples and Hall effect. Hopping semiconductors, polarons, liquid crystals and glasses. Pauling's rules in Polyhedral structural chemistry.

UNIT - V : QUANTAM CHEMISTRY

18 Hrs.

Ploy atomic molecules - hybridisation and non-equivalent hybrids constructions of sp , sp^2 , sp^3 , dsp^2 and d^2sp^3 hybrids and non-equivalent sp , sp^2 and sp^3 hybrids.

Huckel and SCF theories: Simple Huckel theory for p-electrons, Frontier orbitals, extended Huckel theory. Advanced MO methods: SCF Theory for molecules, Slater determinants, and electron repulsion integrals. Roothan's equation. ZDO Approximations, PPP, CNDO and INDO Approximations.

Hellman-Feynman theorem: Some simple application (qualitative treatment only)

BOOKS RECOMMENDED:

1. PHYSICAL METHODS IN CHEMISTRY - R.S.Drago - W.B.Saunders - 1987.
2. STRUCTURAL METHODS IN INORGANIC CHEMISTRY - E.A.V.Ebsworth, D.W.H.Rankin and S.Crodack, ELBS
3. NMR, NQR, EPR AND MOSSEBAUER SPECTROSCOPY IN INORGANIC CHEMISTRY - R.V.Parish, Ellis Horwood.
4. PRACTICAL NMR SPECTROSCOPY - M.L.Martin, J.J.Delpeuch and G.J.Martin, Heydeen.
5. INORGANIC ELECTRONIC SPECTROSCOPY - A.P.B.Lever, Elsevier.
6. MODERN METHODS IN ORGANIC SYNTHESIS - W.Caruthers - Academic press - 1989.
7. DESIGNING ORGANIC SYNTHESIS - S.Warren - Wiley.
8. PRINCIPLE OF ORGANIC SYNTHESIS - R.Norman and J.M. Coxon - Blackie.
9. MODERN SYTHETIC REACTIONS - H.O.House and W.A.Benjamin.

10. ADVANCE ORGANIC CHEMISTRY – Part B - F.A.Carey and R.J.Sundberg – Plenum press - 2000.
11. PRINCIPLES OF SOLID STATE – H.V. Keer
12. SOLID STATE CHEMISTRY AND ITS APPLICATIONS – W.R. West
13. SOLID STATE CHEMISTRY- D.K.Chakrabarty
14. COULSON'S VALENCE- R.Mc WEENEY
15. ATOMS MOLECULES- Karplus and Proter
16. MOLECULAR QUANTUM MECHANICS- P.W. Atkins
17. QUANTUM CHEMISTRY- I.N. Levine

CH - 582A - ENVIRONMENTAL CHEMISTRY 90 Hrs.

UNIT - I : ENVIRONMENT

18 Hrs.

Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, biogeochemical cycles of C,N,P,S and O, biodistribution of elements.

UNIT - II : HYDROSPHERE

18 Hrs.

Chemical composition of water bodies - lakes, streams, rivers, and wet lands etc., hydrological cycle.

Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

UNIT - III : SOILS AND ATMOSPHERE

18 Hrs.

Soils - composition, micro and macro nutrients, pollution - fertilisers, pesticides, plastics and metals. Waste treatment.

Atmosphere - chemical composition of atmosphere - particles, ions, radicals and their formation.

Chemical and photochemical reactions in atmosphere, smog formation, oxides of N,C,S and O and their effects, Pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments.

UNIT - IV : INDUSTRIAL POLLUTION

18 Hrs.

Cement, sugar, distillery, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. disposal of waste and their management.

UNIT - V : ENVIRONMENTAL TOXICOLOGY

18 Hrs.

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes, Bhopal gas tragedy, Chermobyl, three Mile Island, Sewozo and Minamata disasters.

BOOKS RECOMMENDED:

1. ENVIRONMENTAL CHEMISTRY - S.E.Manahan, Lewis publishers.
2. ENVIRONMENTAL CHEMISTRY - Sharma & Kaur, Krishna publishers.
3. ENVIRONMENTAL CHEMISTRY - A.K.De, Wiley-Eastern publishers.
4. ENVIRONMENTAL POLLUTION ANALYSIS - S.M.Khopkar, Wiley-Eastern publishers.
5. ENVIRONMENTAL TOXICOLOGY - ED. J.Rose, Gordon and Breach Science Publications.
6. STANDARD METHODS OF CHEMICAL ANALYSIS - F.J.Welcher Vol. III, Van Nostrand Reinhold Co.
7. ELEMENTAL ANALYSIS OF AIR BORNE PARTICLES - Ed. S.Landsberger and M.Greatchman, Gordon and Breach Science Publications.
8. ENVIRONMENTAL CHEMISTRY - C.Baird, W.H.Freeman.

CH-582B - NATURAL PRODUCTS CHEMISTRY AND HETEROCYCLICS 90 Hrs.

UNIT - I : TERPENOID AND CAROTINOIDS

18 Hrs.

Classification, nomenclature, occurrence, isolation, general methods of structural determination, isoprene rule,

Biosynthesis and Synthesis of Citral, α -terpineol, Menthol, Farnesol, Aboetic acid and β -carotene

UNIT - II : ALKALOIDS

18 Hrs.

Definition, nomenclature and physical action, occurrence, isolation, general methods of structural elucidation, degradation and classification.

Structure, synthesis and biosynthesis of Ephedrine, (+)-Coniine, Nicotine, Atropine, Quinine, and Morphine

UNIT - III : STEROIDS

18 Hrs.

Occurrence, nomenclature, basic skeleton, Deils hydrocarbon and stereochemistry.

Isolation, structure determination and synthesis of Cholesterol, Bile acids, Testosterone, Progesterone, Aldosterone. Biosynthesis of Steroids.

UNIT - IV : HETEROCYCLIC SYNTHESIS

18 Hrs.

Three membered and four membered heterocyclics synthesis and reactions of aziridines, Oxiranes, azetidines, oxitanes, thiiranes and theitane

Synthesis and reactions of benzopyrrole, benzofuran and benzothiophens.

UNIT - V : SIX MEMBERED HETEROCYCLICS WITH 1,2 OR MORE HETERO ATOMS

18 Hrs.

Synthesis and reactions of Pyrollium salts and pyrones and their comparison with pyridinium and thiopyrilium salts and pyridones.

Synthesis and reactions of diazines, triazines, tetrazines and thiozines.

BOOKS RECOMMENDED:

1. NATURAL PRODUCTS CHEMISTRY AND BIOLOGICAL SIGNIFICANCE- J.Mann, R.S.Davidson, J.B.Hobbs, D.V.Banthrope and J.B.Harborne - Longman.
2. ORGANIC CHEMISTRY - VOL. ii - I.L.Finar - ELBS.
3. STEREOSELECTIVE SYNTHESIS: A PRACTICAL APPROACH - M.Nogradi, VCH
4. NEW TRENDS IN NATURAL PRODUCTS CHEMISTRY - Atta-ur-Rahman and M.I.Choudhary, Harwood academic pub.
5. HETEROCYCLIC CHEMISTRY VOL. 1 - 3 - R.R.Gupta, M.Kumar and V.Gupta, Springer - Verlag.
6. THE CHEMISTRY OF HETEROCYCLICS- T.Eicher and S.Hauptmann, Thieme.
7. HETEROCYCLIC CHEMISTRY - J.A.Joule, K.Mills, G.F.Smith, Chapman & Hall
8. HETEROCYCLIC CHEMISTRY - T.L.Gilchrist, Longman.

UNIT I : INTRODUCTION TO COMPUTERS

18 Hrs.

Introduction to Computers- Generations of Computers – Classification of computers - Anatomy of a Digital Computer -Input Devices - Keyboard, Mouse - Output Devices - Monitor, Printer - Memory Units -RAM, ROM, PROM, EPROM, and EEPROM - Auxiliary Storage Devices- Magnetic storage devices-Floppy Diskettes, Hard disks, Magnetic Tapes. Optical Storage - CD-ROM- - Programming Languages - Machine Language, Assembly Language, High Level Language, Types of High Level Language – Translators : Assembler - Compiler and Interpreters- Introduction to algorithms and flow charts.

UNIT II :

18 Hrs.

Introduction to C-C character set, Identifiers and keywords. Data types - Declarations, Operators and expressions - Arithmetic, Unary, Logical, bit-wise, assignments and conditional Operator. Expressions, statements and symbolic constants, Input-Output statements - Pre-processor commands.

UNIT III :

18 Hrs.

Decision making and Branching - Decision making with IF - Simple IF - IF ... ELSE - Nesting of IF ... ELSE - ELSE .. IF ladder - Switch - ?: operator - GOTO statements - Decision making and Looping - WHILE statement - DO statement - FOR statement - Jumps in loops . ARRAYS - One dimensional Arrays - Two dimensional arrays - Initializing two dimensional arrays - Multi-dimensional arrays.

UNIT - IV :

18 Hrs.

User Defined Functions -Need for functions - Form of C functions - Return values and Types - Calling a function - Category of Functions -Passing arguments, Recursion. Use of library functions, Storage classes - Automatic, external and static variables - Structures and Unions - Definition - Giving values to members - Initialization - Comparison of structure variables - Array of Structures - Arrays within structures - Structures within arrays - Structures and function -Unions - Size of structures.

UNIT - V:

18 Hrs.

Development of small computer codes involving simple formulae in chemistry, such as Van der waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such a Cambridge data base.

BOOKS RECOMMENDED :

1. INTRODUCTION TO COMPUTERS, Alexis Leon and Mathews Leon, Leontech World, 1999.
2. PROGRAMMING IN ANSI C - E. Balaguruswamy - Tata McGraw Hill
3. PROGRAMMING WITH C, B. S. Gottfried, Schaum's Outline Series, 2nd Edition, Tata McGraw Hill, 1998.
4. PROGRAMMING IN C, Kris A. Jamsa, Galgotia Publications P.Ltd, 1988.
5. THE C PROGRAMMING LANGUAGE - Kernighan B.W. and Ritchie D.M., Prentice - Hall of India, 1989.
6. INTRODUCTION TO COMPUTERS - Peter Norton, 2nd Edition, Tata McGraw Hill, 1998

7. COMPUTATIONAL CHEMISTRY – A.C.Norris, John Wiley
8. COMPUTERS IN CHEMISTRY – K.V.Raman, Tata McGraw Hill.

UNIT - I : BASICS

18 Hrs.

Importance of polymers, basic concepts, monomers, repeating units, degree of polymerisation. linear, branched and network polymers. classification of polymers. polymerisation, condensation, addition, radical, chain-ionic and coordination and copolymerisation. Polymerisation conditions and polymer reactions. polymerisation in heterogeneous and homogeneous systems.

UNIT - II : POLYMER CHARACTERISATION

18 Hrs.

Polydispersity- molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution, practical significance of molecular weight, measurement of molecular weight. End group, Viscosity, light scattering, osmotic and ultra centrifugation methods. analysis and testing of polymers - chemical analysis of polymers, spectroscopic methods, x-ray diffraction study. Microscopy, thermal analysis and physical testing - tensile strength. Fatigue, impact. Tear resistance hardness and abrasion resistance.

UNIT - III : STRUCTURE AND PROPERTIES

18 Hrs.

Morphology and order in crystalline polymers - configurations of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers, strain induced morphology, crystallisation and melting. Polymer structure and physical properties - crystalline melting point T_m - melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. the glass transition temperature, T_g - relationship between T_m and T_g , effects of molecular weights, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilisation.

UNIT - IV : POLYMER PROCESSING

18 Hrs.

Plastics, elastomers and fibres. compounding. Processing techniques - calendaring, dyecasting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, reinforcing and fibre spinning.

UNIT - V : PROPERTIES OF COMMERCIAL POLYMERS

18 Hrs.

Polyethylene, PVC, Polyamides, Polyesters, Phenolic resins, Epoxiresins, Silicone polymers. Functional polymers - Fire retarding polymers and electrically conduction polymers. Biomedical polymers - contact lenses, dental polymers, artificial heart, kidney, skin and blood cells.

BOOKS RECOMMENDED:

1. TEXT BOOK OF POLYMER SCIENCE - F.W.Billmeyer, Wiley
2. POLYMER SCIENCE - V.R.Gowariker, N.V.Viswanasthan and J.Sreedar, Wiley - Eastern.
3. FUNCTIONAL MONOMERS AND POLYMERS - K.Takemoto, Y.Inaki and R.M.Ottanbrite
4. CONTEMPORARY POLYMER CHEMISTRY - H.R.Alcock and F.W.Lambe - Printice Hall.
5. PHYSICS AND CHEMISTRY OF POLYMERS - J.M.G.Cowie, Blacke Academic press.