MADURAI KAMARAJ UNIVERSITY

DIRECTORATE OF DISTANCE EDUCATION

DEPARTMENT OF CHEMISTRY

PROGRAMME STRUCTURE AND SYLLABI

for

MASTER OF SCIENCE IN CHEMISTRY

(SEMESTER PATTERN)

ANNEXURE-I

PROGRAMME STRUCTURE AND DESCRIPTION OF COURSES IN M.Sc. CHEMISTRY DEGREE (CBCS - SEMESTER PATTERN)

(With effect from the academic year 2021-2022 onwards)

Semester	Part	Subject	Credits
ONE	Core – 1	Introduction to Organic Reactions	5
	Core - 2	Chemical Bonding, Solid state, Metallurgy and Inorganic Polymers	4
	Core - 3	Thermodynamics, Chemical Equilibrium and Electrochemistry	4
	Major Elective (any one):	1. Medicinal Chemistry	5
		2. Biochemistry	
	Core Practical - I	Organic preparation and Qualitative and Quantitative analyses- Practical	5
		Total	**23**
TWO	Core – 4	Stereochemistry and Organic Reactions	4
	Core - 5	Coordination, Organometallic and Bioinorganic Chemistry	5
	Core - 6	Group Theory and Spectroscopy	4
	Major Elective (any one):	1. Computer Applications in Chemistry	5
		2. Industrial Chemistry	
	Core Practical - II	Inorganic Qualitative and quantitative analyses and preparations-Practical	5
		Total	**23**
THREE	Core – 7	Organic Spectroscopy and Natural Products	4
	Core - 8	Inorganic Spectroscopy, Nanochemistry and f-block elements	4
	Core – 9	Quantum, Nano and Macromolecular Chemistry	5
	Non-major Elective (any one):	1. Chemistry for Competitive Examinations	5
		2. Environmental Science	
	Core Practical - III	Conductometric & Potentiometric Titrations & Kinetic, Adsorption & Spectral Measurements- Practical	5
		Total	**23**
FOUR	Core – 10	Biomolecules, Rearrangements and Synthetic Methods	4
	Core – 11	Nuclear Chemistry, Electroanalytical and Thermal Methods	4
	Core - 12	Chemical Kinetics, Surface, Biophysical and Photochemistry	4
	Major Elective (any one)	1. Polymer Chemistry	5
		2. Introduction to Nanoscience	
	Project & Viva-voce	Project & Viva-voce	4
		Total	**21**
		Total Credits	**90**

* denotes laboratory courses for which the sessions will be scheduled separately.

Core (Theory + Practical) 12+3 = **15 papers**; Elective = **4 papers**; Project = 1
Total papers: 20; Total marks: 20 x 100 = 2000 marks. Total credits = 90

ANNEXURE- II

DETAILED SYLLABI – MSc CHEMISTRY (CBCS - SEMESTER PATTERN)

(With effect from the academic year 2021-2022 onwards)

Semester I

Paper I - Introduction to Organic Reactions

Unit I : Electron Displacement Inductive and field effects – bond distances – bond energies – delocalized bonds – cross conjugation –rules of resonance – resonance energy – resonance effect – steric inhibition of resonance – Hyper conjugation – hydrogen bonding – additional compounds – EDA complexes – Crown ether complexes – inclusion compounds – effect of structure on the association constants of acids and bases – concept of hard and Soft acids and bases.

Unit II : Introduction to Reaction Mechanism : Reaction intermediates – free radicals, carbenes, nitrenes, carbanions, carbocations formation and stability of reaction intermediates – methods of determination of reaction mechanism – kinetic and thermodynamic control of chemical reactions. Kinetic and non-kinetic methods for determining organic reaction mechanism. Principle of microscopic inversibility – Energy profile diagram – Hammond postulate.

Unit III : Aliphatic nucleophilic substitution : Nucleophilicity and basicity – SN1and SN2 mechanisms – effect of substrate structure – effect of the attacking nucleophile – effect of the leaving group – effect of the reaction medium – ambident nucleophiles – ambident substrates – neighbouring group participation of n π and σ electrons. SNi mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophile substitution at an allylic carbon – nucleophilic substitution at a vinyl carbon.

Aliphatic Electrophilic substitution : Electrophilic substitution at saturated caron – SE1 and SE2 mechanisms.

Unit III: Stereochemisty I : Symmetry elements and point group classification – Concept of chirality necessary and sufficient conditions for chirality – Relationship between substrate symmetry and chirality. Projection formulae – Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereogenic centre (chiral centre) and molecules with more than one chiral centre.Propernes of enantiomers and diastereoisomers.Erythro and threo nomenclature. Configuration – determination of configuration. Cahn, Ingold and Prelog system of designation of configuration. **Symmetrical Isomerism :**E – Z nomenclature – determination of configuration of symmetrical isomers using physical and chemical methods – stereoisomerism in monocyclic compounds (upto six membered ring).

Unit IV : Aromatic Character Aromatic character in benzene, six-membered rings, five, seven and eight membered rings – other systems with aromatic sextets – Huckel's rule-Craig's rule concept of homoaromatically and antiaromatically – systems with 2,4,8 and 10 electromagnetic systems with more than 10 electron – Alternant and nonalternant

hydrocarbons, Chemicals of cyclopentadienyl anion – Fulvene, Azulene, Tropolones, Syndnones and Annulenes

Novel ring systems: Nomenclature of bicyclic and tricyclic systems – chemist adamantine, diamantine (congressane), cubane and catenanes.

Unit V: Oxidation and Reduction : Elimination of hydrogen and aromatization reactions - catalytic dehydrogenation – mechanism, applications and stereochemical aspects of the following oxidation – reduction reactions: Oxidation reactions involving CrO_3, SeO_2 lead tertraacetate, periodic acide, N- bormosuccinimide, H_2O_2- - Oppenauer oxidation. Catalytic hydrogenation – reactions involving lithium aluminium by trilsobuty1 aluminohydride, DIBAL and sodium borohydride – Birch reduction Meerweion – pondorf- Verley reduction – Wolff-Kishner reduction – Huang- Minlon modification – hydroboration – selectivity in oxidation and reduction.

Reagents in Organic Synthesis : Gilman's reagent (lithium,dimethylcuprate, diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3- dithiane, trimethylsilyl tri-n-butyltin hydride, Woodward and Provost hydroxylation, DDQ, Merrifield phase transfer catalysts, Peterson's Synthesis, baker's Yeast.

Suggested reading:

1. P. Sykes, Guidebook to Mechanism in Organic Chemistry, Orient Longman.
2. Jerry march, Advanced Organic Chemisty, John Wiley & Sons, 4th edn., 2000.
3. E.S. Gould, Mechanism and Structure in-Organic Chemistry, Henry Holt &Co., New York 1959.
4. J. Shorter, Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford, 1973.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry prntice Hall, 6th edn., 2001.
6. I.L. Finar, Organic Chemistry, Vol. I and II, 5th edn. ELBS, 1975.
7. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry.
8. ReinhardBrukner, Advanced Organic Chemistry, Reaction Mechanisms,
Academic Press, 2002.
9. F.A. Carey and F.J. Sundberg, Advanced Organic Chemist, Part B, 4th edn. Plenum Publishers, 2001.
10. R.O.C Norman, Organic Synthesis 3rd edn.1993.
11. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge University Press, 2nd edn., 1982.
12. H.O. House, Modern Synthetic reactions, W.A. benkajamin Inc., California edn., 1972.
13. P.S. Kalsi, Spectroscopy of Organic compounds, 6th edn., New Age International (P) Limited, 2004.
14. P. Ramesh, Basic Principles of Organic Stereochemistry, Meenu Publications, Madurai, 2005.

Paper II - Chemical Bonding, Solid state, Metallurgy and Inorganic polymers

Specific Objective: To introduce the basic inorganic chemistry concepts and bond properties and solid sate structure and properties, metallurgy of important metals and their properties.

Learning Outcomes: Students will be exposed to the nature of chemical bonds and their properties, structure of inorganic compounds, solid state of inorganic crystals and their

properties and applications. Students also learn about inorganic chains, rings and cages compounds, detailed metallurgy of Be, Cu, Ti, Zr, Th, V, Pu, U and Pt metals.

Unit I: Nature of chemical bonds Covalent bond: Hybridization – Calculation of s and p characters – Bent's rule – VSEPR theory – VBT applied to odd electron molecules like ClO_2, NO, NO_2 etc., M.O. theory; LCAO approximation – application of MOT to heteronuclear molecules like NO, CO, $BeCl_2$, BeH_2 and H_2O – Walsh diagram (diatomic & triatomic molecules) – concept of multicentered bond as applied to electron deficient molecules like diborane and metal alkyls.

Unit II: Bond properties and ionic bonding Ionic radii – covalent radii – van der Waals radius – bond length, bond order, bond energy, bond polarity – partial ionic character of covalent bonds – electronegativity & electron affinity and their applications – lattice energy – Born Haber cycle – Covalent character in Ionic compounds – Fajans rule - Different types of electrostatic interactions – Hydrogen bond and their applications

Unit III: Solid State Chemistry Crystal systems and lattices, miller planes, crystal packing- Evaluation of crystal parameters (density, Avogadro number) - Crystal defects – point, line and plane defects – Colour centers – Electronic structure of solids – Free electron and band theories – Electrical conductivity and superconductivity – High temperature superconductors – Types of semiconductors – Thermo-electric power and Hall effect – Photovoltaic effect – Semiconductors in solar energy conversion.

Unit IV: Inorganic Chains – Rings and Cages: Silicates: Various silicate structures – Structure, property, correlation – Silicones. **Poly acids:** Poly acids: Classification – Isopoly acids polymolybdate, polyvanadate and polytungstate – their structures – heteropolyacids: 12A, 12B, 9 and 6 heteropolyacids – preparation and structures.

Phosphazenes and its polymer – Phosphonitrillic compounds – S_4N_4 – Polymeric sulphur nitride (Polythiazyl) Cage compounds: Nomenclature of Boranes and Carboranes – Wade's rule – Stylx number – preparation and structure of B_4H_{10}, $C_2B_{10}H_{12}$, $(B_{12}H_{12})_2$– borazine.

Unit V: Metallurgy Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Ti, Zr, Th, V, Pu, U and platinum metals and compounds like $BeCl_2$, Beryllium acetate, TiCl4, Titanates, TiO_2, ZrO_2, Thoria, VF_5, $VOSO_4$,V_2O_5,Uranyl halides, Uranyl nitrate, Plutonium halides

References:

1. James E. Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4th End. Harper Collins College Publishers, New York, 1993.

2. Asim K Das, Fundamental concepts of Inorganic Chemistry, Vol 1, 2 and 3, 2nd edition, CBS publisher and Distribution Pvt. Ltd, 2016.

3. G.L. Miessler & D.A. Tarr. Inorganic Chemistry, 3rd Edn. Pearson Education, 2016.

4. P.W. Atkins, D.K. Shriver and C.H. Langfood, Inorganic Chemistry, Oxford-ELBS, U.K. 1990.

5. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edn, John Wiley & Sons, Singapore, 1998.

6. K.M. Mackary and R.A. Mackay, Introduction to Modern Inorganic Chemistry, 4th Edn. Prentice Hall, New Jersey, 1989.

7. K.F. Purcell and J.C. Koltz, An introduction to Inorganic Chemistry, W.B. Saunders Company, Philadelphia, 1980.

8. Anthony R West, Solid state Chemistry and its applications, Wiley, ND, 2016 9. Glen E. Rodgers, Inorganic Chemistry, 3rd Edn, CENGAGE, Learning, 2011.

Paper III - THERMODYNAMICS. CHEMICAL EQUILIBRIUM AND ELECTROCHEMISTRY

Unit I: Application of Chemical Thermodynamics: Maxwell relations – Thermodynamics equations of state- applications in the evaluation of Cp – Cv for solids and for vanderwaalsgases.Partial molar properties partial molar face energy – Gibbs – Duhem equation – Determination of chemical potential (Direct method and method of intercept).Thermodynamic properties of real gases-fugacity concept-Calculation fugacity of real gas – concept of activity and activity co-efficient – experimental determination of activity and activity co-efficient – Third law of thermodynamics – Absolute entropies – Determination of absolute entropies – Exception to third law – Unattainability of absolute zero.

Unit II: Chemical and Phase Equilibria: Thermodynamic derivation of equilibrium constant K for reaction involving ideal and real gases – extent of deviation – Temperature dependence – pressure dependence equilibrium constant – Thermodynamics of chemical reactions (reaction potential), principal of Lechatelier – and Braun – chemical equilibria.
Standard reaction free energy – free energy calculation from thermodynamical, electrochemical and equilibrium data. Gibbs phase rule – its thermodynamic derivation-application of phase rule to three component systems. Formation of one pair, two pairs and three pairs of partially miscible liquids – systems composed of two solids and a liquid.

Unit III: Statistical Thermodynamics : Need for statistical thermodynamics- definition of state of a system- ensembles (micro, macro and grand canonical)- Thermodynamic probability – probability theorems - Boltzmann distribution law and its derivation-Boltzmann-Planck equation- partition functions- thermodynamic properties from partition functions- partition function and equilibrium constant- Quantum statistics- Fermi-Dirac and Bose-Einstein statistics photon gas and electron gas according to such statistics- population inversion- Einstein's and Debye's theories of heat capacities of solids. Nuclear spin statistics-statistical basis of entropy of H_2 gas- ortho and para nuclear states- calculation of residual entropy of H_2 at 0 K in terms of ortho-para ratio – Tetrode equation.

Unit IV: Electrochemistry I : Conductivities of ions – Conductance of strong and weak electrolytes – Determination of equivalent conductance of weak electrolyte at infinite dilution. Kohlrauschs law and its applications – transport numbers and mobilities of ions – measurement of transport numbers – Ionic activities and activity co- efficient and their determinations. Electrodes – types of electrode – Electrochemical cells – Nernst equation –

Emf and its measurements – Application of EMF measurement- determination of equilibrium constant, dissociations constant, solubility product and potentiometric titrations. Theory of electrolytic conductance –Arrhenius ionization theory – Debye Huckel theory – Derivation of Debye – HuckelOnsagar equations – Experimental verifications – Debye Falkenhagen and weineffects – Debye – Huckel limiting law. Applications of conductance measurements – Determination of solubility of sparingly soluble electrolytes – Determination of dissociation constant of weak acid – conducto metric titrations.

Unit V: Electrochemistry II: Introduction to electrical double layer – Evidence for electrical double layer – Electrocapillary phenomena – Electro capillary curves ,Surfactants – lipmanns equations, interpretation and electro kinetic phenomena , zeta potential and its applications – structure of electrical double layer – Helmholtz – perrin , Groy – Chapmonn and stern models of electrical double layer – Applications and limitations . Dynamics of electron transfer – Marcus theory – tunneling – the rate of charge transfer- current density – Butler – Volmer equations – Tafel equations – polarization and overvoltage – mechanism of hydrogen evolution and oxygen evolution reactions. Principles of electro deposition of metals – corrosion and passivity – pourbaix and Evans diagram – methods of protection of metal from corrosion. Power storage systems – fuel cells – construction and functioning – applications – photovoltaic cells.

References:

1) S. Glasston, Thermodynamics for Chemists, East-West Press Private Ltd., New Delhi.

2) J.Rajaram and J.C.Kuriakose, Thermodynamics (III Edn.,) ShobanLalNagin, Chand & Co., Ltd., New Delhi (1999).

3) B.R.Puri, L.P. Sharma and M.S.Pathania, Principles of Physical Chemistry (Millennium Edn,) Vishal Publishing Co., (2003)

ELECTIVE
OPTION 1 - MEDICINAL CHEMISTRY

UNIT-I-Drug Design 1

Define-biopharmaceutics, drug, drug- like molecule, druggable target pharmacophore, toxicophore, metabophore; the processes involved in drug therapeutics (with flowcharts\diagram). Concept of receptors: a) nature, criteria, define, druggable target, drug, drug-like elementary treatment of drug-receptor binding interactions: covalent, ionic, dipole-dipole, hydrogen bonding, charge transfer, hydrophobic, and vanderwaals, selection of these in drug design. b) Definition of classical binding terms: dose-response curve, agonist, antagonist, partial agonist, inverse agonist, auto receptor, affinity, efficacy, potency, LD50, ED50, TD50 tolerance. Theries of drug activity :L occupation theory(derivation),rate theory, induced fit theory. Experimental quantification: direct, titration, double reciprocal. Dixon, Scatchard and Hill plots. Receptor selection for drug design: disease, systems, pathological process and molecular process-centered. Drug-Drug interactions in drug design (rational polypharmacy)

UNIT-II- Drug design-2

Multiphore method of drug design-concept of lead compound, lead optimization: analog synthesis by variation of substituents, chain length, double bonds, rings, isosteric, bioisosteric

and physico chemical characters (QSAR) concept of prodrugs and soft drugs, structure-activity relation(SAR)- factors affecting bioactivity based on physical ,chemical, electronic, stereo and geometric considerations: hydrophilicity, lipophilicity, partition coefficient, Shelton and surface activity parameters, bioavailability, geometric, conformational, topological, steric, optical, resonance, inductive, bonding, polarizability, Hammett correlation, ionization constant, redox potentials. ID-QSAR: Hansch, Free –Wilson approach.

UNIT-III-Drug design-3

Introduction to drug adsorption, disposition ,metabolism, elimination (KADME) using pharmaco kinetics and dynamics, discuss various parameters involved, Models-compartment, Non-compartment, physiological- advantage, disadvantage, Explain kinetics and dynamics of intravenous bolus administration and infusion. Mean residence time, statistical moment analysis, pharmacodyunamic models: linear, logarithmic, Emax models, enzyme stimulation, inhibition, drug metabolism, xenobiotics, biotransformation. Scope, importance of pharmacognosy, Indian system of medicinies-Ayurveda, Siddha, Unani, Homeopathi and Aromatherapy. Drugs obtained from plants, animals,marine organisms, minerals and microbes (examples and uses) enzymes in plants and animals-preparation, uses-papain, asparginase, rennin, trypsin, urokinase, pancreatin.

UNIT-IV- Chemotherapeutic agents-I

a) Antineoplastic agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mecholrethamine, cydophosphamide, melphalan, uracil, mustards, 6- mercaptopurine. Recent development in cancer chemotherapy.Hormone and natural products.

b) Cardiovascular drugs:Introduction,cardiovasculardiseases,drug inhibitors of peripheral sympatheticfunction,central intervention of cardiovascular output.Direct acting arteriolar dilators. Synthesis of amylnitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

c) Antimalarialdrugs: Classification, synthesis, assay; chloroquin, primaguine, amaodiaquine, proguanilprimethamine.

UNIT-V Antibiotics and Anti infective drugs

a) Local anti infective drugs: general mode of action, synthesis of sulphonamides, furazoildone, nalidixic acid, ciprofloxacin, nor floxacin, dapsone, aminosalicylic acid, fluconazole, econozole, griseofulvin

b) Antibiotics: cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of ampicillin, amoxycillin, cephalosporin, tetracycline, streptomycin.

References:

1. Introduction to medicinal chemistry, A.Gringuage, Wiley VCH.
2. Wilson and Gisvold's Text book of organic medicinal and pharmaceutical chemistry, Ed. Robert F.Dorge
3. An introduction to Drug Design, S.S Pandya, J.R. Dimmock, New Age International
4. Burger's medicinal chemistry and Drug discovery, vol-I, M.E.Wolff, Johnwiley.
5. Goodman and Gilman's Pharmacological basis of therapeutics, McGraw-Hill
6. Organic chemistry of drug design and drug action, R.B.;Silverman, Academic press.
7. Strategies for organic drug synthesis and design, D.Lednicer, Johnwiley.
8. Biopharmaceutical and pharmacokinetics- G.R.Chatwal, Himalaya.

9. T.Nogrady, Medical chemistry, A biochemical approach, Oxford university press Edn.III.
10. C. Laxmi, Medicinal chemistry, S. Chand.
11. JeyasreeGhosch, pharmaceutical chemisty, S.Chand.
12. Foye's principles of medicinal chemistry, VI Edn. L.Lemke, A.Williams, F.Roche, William zito; Wolterskluwer

ELECTIVE
OPTION 2 - BIO-CHEMISTRY

Unit I: Enzymes Classification, nomenclature, properties of enzymes, some features of active sites of enzymes, enzyme kinetics – Michaelis – Menton model – significance of KM and VMaxvalues.Enzyme inhibition – competitive and non-competitive.Allosteric interaction – Mechanism of enzyme action.Lysozyme and carboxypeptidase.

Unit II: Generation and Storage of Metabolic energy Metabolism – basic concepts and design: glycolysis – citric acid cycle – oxidative phosphorylation – pentose pathway and gluoneogenesis. Glycogen and disaccharide metabolism, fatty acid metabolism – amino acid degration and urea cycle – photosynthesis.

Unit III: Information, Storage, Transmission, Expression of genetic information DNA – Genetic role structure and replication: messenger RNA and transcription genetic code and gene protein relationship – protein synthesis, control of gene expression – Eucaryotic chromosomes, Recombinant DNA technology and viruses.

Unit IV: Bio-inorganic chemistry: Metalloproteins and enzymes – Blue copper proteins – copper proteins as oxidases / reductases – Nickel containing enzymes – structure of DNA – types of nucleic acid interactions – coordination, intercalation and hydrogen bonding – interactions of metal ions with nucleic acid – redox chemistry, hydrolytic chemistry – monitoring the DNA binding by UV, IR, NMR and CV spectral techniques.

Unit V: Biophysical aspects Electron transport and oxidative phosphorylation – Thermodynamic and kinetic aspects – Photosynthesis – An overview – Photosystem II – The light harvesting chlorophyl II – protein complexes of photosystem II – Role of carotenoids in photosynthesis – The primary electron donor of photosystem II, P680 – The stable primary electron acceptor QA and the secondary electron acceptor QB – the transient intermediate electron acceptor of photosystem II, pheophytin – Oxygen evolution – The role of manganese – The electron donor to P680+ - Charge recombination in photosystem II – Photosystem I – Light-harvesting chlorophyl II – protein complexes of photosystem I – The primary electron donor of photosystem I, P700 – The Primary electron acceptor A0 of photosystem I – The intermediate electron acceptor A1 of photosystem I – Mobile electron carriers plastocyanin and ferredoxin and NADP+ - reductase.

References:
Unit I-III

1. B.D. Hames and N.M. Hooper, Biochemistry, Viva Books Pvt. Ltd., 2003.
2. J.M. Berg. J.L. Tymoczko and L. Stryer, Biochemistry, 5thEdn. W.H. Freeman and Company, New York, 2002. 3. A.L. Lehninger, Biochemistry, Nath Publishers. 2798

Unit IV:

1. I. Bertini, H.B. Gray, S.J. Leppard and J.S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998.
2. B. Ke. Advances in Photosynthesis, Vol. 10 Photosynthesis – Photobiochemistry and photobiophysics, kluwer Academic Publishers, Dordrecht, 2001.

Unit V:

1. B.Ke. Advances in Photosynthesis, Vol. 10 Photosynthesis – Photobiochemistry and photobiophysics, kluwer Academic Publishers, Dordrecht, 2001.

PRACTICALS
Semester I

Organic preparation, Qualitative and Quantitative Analysis

Separation and analysis of two component mixtures. Identification of the components and preparation of solid derivative.

1. Quantitative analysis

a) Estimation of glucose by Lane and Eynon method and Bertrand method.
b) Estimation of glycine
c) Estimation of formalin
d) Estimation of methylketone

2. Organic preparations (only for class work) - About THREE two stage preparations :

a) p - Nitroaniline from acetanilide
b) P-Bromoaniline from acetanilide
c) m – Nitrobenzoic acid from methyl benzoate
d) Benzanilide from benzophenone
e) sym – Tribromobenzene from aniline.

3. Spectral analysis of synthesised compounds using FTIR, NMR, LC-MS, etc

*****

Semester II

Paper I - Stereochemistry and Organic Reactions

Unit I : Stereochemistry II : Prochirality and prosteroisomerism, enantiotopic and diasterotopic ligands and faces and their nomenclature pro-R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions. A symmetric synthesis, Cram and Prolong rules; Optical isomerism due to axial chriality – biphenyls, allenes and spiranes, -molecules with plannar chirality – paracyclophanes, trans cycloctene, ansa compounds.

Unit II : Conformational analysis : Configuration and confirmation – conformations of ethane and n-butane conformation analysis p stereoelectronic and steric factors – conformation of simple cyclic compounds – confirmations of monosubstituted and disubstitutedcyclohexanes correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties – conformational free energy – Curtin – Hammett principle – quantitative treatment of mobile system – Eliel – RO Equation – conformations and reactivity of cyclobexanones – conformational analysis of aldohexopyranoses.

Unit III : Addition to multiple bands : Electrophilic, nucleophilic and free radical additions – addition to conjugated systems – orientation of the addendum – stereochemical factors in reactions like addition of hydrogen, halogens, hydrogen, halides and hypohalous acids, hydroboration and hydroxylation – epoxidation. \ Addition to carbonyls groups – mechanism – Aldolcondenstation – Perkin reaction - Knoevenagel reaction – Manmch reaction – Cannizaro reaction – benzoil condensation – Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Writing reaction – Grignard reaction. Addition to α, β unsaturated carbonyl groups – addition of Grignard reagent to α, β unsaturated carbonyl compounds – Michael addition – Diels – Alder reaction – addition to carbenes and carebenoids to double and triple bonds. Esterification of acids and hydrolysis of esters – decarboxylation of carboxylic acids.

Elimination : α – elimination – β – elimination – E1, E2, and E1CB mechanisms – stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E1, E2 and E1cB reactions – elimination vs substitution – pyrolyticcis eliminations – Bredt's rule.

Unit IV :Terpenes : Classfication of terpenoids – structure, stereochemistry and synthesis α, pinene, camphor, zingiberene, cadinene, α-santonin, abietic acid and squalene.

Vitamins : Structure and synthesis of Vitamins A, B1, B2, B6, B12 (structural features only) E, H & K.

Unit V : Aromatic electrophilic substitution – orientation – reactivity – mechanism of nitration, halogenations, Friedal-Craft's reaction and sulphonation – partial rate factors – ortho / para ratio – Quantitative treatment of reactivity of the electrophile (the selectivity relationship) – Aromatic nucleophilic substitution reactions – SNAr, SN_1 and benzyne mechanisms. Quantative treatment of the effect of structure on reactivity – The Hammett relationship – significance of reaction and substituents constants – application of the Hammett equation in reaction mechanism – limitations and deviations.

Suggested readings:

1.E.L.Eliel. S.H.Wilen& L.N.Mander, Stereochemistry of Carbon Compounds, John Wiley & Sons, 2003.
2. V.M. Potapoy, Stereochemistry, MIR Publishers, Moscow, 1979
3. L.L. Finar, Organic Chemistry, Vol.II, 5th edn.ELBS, 1975.
4. D. Nasipuri, Stereochemistry of Organic Compounds, principals and Applications, New Age International (P) Limited, 2ndedn., 1994.
5. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, New Aged International (P)Limited, 4th edn.1997.
6. T.H.Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry.
7. Jerry March, Advanced Organic Chemisty, John Wiley & Sons, 4thedn., 2000.
8. E.S. Gould, Mechanism and Structure in Organic Chemistry, Henry Holt & Company, New York, 1959.
9. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Academic Press, 2002.
10. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part B – 4th edn., Plenum Publishers, 2001.
11. Paul de Mayo, Chemistry of Terpenoids, Vol. I & II, academic press.
12. L. Fieser and Mary Fieser, Steroids, Rerinhold 1953
13. W.Klyne, The Chemistry of Steroids, Methuen & Co – New York, 1965.
14. S.F. Dyke, Chemistry of Vitamins, Interscience Publisher 1965.

Paper II - Coordination, organometallic and Bio-inorganic chemistry

Unit I: Coordination Compounds IUPAC Nomenclature of coordination compounds – isomerism in coordination compounds – Types of ligands – monodendate, ambidentate and macro cyclic ligands – Chelate and Chelate effect - Stability constant – Factors affecting stability of complex compounds – Determination of stability constant spectrophotometry, Jobs method and polarographic methods. Theories of bonding – VB – CFT — Splitting of d-orbitals in Oh, Td, square planar and trigonalbipyramidal geometries – CFSE calculation in terms of Dq – Factors affecting crystal field splitting – Spectrochemical series –Jahn-Teller Theorem- MO theory of octahedral complex- Magnetic properties of transition metal complexes – calculation of spin-only and orbital quenching magnetic moments.

Unit II: Reaction mechanism of coordination compounds: Substitution reactions of octahedral complexes – labile – inert complexes – mechanism of acid hydrolysis – and anation reactions. Substitution reactions of square planar complexes – Factors affecting reactivity of square planar complexes – Trans – effect and its applications – Electron transfer reactions – complementary and non-complementary reactions – outer sphere and inner sphere electron transfer mechanisms – Synthesis of coordination compounds using electron transfer and substitution reactions, Macrocyclic ligand and Template effect.

Unit III: Bio-inorganic Chemistry-I Porphyrin ring system – metalloporphyrins – hemoglobin and myoglobin – structures and work functions – synthetic oxygen carries – cytochromes – structure and work function in respiration – chlorophyll – structure – photosynthetic sequence – iron-sulphur proteins (non-heme iron protein) – Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases – copper proteins as oxidases – cytochrome C oxidase – mechanistic studies of Cytochrome C oxidase – Hemocyanin.

Unit IV: Bio-inorganic Chemistry-II Carboxypeptidase A: structure, function – carbonic anhydrase – inhibition and poisoning – corin ring system – vitamin B12 and B12 coenzymes – *in-vivo* and *in-vitro* nitrogen fixation – essential and trace elements in biological systems – metal ion toxicity and detoxification – molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps – chelate therapy – *cis*platin.

Unit V: Organometallic Chemistry Synthesis, structure and bonding in metal carbonyls, nitrosyls, dioxygen complexes and dinitrogen complexes – Application of EAN and 18 electron rules- Synthesis, properties, structure and bonding in Ferrocene, Arene, olefin, acetylene and allyl complexes. Oxidative addition – reductive elimination – insertion reaction – catalytic mechanism in the following reactions: hydrogenation of olefins (Wilkinson catalyst) – Tolman catalytic loops – hydroformylation (oxo process) – acetic acid from ethanol – oxidation of alkenes to aldehydes and ketones (Wacker process) – catalysis in the formation of synthesis of gas-olefin polymerisation (Ziegler – Natta) – Cyclooligomerisation of acetylenes (Reppe's or Wilke's catalysts) – olefin isomerisation using Ni catalyst.

Suggested Readings:

1. W.E. Addison, Structural Principles of Inorganic Chemistry, Wiley, 1961.
2. B.D. Gupta and A.J. Elias, Basic organometallic chemistry, 2nd Edition, University Press, 2017.

3. Asim K das, Fundamental concepts of Inorganic Chemistry, Vol 4-6, 2nd edition, CBS publisher and Distribution Pvt. Ltd, 2016.
4. A.F. Wells, Structural Inorganic chemistry, 4th edition, Oxford, New York, 1975.
5. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6thEdn., John Wiley & Sons, Singapore, 2017.
6. K.P. Purcell and J.C. Koltz, An introduciton to Inorganic Chemistry, W.B. Saunders Company, Philadelphia, 1980.
7. James E.Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4h Edn, Harper Collins College Publishers, New York, 1993.
8. F. Basalo and R.G. Pearson, Mechanism of Inorganic reaction, 2ndEdn., Wiley, New York, 1967.
9. I.Bertini et al. Bioinorganic Chemistry, Viva Books Private Ltd., Chennai, 1998.

Paper III - GROUP THEORY AND SPECTROSCOPY

Unit I: Molecular Spectroscopy I: Characterization of Electromagnetic radiation - Types of molecular energies- Adsorption and emission spectra - signal to noise ratio- the width and intensity of spectral transition – microwave spectra of rigid and non rigid di atomic molecules and simple polyatomic molecules- Einstein's coefficient- induced emission and absorption- Rotational spectra of rigid diatomic molecules- effect of isotopic substitution relative intensity of rotational spectral lines – stark effect in microwave spectra – microwave spectrometer – Application of microwave spectra. Infrared spectroscopy – energy of a diatomic molecule based on harmonic and anharmonic oscillator model – selection rule – diatomic vibrating rotator – P.Q.R branches – Break down of Oppenheimer approximation – Influence of rotation on the spectra of polyatomic molecules – overtones , combination and difference bands – concept of group frequencies – coupling interaction – Fermiresonance – Fourier transform infrared spectroscopy . Application of IR spectra.

Unit II: Molecular spectroscopy II: Raman spectroscopy – qualitative quantum theory of Raman scattering, pure rotational, vibrational and vibrational – rotational Raman spectra – selection rules – Mutual exclusion principle – laser Raman spectra – Electronic spectra of diatomic and polyatomic molecules – Born – opperheimer approximation – vibrational coarse structure – Frank – condon principle – dissociation energy – rotational fire structure of electronic – vibration transitions – fortrat diagram- predissociation. Photoelectron spectroscopy – theory – XPS – UV –PES – Instrumentation – evaluation of ionization potential – ESCA – chemical information from ESCA – Auger electron spectroscopy – basic idea

Unit III: Spin Resonance Spectroscopy: NMR – Principle – Relaxation process – chemical shift- spin – spin splitting, relaxation times – line shape and line width, experimental technique – double resonance technique, ENDOR , Overhauser effect, FT – NMR Spectroscopy, Lanthanide shift reagents – NMR imaging. NQR –Principles – Characteristics of quadrapolar nucleus – effects of field gradient and magnetic field upon quadrapolar energy levels – NQR transitions – application of NQR spectroscopy. ESR – Principles – hyperfine spilliting – factors affecting the magnitude of g value – ESR spectra of free radicals in solutions – Anisotropic systems –Systems in triplet state – Zero field splitting and Krammers degeneracy

Unit IV Group theory: Molecular symmetry elements and symmetry operations – Group

postulates and types of groups- point groups – assignment of point groups to molecules – order of a group, sub groups, similarity transformations – conjugate elements and classes- Group multiplication table- cyclic and inverse rule – Matrix representation of symmetry operations, character of the matrix – reducible and irreducible representation - properties of irreducible representation – Mullikans notation- statement and proof of Great orthogonality theorem and its consequences- construction of character tables- C2v,C3v,C4v,C2h and D2α point groups – Determinations of symmetry species for translation and rotations – Direct product concept – Symmetry of hybrid orbitals.

Unit V Application of Group theory: Standard reduction formula relating reducible and irreducible representations – symmetries of normal modes of vibrations in linear and non-linear molecules – physical basis of spectroscopic selection rule – properties of dipole moment, polarizability and definite integrals. Selection rules for vibrational spectra –IR and Raman active mutual exclusion principle with illustrations Symmetries of molecular orbitals and symmetry selection rule for electronic transition in ethylene formaldehyde and benzene. Projection operators- SALC procedure – Hybridization schemes for atoms in CH4, BF3, Ptcl42-, and SF6. Wave functions as basis of irreducible representation – HMO theory – HMO Calculation and delocalization energy for cyclopropeny, butadiene and benzene systems.

References:

1) F.A.Cotton, Chemical Applications of Group Theory, 3rd, Edn., John Wiley & Sons, New York (1999).
2) G.Davidson, Introduction to Group Theory for Chemist, Applied Science Publishers Ltd., London (1971).
3) V.Ramakrishnan and Gopinath, Group Theory in Chemistry, 2nd edn., Vishal Publications, 1991.
4) K.V.Raman, Group Theory and its Application in Chemistry, Tata McGrew-Hill, (1990).
5) A.Streitweiser, Molecular Orbital Theory for Organic Chemistry, John Wiley & Sons.
6) C.N.Banwell and E.M.McCash, Molecular Spectroscopy. Tata McGraw Hill, 4th Edn., (1995). 7) G. Aruldhas, "Molecular Structure and Spectroscopy", Prentice-Hall of India Ltd., New Delhi (2001).
8) R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977)
9) D.C.Harris and M.D. Bertolucci, Symmetry and Spectroscopy-An Introduction to Vibrational and Electronic Spectroscopy, Oxford University Press, New York, (1978).
10) G.H.Barrow, Introducation to Molecular Spectroscopy, McGraw Hill.
11) R.Chang, Basic Principles of Spectroscopy, McGraw Hill, London (1976).
12) B.F.Straughan and S. Walker (eds.). Spectroscopy, Vol 1.2 and 3, Chapman & Hall, London (1976).
13) P.W.Atkins, Physical Chemistry, 6thedn., Oxford University Press, Tokyo (1998). 14) E.B.Becker, High Resolution NMR, 2nd edn., Academic Press, 1990
15) A.Carrignton and A.D.McLachian, Introduction to Magnetic Resonance, Harper and Row. 16) D.Shaw, Fourier Transform NMR Spectroscopy, Elsevier.

ELECTIVE OPTION 1 - COMPUTER APPLICATIONS IN CHEMISTRY

Unit I: Basic Concepts of Communications systems
Computer networks: An overview – communication processors – protocols – network architecture Net working – types of network-Net work topology Communication systems: Satellites – RADAR – optical fibers – advantages and disadvantages – ISDN – distributed systems – advantages and disadvantages. Telecommunications: Analog and digital signals – types and needs of modulations – MODEMS – Telecommunication software.

Unit II: Basic concepts of Internet and Applications in Chemistry Internet: History of internet – the working way of internet – getting connected to internet – Internet protocols – Internet addressing – domain names – internet services- Characterization – advantages – drawbacks – need for intranet – extranet. **WWW:** Web pages – home pages – web browsers – search engines – internet chat – chatting on web. **Application of Internet in Chemistry:** Websites in Literature survey in chemistry – popular websites in chemistry –opening, browsing and searching a website – literature searching online. Desktop chemical software - Structure drawings programs using Chemdraw – Graph drawing and calculation of Linear and Multi regression and correlation coefficient using Ms Excel.

Unit III: Basic Concepts VB Introduction to Visual Basic – the integrated development environment – the menu bar, the tool bar, the project explorer, the tool box, the properties of window, the form designer, the form lay out, the immediate window, the elements of the interface –customizing the environment. Working with Forms: The appearance of form – the start up form – loading, showing and hiding forms – elementary concepts of drag and drop operations. Elementary concepts of the Text Box control, the List Box and Combo Box controls. Variables – declaring variables – variable types – strings, numeric and data variables – scope and life forms of variables – constants.

Unit IV: The Language Forms and Basic Active Controls Control flow statements: If ... Then and If ... Then ... Else Loop statements: DO... Loop, For ... Next and While – Wend-nested control statement – the Exit statement. Arrays: Declaring arrays – specifying arrays – multi dimensional arrays. Procedures: Subrouties, functions, calling procedures

Unit V: Applications of VB in Chemistry Writing Simple VB programs in Chemistry: 1. Calculation of different types of velocity 2. Ionic strength of an electrolyte. 3. Different velocities of a gas. 4. Average rate constant. 5. Unit cell dimensions in solid state 6. Thermodynamic parameters. 7. Reduced mass. 8. Empirical formula of an organic compound containing C, H and O. 9. Normality, molality and molarity of a solution. 10. Half life period of a radioactive material. 11. Temperature in Kelvin scale into Celsius scale and vice-versa.
Practical (Class work Only) Salient feature of windows and MS Word for typing texts equations in Chemistry To learn creating, receiving and sending e-mail Drawing chemical structure and predicting NMR spectrum in ChemDraw To search a particular topic in chemical literature sources for physical data, reactions, syntheses, techniques or concepts. To learn the data analysis correlation and curve fitting using MS Excel Data interpretations of some physical chemistry experiments like CST, Ester hydrolysis, Phase Diagram To develop a visual basic application for displaying the contents of the selected file using the file list box, directory list box and drive list box. To learn the integrated development environment – the menu bar, tool bar, the project explorer, the tool box, Different types of window Form designer, the Message box and Input box Construction of programs in VB language,

compiling, debugging and making executive files, printing the output. Running VB programs in Chemistry to calculate/determine the problems given in Unit V

References:

1. Evangelos Petroutsos, Mastering "Visual Basic 6", BPB Publication, First Indian Edition, New Delhi, 1998, pp 1-51, 99-174, 177-180, 209-211, 227-262.
2. David Jung, Pierre Boutquin, John D. Conley III, Loren Eidahl, Lowell Mauer and Jack Pudum, "Visual Basic 6 Super Bible", First Indian Edition, Techmedia, New Delhi, 1999.
3. Gary Cornell, "Visual Basic 6", Tata-McGraw Hill, New Delhi, 1998.
4. Barbara Kasser, "Using the Internet", Fourth Edition, EE Edition, New Delhi, 1998.
5. K.V. Raman, "Computers in Chemistry", Tata – McGraw Hill Publishing Company, New Delhi, 1993.
6. Alexis Leon and Mathews Leon, "Fundamentals of Information Technology", (Chapters 17-19 & 21-23), Leon Vikas, Chennai (1999).

ELECTIVE OPTION 2 - INDUSTRIAL CHEMISTRY

Unit : I PRINCIPLES OF CHEMICAL TECHNOLOGY Introduction – basic principles of chemical technology – importance of chemical technology – classification of technological process – designing and modeling of chemical plants – unit process and unit operations. Basic requirements of industrial reactors – choice and selectivity of reactor – basic principles of homogeneous and heterogeneous processes and reactors with examples.

Unit : II RAW MATERIALS AND ENERGY FOR CHEMICAL INDUSTRY Raw materials – Characteristics of raw materials and their resources – methods of raw material concentration – integral utilization of raw materials. Energy for chemical industry – power and fuels – classification of fuels – coal – fuel gases and liquid fuels – petroleum – cracking – chemical corrosion – types of corrosion and preventive measures.

Unit : III SMALL SCALE CHEMICAL INDUSTRIES Electro-thermal and electro-chemical industries: electroplating – surface coating industries – oils, fats and waxes – soaps and detergents – cosmetics. Match industries and Fire Works: Manufacture of some industrially important chemicals like potassium chlorate, potassium nitrate, barium nitrate and red phosphorous – metal powders.

Unit : IV LARGE SCALE CHEMICAL INDUSTRIES Manufacturing process – raw materials – composition and uses of products in Portland cement – ceramics – plastics, synthetic fibres –synthetic rubber – fertilizers – insecticides and pesticides – photo film industries – commercial aspects of starting an industry

Unit : V INDUSTRIAL SAFETY

Safety signs and colours used in industries – Industrial Hazards and Accidents – Classification of Hazards – Physical, chemical Biological, Ergonomic and stress Hazards – Causes, prevention and control – case study on industrial accidents – Bhopal gas Tragedy – Heat stress – sources and control – Noise pollution in industry – sources and control.

References:

1. Mukhlynov (ed.), Chemical Technology, Vol.1, Mir Publication, Moscow, III edn., 1979.
2. A. K. De, Environmental Chemistry, Wiley Eastern Ltd., II edn., Meerut 1989, Chs, 5 – 7.

3. R.K. Goel, Process know-how and material of construction for Chemical Industries, S.B. Publ., Delhi, 1977.
4. B.N. Chakrabarthy, Industrial Chemistry, Oxford and IBH Publ., Now Delhi, 1984.
5. R. Norris Shreve and J.A. Brink, Jr. Chemical Process Industries, IV edn., McGraw Hill, Tokyo, 1977.
6. Industrial Safety and Environment – A.K. Gupta – University Science press, New Delhi.

Semester II Practicals
Inorganic Qualitative and Quantitative Analysis & Preparations

1. Semimicro Qualitative Analysis:

Analysis of mixture containing two familiar and two less familiar cautions from the following:

Less familiar W, Mo, Se, Te, Ce, Th, Zr, Ti, V, U, Li,

Familiar: Pb, Cu, Bi, Cd, Cr, Mn, Zn, Co, Ni, Ca, Sr and Mg

(Insoluble and Interfering anions may be avoided)

2. Estimation: Estimation of one metal ion (Cu, Mg, Ca) in the presence of impurity (Pb) by complexometric titration.

3. **Inorganic Preparations:** Preparation of at least three inorganic complexes.

1)	*$VO(acac)_2$*	*9)*	*$[Ni(DMG)_2]$*
2)	*$K_3[Fe(C_2O_4)_3]$*	*10)*	*$[Cu(NH_3)_4]SO_4.H_2O$*
3)	*Prussian Blue, Turnbull's Blue*	*11)*	*$K_3[Cr(C_2O_4)_3]$*
4)	*Cis – $[Co(trien)(NO_2)_2]Cl.H_2O$*	*12)*	*$[Cu(thiourea)_3]Cl$*
5)	*$Na[Cr(NH_3)_2(SCN)_4]$*	*13)*	*$[Co(NH_3)_5(NO_2)](NO_3)_2$*
6)	*$Hg[Co(SCN)_4]$*	*14)*	*$Mg(C_9H_6ON)_2].2H_2O$*
7)	*$[Co(Py)_2Cl_2]$*	*15)*	*$[Fe(acac)_3]$*
8)	*$[Ni(NH_3)_6]Cl_2$*		

4. **Inorganic Quantitative Analysis (Any two)**
Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe, Ca-Ba, Cu-Zn, Fe-Ni etc. involving volumetric and gravimetric methods.

5. Spectral characterization of any two synthesized inorganic complexes – Demonstration only
a) Evaluation of 10Dq, β'and β from UV-Visible spectrum.
b) Evaluation of IR frequencies of stretching and bending vibration of selected inorganic complexes.
c) Calculation of g and A values from EPR spectrum evaluation.
d) Evaluation of thermal stability of inorganic complexes by TGA, DTA and DSC studies.

SEMESTER III
Paper I - Organic Spectroscopy and Natural Products

Unit I : Spectroscopy I : UV Spectroscopy : Principle – absorption spectral of conjugated dienes ; α, β unsaturated carbonyl compounds – Woodward – Fieser rules. **IR Spectroscopy:** Molecular vibrations – vibrational frequency – factors influencing group frequencies – quantitative studies. **Mass Spectroscopy:** Principle – type of ions – base peak – parent ion, metastable and isotopic peaks – fragmentation – general rules – pattern of fragmentation for various classes of compounds – Mc Lafferty rearrangement – Retro Diels – Alder reaction.

Unit II – Spectroscopy II : NMR Spectroscopy : Origin of NMR / spectra – chemical shift – spin-spin coupling – coupling constant – first and second order spectra – spin – spin splitting – influence of stereochemical factors on chemical shift of protons – simplification of complex spectra - deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect – CIDNP-NMR concept of aromaticity. **NMR Spectroscopy :** Basic principle of FT technique – Relaxation time – assignment of signals – Off resonance decoupling – additivity relationship – calculation of chemical shifts for aromatic and alphatic compounds – DEPTC spectra – 13C -13C correlation COSY, HETCOR, ROESY, NOESY and TOCSY – Inadequate.

Unit III – Chiroptical and Analytical techniques ORD and CD – Principle – Cotton effect – type of ORD curves – α – haloketone rules – Octant rule – applications to determine the configuration and confirmation of simple monocyclic and bicyclic ketones – comparison of ORD and CD. **Chromatographic techniques:** Column, TLC, Paper, GLC, HPLC, Exclusion and Ion exchange.

Unit IV : Steroids : Classification – configurational and conformational aspects of A/B cis and A/B trans steroids – complete chemistry and stereochemistry of cholesterol (includes bile acids), chemistry of ergosterol and Vitamin D – male sex harmones – androsterone and testosterone - female sex harmones – oestrone, equilenin and progesterone – A basic idea about adernocorticalharmones – cortisone (synthesis not included). Prostaglandins. General study of prostaglandins, Structures, Chemistry of PGE1 and PGF1α.

Unit V : Alkaloids and antibiotics : General methods of structural determination- Hofmann, Emde and Von Braun degratations. Structure and synthesis of quinine, papaverine, atropine, narcotine, morphine, reserpine and Iysergic acid. **Antibiotics :** Definition, classification of antibiotics, structure, stereochemistry and synthesis of penicillin, chloramphenicol.

References:

1. John R. Dyer, Application of absorption, Spectroscopy, prentice – hall William Kemp, Organic Spectroscopy, ELBS, 3rd edn.,
2. William Kemp, Organic Spectroscopy, ELBS, 3rd Edn.
3. Robert M. Siverstelin, Francis X, Webster, Spectrometric Identification of Organic Compounds, 6thedn., John Wiley & Sons, Inc., 2004.
4. I.L. Finar, Organic Chemistry, Vol.II, ELBS, 1975
5. Paul de Mayo, Chemistry of Terpenoids, Vol. I & II Academic Press.
6. L. Fieser and Mary Fieser, Steroids, Reinhold 1953
7. W. Klyne, The Chemistry of Steroids, Methuen & Co., New York.1965.
8. E.L. Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, 1962

9. P. Crabbe, ORD and CD in Chemistry and Biochemistry, Academic Press 1972.
10. A Braithwaite and F.J. Smith, Chromatographic methods, Chapman and Hall 4th edn., 1985.
11. K.W. Benty, Alkaloids, Vol I &II Interscience 1957.

Paper II - Inorganic Spectroscopy, Nanochemistry and f-block elements

Unit I: Application of spectroscopy to the study of Inorganic Compounds I Electronic spectra of transition metal complexes and Photochemistry, d-d transition-charge transfer transition – selection rules – mechanism of breakdown of selection rules – bandwidths and shapes – Jahn Teller effect – Tanabe – Sugano diagram – evaluation of 10Dq and for octahedral and tetrahedral complexes of d3, d6, d7 and d8 configurations – photochemistry – photo redox and substitution reaction occurring in Co(III) and Cr(III) complexes – photochemistry of ruthenium polypyridyls.

Unit II: Application of spectroscopy to the study of Inorganic Compounds II Application of IR and Raman spectra in the study of coordination compounds – application to metal carbonyls and nitrosyls – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding – stretching mode analysis of metal carbonyls. Mossbauer and Photoelectron spectroscopy (PES): Mossbauer effect resonance absorption – Doppler effect – Doppler velocity – Experimental technique of measuring resonance absorption – isomer shift – magnetic hyperfine splittings application of Mossbauer spectroscopy in the study of iron and tin complexes. Photoelectron spectroscopy: Theroy – XPS – UV-PES – Instrumentation evaluation of ionisation potential – Chemical identification of elements – Koopmann's theorem – chemical shift – UPS – XPES of N_2, O_2 and HCl - evaluation of vibrational constants from UPS – spin-orbit coupling – Auger spectroscopy – principle and its applications.

Unit III: Application of spectroscopy to the study of inorganic compounds III NMR Spectroscopy:31P, 19F and 15N – NMR – introduction – applications in structural problem – evaluation of rate constants – monitoring the course of reaction – NMR of fluxional molecules – NMR of paramagnetic molecules – contact shifts and shift reagents.
ESR Spectroscopy: Principles – presentation of the spectrum – hyperfine splitting – evaluation of g- and A tensors – factors affecting the magnitude of g-values – zero field splitting – Kramer's degeneracy – ESR of d3 octahedral – complexes – anisotropy and hyperfine splitting constant – Application of ESR in the study of transition metal complexes – Jahn-Teller distortion studies in Cu(II) complexes – evaluation of spin-orbit coupling.

Unit IV: Nanochemistry Basic idea of nanochemistry –Challenges and Future prospects-Defining nanoassembles – measurements – examples – Applications of nanomaterials – zero dimensional, one dimensional and two dimensional arrangements. **Nanotubes:** Structure and characterization of single walled carbon nanotubes – nanotubes properties – application of nanotubes. **Nanowires:**Vapour phase – Oxide assisted – carbothermal growth of nanowires – properties. **Nanorods:** Seed mediated growth of inorganic nanotubes and nanorods. **Nanostructured polymers:** Conducting polymers – block-co-polymers – nanocages.

Unit V: f-block elements Chemistry of Lanthanides and Actinides: Lanthanides – Occurrence, extraction from ores – Separation procedure – iron exchange method – solvent extraction method. Physical and chemical properties – Electronic configuration – common

oxidation state – lanthanide contraction and its consequences – colour of lanthanide ions – magnetic properties of lanthanides – separation of actinide elements – separation of Pu from fission products – electronic configuration – oxidation state – comparison of lanthanides and actinides – Position in the periodic table.

References:

1. Asim K das, Fundamental concepts of Inorganic Chemistry, Vol 5 and 7, 2nd edition, CBS publisher and Distribution Pvt. Ltd, 2016.
2. Adamson, Concept of Inorganic Photochemistry, Wiley, New York, 1975.
3. S.F.A. Kettle, Coordination Chemistry – An Approach, Spectrum Academic Publishers, Oxford, 1996.
4. R.S. Drago, Physical Methods in Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, London, 1977.
5. B S Murty, P Shankar, Baladev, B BRath and J Murday, Text book of Nano Science and Nanotechnology, University Press, 2012.
6. ChatwalBhagi and Agarwal, Bioinorganic Chemistry, Sultan Chand Co., New Delhi, 2001.
7. M.A.O.Hill and P.Day (Eds.), Physical Methods in Advanced Inorganic Chemistry, Interscience, New York, 1968.
8. Charles P.Poole Jr. and Franck Owens, Introduction to Nanotechnology,Wiley-Interscience.
9. C.N.R.Rao, A.Muller and A.K. Cheetham, The Chemistry of Nanomaterials – Synthesis, Properties and Applications, Volumes 1 and 2, Wiley – VCH – Verlag GmBH& Co., Wilhelm, 2004.
10. K.F. Purcell and J.C. Koltz, An Introduction to Inorganic Chemistry, W.B. Saunders Company, Philadelphia, 1980.

Paper III - Quantum, Nano and macromolecular Chemistry

Unit I: Quantum mechanics – An Introduction: Failure of classical mechanics and the success of quantum theory in explaining block body radiation. Photo electric effect – Bohrs theory of hydrogen atom – hydrogen spectra – Compton effect – de-Broglie concept of matter waves – distinction between matter waves and electromagnetic radiation – experimental verification of matter waves – Heisenbergs uncertainty principle – Hypothetical (gedenkan) experiments of Heisenberg – Bohrs complementarity principle. Postulates of quantum mechanics – operator algebra – Expressions – addition, subtraction and multiplication – linear operators – Laplacian operator – vector operator – ladder operator- quantum mechanical operator for the following observables: position, linear momentum, kinetic energy, potential energy, total energy and angular momentum. Commutate algebra – evaluation of commutators.

Unit II : Application of quantum mechanics to simple system: Derivation of Schrodinger wave equation- Application of SWE to simple system – particle moving in one dimensional box quantization of energy – characteristics of wave functions , probability of a particle, component of momentum, uncertainty principle through one dimensional box and electronic transition selection rule. Particle moving in three dimensional box- concept of degeneracy and distortion – Rigid rotator – rotational energy levels – simple harmonic oscillator – zero point energy – Hydrogen atom problem – Radial wave functions – radial probability distribution – shapes of various atomic orbitals – Term symbols – L -S & J-J coupling schemes – spectroscopic states.

Unit – III Approximation methods in Quantum mechanics: Need for approximation methods – the perturbation theory (first order only) – application of the perturbation method to Hydrogen and the He atom – the variation method – application of variation method to Hydrogen and He atom. Hartree – Fock self consistent field (HFSCF) method – application to He atom – Electron spin and pauli principle – Anti symmetric nature of the wave functions – slater determinants – approximate wave function of many atoms – Molecules – Born – oppenheimer approximation- molecular Hamiltonian operators – VB treatment to hydrogen molecule – Coloumbic integral – exchange integral and overlap integral – MO treatment of hydrogen molecular cation, homonuclear and heteronuclear diatomic molecules – Molecular term symbol. Hybridisation – HMO theory – ethylene and butadiene.

Unit IV : Chemistry of nano- materials: Definition and historical perfective, Effect of nano science and nanotechnology in various fields. Synthesis of nanoparticles by chemical routes. Microscopic techniques for the characterization of nanomaterials- UV – visible and fluorescence spectroscopy - AFM, SEM, TEM, X-ray diffraction and Microanalysis.

Unit V :Macromolucules : Polymer – definition – types of polymers – properties of polymers – kinetics and mechanism of free radical , ionic , condensation and zeigler – natta polymerization processes. Emulsion and suspension polymerization techniques – polymer molecular weight distribution – molecular weight determination – osmotic pressure method – light scattering method – ultra centrifuge method and viscosity method. Conducting polymers – chemical structure and electronic behavior of polymers – doping of conducting polymers – polymer electrodes.

References:

1. A.K. Chandra, Introductory Quantum Chemistry, 3rd Edn., Tata McGrawhill Publishing Co., New Delhi (1988)
2. M.W. Hanna, Quantum Mechanics in Chemistry, 2nd Edn., The Benjamin/Cummings Publishing Co., London (1969)
3. D.A.McQuarrie, Quantum Chemistry, 1st Indian Edn., Viva Books (P) Ltd., New Delhi (2003).
4. P.W. Atkins, Molecular Quantum Mechanics, 2nd Edn., Oxford University Press, (1986).
5. C.P.Poole and F.J.Owens Introduction to Nanotechnology, (2004).
6. C.C.Koch Nano Structured Materials.
7. R.Preidt, L.Costlow and A. Peter Introductory Nanotechnology
8. F.W. Billmeyer, Text Book of Polymer Science, 3rd Edn., Wiley-Interscience publishers, New York, (1984).
9. V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, Wiley Eastern Ltd., New Delhi (1986).

ELECTIVE – OPTION I
CHEMISTRY FOR COMPETTIVE EXAMINATIONS

Objective: This is the third of the four semester sequential courses in chemistry. This paper deals with basic chemistry involving metals and non-metals, chemical reactions, gas laws, general chemistry, environmental chemistry and application of chemistry in day to day life.

Unit I: BASIC CHEMISTRY- I: Elements – atoms and molecules – Metals and nonmetal – metaolloid, alloy, ore and minerals - Chemical formulae and symbols – Important basic terms such as pressure, volume, atomic mass, molecular mass, temperature, atomic number – Types of chemical reactions (exothermic and endothermic, Physical and chemical changes, oxidation and reduction) – ideal and real gas - Important laws of Chemistry (Boyle's law, Charle's law, Hess's law, Grahams law of diffusion, Beer's law, Henry's law, Faraday's law, Law of conservation of matter or energy).

Unit II: BASIC CHEMISTRY- II: (Only elementary idea can be given) Different concepts of Acids and Bases (Arrhenius, Bronsted and Lewis) – pH concept (no calculation) – Water – Hard and soft water - Chemical nature of metals- Steel and iron (no manufacture) – heat treatment of steel – Solutions and their types (True, Colloidal and suspension) – uses of colloidal solution – Buffer solution – Nuclear Chemistry – isotopes and radioactivity Definitions of some important chemical processes (Haber's, Contact's, Ostwald's, Process)

Unit III: ENVIRONMENTAL CHEMISTRY: Pollution and types of pollutions – Composition of atmosphere – Major regions of atmosphere and their characteristics – Elementary idea of Green house effects and Acid rain – Air pollution – Control of air pollution and their harmful effects – CFC, Global warming, substitute for CFC (Just name only)-Water pollution – Dissolved oxygen – BOD, COD and TDS (elementary idea only)

Unit IV: CHEMISTRY IN SERVICE OF MAN –I: (Only elementary idea can be given) Plastics – Classification with examples – Polymer (natural and synthetic) – Soaps and Glass – Annealing of glass – Cement – Constituents and setting and hardening of cement – Rubber – Types with examples and vulcanization of rubber- Corrosion of metal – prevention – Lubricants (definition and classification) – Fuel – Classification with suitable examples - calorific value – LPG and Rocket fuel.

Unit V: Chemistry in service of man –II: (Only elementary idea can be given) Food adulterants – common food adulterants and their harmful effects and tests to identify them– Classification and biological functions of Vitamins A, B6, B12, C, D, E and K (structural elucidation not required) – Classification and biological functions of antibiotics – penicillin, chloroamphenicol, streptomycin and tetracycline.

Reference Books:

1. A Text book of Environmental Chemistry, O.D.Tyagi, M. Mehra, Anmol Publication, 1990.
2. Applied Chemistry, K. Bagawathi Sundari, MJP Publishers, Chennai – 2006.
3. General Studies Manual, The TMH Publishers, 2008

ELECTIVE OPTION-II
ENVIRONMENTAL SCIENCE

Unit I: Introduction and Classification Introduction – Environmental science – Environmental chemistry – Ecology – Definition – Eco-system – Cycling of mineral elements and gases – Phosphate cycle – Carbon cycle – Hydrogen cycle – Nitrogen cycle – Hydrological cycle – Environmental segments – Pollution and its types: air pollution – water pollution – soil pollution – radioactive pollution – thermal pollution – noise pollution – marine pollution – other types of pollution – and its effects and control – remedial measures.

Unit II: Air Pollution Introduction – Sources of air pollution – air pollutants – classification and effects of air pollutions – oxides of nitrogen, sulphur and carbon – acid rain – effects and control – hydrogen sulphide – effects and control – carbon mono oxide – effects and control – photochemical smog – effects and control fly ash – effects and control – green house effect – global warming – effects and control – ozone layer – ozone depletion – cholorofluoro carbons – effects and control.

Unit III: Water Pollution Introduction – types of water – water pollution – sources of water pollution – water pollutants – classification – physical, chemical and biological – inorganic pollutants and toxic metals – organic pollutants – radioactive pollutants in water-pesticides and fertilizers – suspended particles – water quality – water quality index – ill effects of water pollutants – fluorosis – water pollution control – water treatment – primary, secondary and tertiary treatment – desalination – reverse osmosis – sewage and industrial waste water treatment.

Unit IV: Soil Pollution Introduction – types of soil – soil pollution – types – indicators of soil pollution – plants as indicators of pollution – sources of soil pollution – fertilizers and pesticides – radioactive pollutants – solid wastes – soil sediments as pollutant – soil erosion – treatment of soil pollutants – treatment of solid wastes thermal methods – land filling compositing – land protection – remedial measures for soil pollution.

Unit V: Analysis of Pollutants

Introduction – analysis of air pollutants – units – sampling – devices and methods for sampling – measurement: UV–Visible spectrometry – IR spectrometry – emission 2815 spectrometry – turbidimetrynephelometry – gas chromatography – HPLC – chemiluminescence of nitrogen oxides – IR photometry – conductometry – analysis of water pollutants – units – sampling – devices and methods for sampling – measurement: UV-Visible spectrometry – titration – analysis of different water quality parameters – BOD-COD – analysis and monitoring of pesticides and industrial pollutants.

Suggested Readings:

1. B.K. Sharma and H. Kaur, Environmental Chemistry, Krishna Prakashan, Meerut, 1997.
2. A.K. De, Environmental Chemistry Wiley Eastern Ltd., Meerut, 1994.
3. A.K. Mukherjee, Environmental Pollution and Health Hazards – Causes and Control, Galgotia Press, New Delhi, 1986.
4. N. Manivasakam, Physico-chemical Examination of Water, Sewage and Industrial Effluents, Pragati Prakashan Publication, Meerut, 1985.

Semester III Practicals

Conductometric and Potentiometric Titrations and, Kinetic, Adsorption and Spectral Measurements

I. Electrochemistry

a. Conductometric titrations

i) Conductivity mixture of acids –base titration.

ii) Conductometric displacement titration.
iii) Conductivity precipitation titration.
iv) Conductometric acid – base displacement titration.
v) Estimation of acetic acid – sodium acetate buffer.

b. Potentiometric titrations
i) Potentiometric redox titration MnO_4^- - I^- system.
ii) Potentiometric redox titration Ce^{4+} - Fe^{2+} system.
iii) Potentiometric precipitation titration Ag^+ - Cl^- - I^- system
iv) Determination of dissociation constant, Kd and Determination of pH of Buffer by potentiometry.

c. Precipitation titration
i) $Na_2CO_3 \rightarrow Pb(NO_3)_2 \rightarrow Na_2CO_3$ ii) $K_2SO_4 \rightarrow BaCl_2 \rightarrow K_2SO_4$

II. Thermochemistry i) Heat of solution – Oxalic acid, Ammonium oxalate and potassium nitrate.

III. Adsorption Isotherm i) Adsorption of oxalic acid on charcoal. ii) Adsorption of acetic acid on charcoal.

IV. Kinetic Experiments
i) $S_2O_8^{2-}$ vs I^- kinetics of salt effect

ii) Kinetics of alkaline hydrolysis of ester by potentiometric method

V. Partition coefficient

VI. Experiments based on UV-Visible and infrared spectrophotometer

VII. Titration using pH meter Determination of the first, second & third dissociation constant of Phosphoric acid.

Semester IV
Paper I - Biomolecules, Rearrangements and Synthetic Methods

Unit I : Carbohydrates, Amino acids, proteins and Nucleic acids : Classification of proteins – peptides – structure of peptides - synthesis of peptides – Chemisty of gluthathione and oxytocin – an elementary treatment of enzymes, coenzyme and nucleic acids – biosynthesis of amino acids – RNA and protein synthesis – Genetic code – DNA and determining the base sequence of DNA. Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used for determination of ring size – conformations of aldohexopyranoses – structure and synthesis of maltose, lactose, sucrose and cellobiose. A brief study of starch and cellulose.

Unit II: Photochemistry & Free radicals : Conservation of orbital symmetry – electrocyclic reactions – cyclo addition reactions and sigmatropic rearrangements – applications of correlatioin diagram approach frontier molecular orbital approach, Huckel Mobius approach and Perturbation molecules orbital approach to the above reactions. Photochemical reactions of ketones – photosensitization – Norrish I and Norrish type reactions – paterno – Buchi reaction – photooxidation – photoreduction – photochemistry of arenes. **Free radicals :**

Formation, detection and stability of free radicals – free radical reactions halogenations, addition, oxidation, reduction and rearrangement reactions – BartoSandmeye, Gomberg, Bachmann, Ultmann, Pschorr and Hundsdiecker reactions.

Unit III: Molecular rearrangements: Mechanism of the following rearrangemetns reactions : Wagner - Meerwein, Pinacol, Demzanov. Beckmann, Hoffmann, Curtius , Wolff, Baeyer - Villeger, Stevans, Sommelet – Hauser , Favorskii, Banzil – benzilic acid, Claisen, Cope, Fries, Dienone – phenol, di-pimethane, hydroxioamino – p-aminophenol and Benzidine rearrangement - Photochemical arrangements.

Unit IV: Green Chemistry – I Principles of green chemistry – planning a green synthesis in a laboratory - general interest for solvent free processes – solvent free techniques – Microwave synthesis : Introduction and characteristics of microwave heating – interaction of microwave radiation with the material – difference between conventional heating and microwave heating. Dielectric polarization – dipolar polarization - applications and advantages of microwave heating over conventional heating.

Unit – V Synthetic methods Planning a synthesis - Relay approach and convergent approach to total synthesis Retrosynthetic analysis of simple organic compounds – functional group interconversions - use of activating and blocking groups in synthesis – stereoselective problems of geometrical and optical isomerism – steric crowding – Transition metal complexes in organic chemistry – Homogeneous hydrogenation – Regioselectivity – Disastereoselectivity – Enantioselectivity – Umpolung synthesis – Robinson annelation – A schematic analysis of the total synthesis of the following compounds; 2,4, dimethyl 1-2 – hydroxypentanoic acid, trans – 9 –methyl – 1- decalone and isonootkatone.

References:

1. A.L. Lehninger, Biochemistry, Nath Publishers.
2. C.H.Depuy and O.L.Chapman, Molecular Reactions and Photochemistry Prentice Hall, 1972.
3. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, McMillan India Ltd., 1978.
4. R.B. Woodward andR.Hoffmann,The Conservation of Orbital Symmetry VerlogChemie GMBH and Academic Press, 1971.
5. Hung, The Chemistry of Free Radicals.
6. I.L.Finar, organic Chemistry, Vol. II, ELBS, 1975.
7. P.De., Mayo, Molecular arrangements.
8. Jerry march, Advanced Organic chemistry, John Wiley & Sons, 4thedn., 2000.
9. K.R.Desai, Green Chemistry (Microwave Synthesis) Himalaya Publishing House, Mumbari 2005.
10. R.Sanghi and M.M.Srivastava, Green Chemistry (Environmental Friendly Alternatives), Narosa Publishing House, New Delhi 2003.
11. A..K.Ahluwallia, Green Chemistry (Environmentally Benign Reactions), Aru Books India, New Delhi 2006.
12. R.E. Ireland, Organic synthesis, Prentice Hall of India Pvt Ltd., 1975.
13. R.T.Morrison, and R.N.Boyd, Organic Chemistry, Prentice Hall 6th edn., 2001.

Paper II - Nuclear Chemistry, Electroanalytical and Thermal Methods Specific

Objectives: To introduce the nuclear and analytical chemistry concepts, data analysis and computers in chemistry.

Learning Outcomes: Ensures the students to understand the structure of nucleus, nuclear fission and fusion, radioactivity of isotopes, electroanalytical, thermoanalytical, spectroanalytical methods. In addition the students must have knowledge of computers in chemistry, internet, browsing and searching a website.

Unit I: Structure of Nucleus and Radioactive Decay Composition of the nucleus – nuclear size, shape and density – principal, radial and magnetic quantum numbers – magnetic and electric properties of nucleus – elementary treatment of shell (independent particle) model – nuclear configuration – parity and its conservation – mass defect and binding energy – nuclear forces theory. **Radioactive decay:** Group displacement law – decay series – rate of disintegration – half life – average life – units of radioactivity – secular and transient equilibria – theories of alpha decay, beta decay, gamma emission, positron decay, nuclear isomerism, internal conversion and electron capture – Auger effect.

Unit II: Nuclear fission and Fusion and application of radioactive isotopes Bethe's notation of nuclear process – nuclear reaction energies (Q value) – fission – energy release in nuclear fission – mass distribution of fission products – theory of nuclear fission – fissile and fertile isotopes – energy from nuclear fusion – thermonuclear reactions in stars – classification of reactors – power nuclear reactor – breeder reactor – nuclear reactors in India. Applications of radioactive isotopes: characteristics of tracer isotopes – chemical investigations – age determination – medical field – agriculture – industry – analytical applications – isotope dilution analysis – neutron activation analysis – biological effects of radiation – waste disposal management

Unit III :Electoanalytical&Thermoanalytical methods: Electroanalytical Techniques: Electrogravimetry: Theory of electrogravimetric analysis – electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell-working electrodes – auxiliary electrode and reference electrode – Coulometric titrations. Voltammey: Cyclic voltammety – Stripping voltammetry – Chronopotentiometry, Amperometry: Amperometric titrations. **Thermoanalytical Methods:** Theory, Instrumentation and applications of thermogravimetry – Differential Thermal Analysis and Differential Scanning calorimetry- Factors affecting TG and DTA curves – Difference between DTA and DSC.

Unit IV: Spectroanalytical Methods and Data handling

i) Spectroanalytical methods: Law of absorption and quantitative law of luminescence – principles and applications of spectrophotometry, fluorimetry, nepheleometry and turbidimetry – Emission spectroscopy and flame spectroscopy – atomic absorption, atomic emission and atomic fluorescence spectroscopy. Optical rotatory dispersion and circular dichroism. ii) Data Analysis: Significant figures and Significant figures in Numerical computations- Mean and standard deviation, significant figures and computation – comparison of results – F-Test and Student's t test – Rejection of results – Q Test – Correlation coefficient and linear regression - method of least square.

Unit V: Computer in Chemistry: History and development of computers, Mainframe, micro and Super computer systems – CPU and other peripheral devices – Evolution of

proramming languages: Machine language, assembly language and higher level language. Internet – History of internet – applications of internet in Chemistry – websites in Literature Survey in Chemistry – popular websites and data bases in Chemistry– downloading the attachment / PDF files – opening, browsing and searching a website – literature searching online. Email: Introduction – working way – mailing basics – e.mail ethics – advantages and disadvantages – creating e-mail id – receiving and sending e-mails.

Suggested Readings:

1. S.Glasstone, Source Book on Atomic energy, 3rd Edn., Van Nostrand Reinhold Company, New York, 1967.
2. G. Friedlander, J.W. Kannedy, E.S. Macias and J.M. Miller, Nuclear and Radiochemistry, John Wiley & Sons Inc., New York, 1981.
3. Asim K das, Fundamental concepts of Inorganic Chemistry, Vol 1 and 7, 2nd edition, CBS publisher and Distribution Pvt. Ltd, 2016 3. F.J.Holler, S.R. Gouch, D.A. Skoog and D.M. West Fundamentals of Analytical Chemistry, 9thEdn, (2014), Cengage Learning India Private Limited., New Delhi.
4. U.N. Dash, Nuclear Chemistry, Sultan Chand Sons, New Delhi, 1991.
5. J.Basset et al. Vogel's Text book of Quantitative Inorganic Analysis, Longman, 5th Edn. ELBS, Essex, 1989.
6. H.H. Willard, LL.Merritt and J.A. Dean, Instrumental Methods of Analysis, East-West Press, New Delhi, 1988.
7. J.G.Dick, Analytical Chemistry, Tata-McGraw Hill, 1973.
8. Alexis Leon and Mathews Leon, "Fundamentals of Information Technology", Leon Vikas, Chennai (1999).
9. Barbara Kasser, "Using the Internet", 4th Edn. EE Edition, New Delhi, 1998.
10. H.I. Arnikar, Essentials of Nuclear Chemistry, 3rd Edn.Wiley Eastern Ltd,
11. Fundamentals of Analytical Chemistry, Saunders College Publishing Co., Philadelphia, 1982.

Paper III - Chemical kinetics, Surface, Biophysical and Photochemistry

Unit I : Chemical kinetics I: Empirical rate laws – influence of temperature on the rate of reaction – Theories of reaction rates – Arrhenius theory , collision theory and transition state theory of reaction rates – potential energy surfaces – kinetic isotope effect- Theory of unimolecular reactions – Lindemanns theory , Hinshelwood theory , RRK theory, RRKM theory and slaters theory – chain reactions – steady state approximations – kinetics of chain reactions – thermal reaction between H_2 and Br_2 – thermal decomposition of N_2O_5 and acetaldehyde – H_2 – O_2 explosive reactions. Reaction in solutions – influence of solvent dielectric constant , ionic strength – Bronsted – Bjerrum equation – primary and secondary salt effect – effect of pressure on reaction rates – significance of volume activation.

Unit II : Chemical Kinetics II and Catalysis : Fast reactions – Fast reactions techniques – flow methods (Continous and stopped flow methods) – relaxation methods (T and P jump methods) – pulse techniques (Pulse radiolysis , flash photolysis) – shock tube method – molecular beam method – life time method – Homogeneous catalysis – acid base catalysis – vant Hoff and Arrhenious intermediates for protolytic and prototropic mechanism. Catalysis in Biological systems- enzyme catalysis – Michaelis – Menten kinetics – Lineweaver and Burk plot – Eadie plot – influence of pH on the enzyme catalysis. Heterogeneous catalysis – kinetics and mechanism of unimolecular and bimolecular reactions – Langmuir –

Hinshelwood and Langmuir – Rideal mechanism – ARRT of surface reactions – NH_3 synthesis, hydrogenation of C_2H_4 and cracking of hydrocarbon.

Unit III: Surface chemistry: Introduction – adsorption of gases on solid – physisorption and chemisorption – adsorption isotherms – Freundlich – longmuir – BET – Temkin adsorption isotherms, Adsorption on liquid surface – surface tension – Gibbs absorption isotherm – surface area determination – solution and interfacial behavior of surfactant – Definition and classification of surfactants – preparation of LB films- Micelles – critical micelles concentration (CMC) – structure – bimolecular reaction occurring in a micellar solution – reverse micelles – micro emulsion –Application of photo electron spectroscopy – ESCA and Auger spectroscopy to the study of surfaces.

Unit IV : Biophysical chemistry : Thermodynamics in biology – concept of irreversible thermodynamics – standard free energy, entropy and chemical potential change in biochemical reactions – Energy flux – Onsager reciprocal relationship – Bio energetics and metabolism – catabolism – anabolism – energy relationship between catabolic and anabolic path ways. High energy metabolites – ATP and its role in bioenergetics – phosphoryl group transfers and ATP – Role of single oxygen in biology – Biophysical application of Mossbauer effect – Mossbauer effect in hemoglobin – spin labeling –molecular recognition. Introduction to supra - molecular chemistry and photochemistry.

Unit V: Photo and Radiation chemistry: Absorption and emission of radiation - Physical properties of the electronically excited molecules – excited state dipole moments, Pka and redox potentials – photo – physical processes in electronically excited molecules – Fluorescence. Phosphorescence and other deactivation processes. Excimer and Exciplex complex formation. Stern – volmer equation and its applications – Electronic energy transfer mechanisms – photosensitization and chemiluminescence. Experimental techniques in photochemistry – light sources – chemical actinometry – measurement of quantum efficiency – photosynthesis – PSI and PSII – photochemical conversion and storage of solar energy.Radiation chemistry – Source of high energy – interaction of high energy radiation with matter radiolysis of water – determination of G-value – mode of reactions of hydrated electrons – Experimental techniques of radiation chemistry – Dosimetry – Application of radiation chemistry in biology and industry.

Recommended Books:

1. K.J.Laidler, Chemical Kinetics, 3rd Edn., Harper International Edn., London (1987).
2. K.J.Laidler, Theories of Chemical Reaction Rates, McGraw Hill Book Co., London (1969).
3. F.Wilkinson, Chemical Kinetics and Reaction Mechanisms, Van Nostrand Reinhold Co., New York (1980).
4. C.Kalidad, Chemical Kinetic Methods, New Age International, 1996.
5. Margaret Robson Wright, Fundamental Chemical Kinetics- An Explanatory Introducation to the Concepts, Horwood Publishing Ltd., West Sussex 1999.
6. A.W. Adamson, Physical Chemistry of Surfaces 5th Edn., John wiley& Sons, New- York (1990).
7. D.Attwood and A.T.Florence, Surfactant Systems- Their Chemistry, Pharmacy and Biology, Chapman and Hall, New-York (1983).
8. K.K.Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern
9. N.J. Turro, Modern Molecular Photochemistry. Benjamin Cummings.

10. Hamil, Williams and Mackay, Principles of Physical Chemistry II Edn., Prentice-Hall of India, Pvt., Ltd., New Delhi (1968). (Radiation Chemistry)

ELECTIVE OPTION 1 - POLYMER CHEMISTRY

Unit I: Classification of Polymers and Chemistry of Polymerization General definition – Nomenclature of polymer-Classification of polymers- Linear polymers, non-linear or branched polymers, cross-lined polymers, homo chain hetero chain, homopolymers co-polymers block polymers and graft polymers. Chemistry of polymerisation: Types of polymerization – mechanism – Chain, growth, free radical, ionic, co-ordination, ring opening, matalhetical, group transfer, polyaddition and polycondensationpolymerisation.

Unit II: Individual Polymers Individual polymers: Monomers required general methods of preparation, repeat units and uses of the following polymers and resins – polyethylene, polystyrene, polyacrylonitrile, polymethylmethacrylate, PVC, polytetra – fluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethylene, glycols, phenol – formaldehyde, urea-formaldehyde, melamine – formaldehyde and epoxy resins – silicone polymers.

Unit III: Properties of Polymers
General properties of Polymer (Rheological, Mechanical, Thermal, optical and electrical) – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotatic, isotatic and atatic polymers. Glass transition temperature: Definition – factors affecting glass transition temperature – relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticiser – importance of glass transition temperature – heat distortion temperature. Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights – molecular weights and degree of polymerization – poly dispersity – molecular weight distribution in polymers – size of polymer molecules – kinetics of polymerisation.

Unit IV: Polymerisation Techniques, Degradation and Uses of Polymers
Polymerisation Techniques Bulk, solution, suspension, emulsion, melt condensation and interfacial polymerisations. Degradation: Types of degradation – thermal, mechanical, ultrasonic and photodegradation – photo stabilisers – oxidative degradation – antioxidants – Uses of polymers in electronics and biomedicine. Thermal (TG, DTA and DSC) and SEM methods of characterization of Polymers

Unit V: Polymer processing and polymer composites
Polymer processing plastics (thermo and thermosettings), elastomers, fibres, compounding, plasticisers, colorants, flame retardants. Compression and injection mouldings – film extrusion and calendaring – die casting and rotational casting – thermofoaming – reinforcing.' Introduction to polymer composites – Types- Role of matrix in composites – Smart composites and smart materials

Reference Books:
1. V.R. Gowariker, N.V.Viswanatha and Jayadev Sreedher, "Polymer Science", Wiely Eastern Ltd., New Delhi, 1986.
2. G. Odian, "Principles of Polymerization", 2nd edn., John Wiley and Sons, New York, 1981.
3. D.W. Van Krevelen and P.J. Hoftyrager, "Properties of Polymers", Elsevier, New York,

1976.
4. B.K. Sharma, "Polymer Chemistry", GoelPublishig House, Meerut, 1989.
5. P.J. Flory, Principles of Polymer Chemistry", Cornell Univ. Press, Ithaca, 1953.
6. F.W. Billmeyer, "Text Book of Polymer Science", 3rd Edn. John Wiley and Sons, New York, 1984.
7. Harry R. Allcock, F.W. Lampe and J.E. Mark, "Contemporary Polymer Chemistry", 3rd Edition, Pearson, Prentice Hall, Delhi, 2005.
8. N B Singh and S S Das, Introduction to Polymer Science and Technology, New Age International Publishers, 2nd edition, 2017.
9. M C Gupta, A P Gupta, Polymer Composite, New Age International Publishers, 2007.

ELECTIVE OPTION 2 - INTRODUCTION TO NANOSCIENCE

Unit I: General Introduction: Forms of Matter – Crystal structures – Electronic properties of atoms and solids – Surface energy and surface tension – Defining nanodimensional materials – 0D, 1D and 2D nanostructures – sizes dependence of properties – special properties resulting from nanodimensionality – Potential uses of nanomaterials.

Unit II: Synthesis of nanomaterials: General approaches – Nucleation process – size of the crystal – Influence of nucleation rate on the size of the crystal – Chemical methods – Sol-gel techniques – Control of grain size – Co-precipitation – Hydrolysis – Sonochemical method – Colloidal precipitation – Bottom up and top down approaches – Kinetically confirmed synthesis of nanoparticles.

Unit III: Principle of Instrumentation Spectrophotometry, XRD, EXAFS, XPS, SEM, TEM, AFM – application to nanomaterials characterization.

Unit IV: Optical properties of nanomaterials: Optical properties of nanomaterials: UV-Vis, IR absorption – PHotoluminescence and stimulated emission – Nonlinear optical mixing – photoconductivity. Magnetic Properties: Concepts of dia, para and ferro-magnetism – Exchange correlation – Exchange interaction. Electrical Properties: Electrical conductivity – Hall Effect – charge carrier density – activation energy, electronic properties – field emission properties.

Unit V: Biological nanomaterials: Biological nanomaterials: Sizes of building blocks – Proteins – DNA double nanowire – Enzymes – Protein synthesis – Micelles and Vesicles – Biomimetric nanostructures – Worm micelles and Vesicles from block copolymers.

Reference Books:

1. C.P. Poole Jr. F.K. Owens, Introduction to Nanotechnology, John Wiley & Sons, 2003.
2. M.D. Ventra, S.Evoy, J.R. Heflin, Jr., (Eds), Introduction to Nanoscale Science and Technology, Kluwer Academic, 2004.
3. G. Cao., Nanostructures &Nanomaterials: Synthesis properties and applications, Imperial College Press.
4. B S Murty, P Shankar, Baladev, B BRath and J Murday, Text book of Nano Science and Nanotechnology, University Press, 2012.
5. C.N.R. Rao, A. Muller, A.K. Cheetham (Eds.) The Chemistry of Nanomaterials: Synthesis,

Properties ad Applications, WILEY-VCH Verlag GmbH & Co., KGaA, Weinheim, 2004.
6. P. Knauth, J. Schoonman (Eds), Nanostructured Materials: Selected Synthesis Methods, Properties and Applications, KLUWER ACADEMIC, 2002.
7. G. Schmid, Nanoparticle: From Theory to Applications, Wiley-VCH Verlag GmbH & Co. KGaA, 2004.
8. P. Dutta, S.Gupta (Ed), Understanding of Nanoscience and Technology, Global Vision Publishing House, 2006.
9. C.C. Koch, Nanostructured Materials: Processing, Properties and Applications, Jaico Publishing House, 2006.
10. Challa S.S.R. Kumar (Ed) Biological and Pharmaceutical Nanomaterials, John Wiley VerlogCmbh& Co., KgaA, 2006.

SEMESTER IV - PROJECT WORK AND VIVA-VOCE

INSTRUCTIONS ON PROJECT WORK

Candidates can select for his / her research project in any one of the areas of chemistry in consultation with The Head, Department of Chemistry, DDE MKU.

The project report should be submitted to The Head, Department of Chemistry one week prior to the commencement of the university examinations. If a candidate fails to submit his/her project report on the date presented above, he/she may be permitted to submit the same four days prior to the date of viva- voce examination with a fine prescribed by the university.

Candidates shall submit **2 copies** of the project report for valuation.

The project report shall contain at least 25 pages excluding bibliography and appendices.

The project report shall be valued for a total of 100 marks out of which the external and guide share 60 and 40 marks respectively. The sum of marks awarded by both the examiners shall be considered to be the final mark. For the pass in the project the candidate shall secure a minimum of 50 marks. If the candidate fails to get the minimum pass mark in the project report he/she shall be permitted to resubmit the project report again within a period of 6 months after the publication of the result.

For candidates who have passed in the evaluation of the project there will be a viva- voce examination pertaining to the project work. The viva-voce carries a minimum of 20 marks and it will be conducted jointly by the guide and the external examiner. The learner should secure a minimum of 10 marks for a pass in the viva-voce examination failing which he/she shall be required to reappear for the same for a month but within a period of 3 months for which he/she will have to pay a fee as prescribed by the University.

Further, for a pass in this paper as a whole a candidate should secure at least 60 marks in project report and viva-voce put together.