MASTER OF SCIENCE IN CHEMISTRY (SEMESTER PATTERN) CHOICE BASED CREDIT SYSTEM SYLLABUS TWO YEARS FULL TIME PROGRAMME

COURSESOF STUDIES (AS PER U.G.C. MODEL SYLLABUS)

P.G. DEPARTMENT OF CHEMISTRY ,GANGADHAR MEHER UNIVERSITY, SAMBALPUR

POST GRADUATE PROGRAMME STRUCTURE DEPARTMENT OF CHEMISTRY

Post graduate programme comprising two years, will be divided in to 4(four) semesters each of six months duration.

Vear		Semesters
Year	Semester I	Semester II
First Year	100	Semester IV
Second Year	Semester III	Jenieste. 17

PART-I; First Semester

PAPER NO	NAME OF THE COURSE	MARKS		Total Marks	Duration(Hrs)of exam(End	Credit
	COOKSE	End term	Mid Term		term)	
	WORGANIC	80	20	100	3	4
101(THEORY)	INORGANIC	-	20	100	3	4
102(THEORY)	ORGANIC	80	-	100	3	4
103(THEORY)	PHYSICAL	80	20		3	4
	POLYMER	80	20	100		4
104(THEORY)	ORGANIC	80	20	100	3	
105(PRACTICAL)			-	500		20
	Total			1000		

PART-II; Second Semester

PAPER NO	NAME OF THE COURSE	MARKS		Total Marks	Duration(Hrs) of exam(End	Credit
		End	MidT erm 20	100	term)	4
		80				
201(THEORY)	INORGANIC	80	20	100	3	4
202(THEORY)	ORGANIC	80	20	100	3	4
203(THEORY)	PHYSICAL	-	20	100	3	4
204(THEORY)	BIOINORGANIC	80	20	100	3	4
205(PRACTICAL)	INORGANIC	80	-	100	3	4
DSE Papers 206A(THEORY)	a.NANOMATERIALS&NANOCHE MISTRY b-SURFACE CHEMISTRY c.COMPUTATIONAL CHEMISTRY	80	20	150		
206B 206C	& MOLECULAR MODELLING			600		24
	Total			600 he onted	by students of	this

^{*}Discipline specific elective paper. Any one paper can be opted by students of this department. Minimum student strength to run the course in elective paper should be 8.

PART-III; Third Semester

PAPER NO	NAME OF THE COURSE	MARKS		Total Marks	Duration(Hrs) of exam(End	Credit Hours
		END Term	MID Term		term)	
301(THEORY)	INORGANIC	80	20	100	3	4
And the second section of the section of the second section of the	ORGANIC	80	20	100	3	4
302(THEORY)	PHYSICAL	80	20	100	3	4
303(THEORY)	SUPRAMOLECULAR	80	20	100	3	4
304(THEORY)		80	20	100	3	4
305(PRACTICAL)	PHYSICAL	-	1000	100	3	4
*IDSE Papers 306A(THEORY) 306B	a.ENVIRONMENTAL CHEMISTRY b-INDUSTRIAL PROCESS c.MATTER & ENERGY HALANCE	80	20	100		
306C	1			600		24
	Total	1			ted by students	of othe

^{*}Inter discipline specific elective paper. Any one paper can be opted by students of other Departments.

PART-IIV; Fourth Semester

PAPER NO	NAME OF THE COURSE	MARKS		Total Marks	Duration(H rs)of exam(End term)	Credit Hours
	COOKSE	End term	Mid			
	2000000	80	20	100	3	4
401(THEORY)	INORGANIC		20	100	3	4
402(THEORY)	BIOORGANIC	80	20	100	3	4
403(THEORY)	PHYSICAL	80	11.021100	100	3	4
404(THEORY)	GENERAL	80	20	100	3	4
405(PRACTICAL)	Project work & VIVA VOCE		50+50		1	20
	Total			500		1,22,000
	110.3977.2011	7	200			88
22 Papers	Grand total	2	200			

^{*}Pass percentage;

- 1. The minimum marks required to pass any paper shall be 40 percent and 40 percent in aggregate of a semester.
- 2. No students will be allowed to avail more than three chances to pass in any paper inclusive of first attempt.

FIRST SEMESTER

Paper - CHE-101: INORGANIC

Full Mark 100- (80+20 Marks)

UNIT -1: Nuclear Chemistry:

- (a) Nuclides, their classification, nuclear stability, nucleus, its size and shape, mechanical effect due to orbiting and spinning of nucleons, magnetic quantum number, principal and radial quantum numbers, Maria-Goeppert notation for nucleons, total angular momentum of nucleus, net magnetic moment of nuclei, Nordheim rule.
- (b) Nuclear models and nuclear reaction: shell model, liquid drop model, proton and neutron configuration, spin and pairity of nucleon, types of nuclear reactions, conservation in nuclear reaction, reaction cross section, compound nucleus theory.
- (c) Nuclear reactor: Fission energy, classification of reactors, uranium reactor, breeder reactor, reactor power.

UNIT-2: Bonding

- (a) Ionic bond: lattice energy, Born-Lande equation, size effect, effects of radius ratio on coordination number of ionic compounds, crystal structures of NaCl, CsCl, CaF₂, TiO₂, lattice energy and hydration energy, their effects on solubility of ionic compounds.
- (b) VSEPR theory, Walsh diagrams (tri-and penta-atomic molecules), $d\pi$ -p π bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

UNIT-3

- (a) Electron deficient compounds: definition and examples, hydrides of boron (boranes), general methods of preparation, properties, structure and bonding in higher boranes (B_4H_{10} , B_5H_9 , B_5H_{11} , B_6H_{10}), metaloborane , carborane, three centred bond, Linnett double quartet approach, applications.
- (b) Isopoly and heteropoly acids: isopoly molybdates, tungstates, and vanadates.

UNIT-4

lanthnides and actinides

- (a) Binary ionic compounds, Ternary and complex oxides, complex compounds of lanthanides and electronic, optical and magnetic properties.
- (b) Electronic and magnetic properties of actinides

Books for reference:

1. Essentials of Nuclear Chemistry - H. J. Arniker.

- 2. Concise Inorganic Chemistry J. D. Lee.
- 3. Text Book of Physical Chemistry S. Glasstone.
- 4. Principles of Physical Chemistry Puri, Sharma and Pathania.
- Physical Chemistry P. C. Rakshit.
- 6. Selected topics in Inorganic Chemistry Mallik W. U., Tuli G. D., Madan R. D.; S. Chand & Co.

Paper - CHE- 102: ORGANIC

Full Mark 100 (80+20) Marks)

UNIT-1

Nature of Bonding in Organic Molecules, Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy levels of π -molecular orbitals, aromaticity, homo-aromaticity, annulenes, antiaromaticity

UNIT -2: Reaction intermediates:

- (a) Non-classical carbonium ion (generation, structure, stability and fate).
- (b) Free radicals, arynes and nitrenes (generation structure, stability and fate).

UNIT-3: Substitution reactions

(A) Nucleophilic substitution reaction

- (i) Aliphatic nucleophilic substitution S_N1, S_N2 & S_Ni reactions, neighbouring group participation reactions (partici-pation by double bonds), aromatic ring substitution, amb-ident nucleophile and substrate effect of nucleophile.
- (ii) Aromatic nucleophile substitution, intermediate Meisenheimer- complex mechanism, S_N Ar mechanism and benzyne mechanism, Sommelet-Hauser reaction, Von Richter rearrangement.

(B) Electophillic substitution reactions

(i) Aliphatic electrophilic substitution S_E1, S_E2, S_Ei reaction, mechanism and stereo chemistry.

- (ii) Aromatic electrophilic substitution sigma and pi complex mechanism orientation and reactivity in substituted benzene ring, ortho-para ratio. Vilsmeier Haack reaction, Bischler-Napieralski reaction, Pechmann reaction, Fries rearrangement.
- (iii) Free radical substitution reactions: free redical substitution ianism (reactions at sp³ and sp² carbon).

UNIT-4: Addition and elimination reactions

- (a) Nucleophilic and free radical addition.
- (b) Elimination reactions: EI, E2 and EI CB mechanisms and orientation, effect of substrate, leaving group and medium, orientation of the double bond, Saytzeff rule and Hoffmann rule, pyrolytic eliminations.

Books For Reference:

- Electronic Structure of Organic molecules L. N. Ferguson.
- Organic Reaction mechanism E. S. Gold.
- 3. Advanced Organic Chemistry: Reaction mechanism and structure Jerry March.
- Organic Reaction Mechanism N. Tiwari, Books & Allied Pvt. Ltd.

Paper - CHE- 103: PHYSICAL

Full Mark 100 (80+20 Marks)

Unit-1: Thermodynamics -1

- (a) Second law of thermodynamics, heat engines and refrigeration engines, entropy and its variation with temperature, pressure and volume, entropy of mixing, entropy correction from ideal behaviour, thermodynamic equation of state, entropy and heat capacities relationships, difference of heat capacities, work function, free energy, Gibb's Helmholtz equation and its application.
- (b) Third law of thermodynamics, its application to solids, liquids and gases, Nernst heat theorem and its applications.
- (c) Entropy and thermodynamic probability, Boltzman-Planck equation for entropy, Maxwell-Boltzmann distribution law (evaluation of MB constants excluded), effect of degeneracy.
- (d) Partition function, molecular and molar partition function, evaluation of translational partition function, entropy in terms of partition function, entropy of monoatomic gases, Sackur Tesrode equation.

UNIT-2: Thermodynamics -II

Classical Thermodynamics Concept of free energy, chemical potential and entropy, Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances and determinations. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient.

UNIT-3: Thermodynamics -III

Non Equilibrium Thermodynamics Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocal relations. Partial molar properties, chemical potential and its variation with temperature and pressure, determination of partial molar properties (1) by direct method (2) from apparent molar properties (3) from equation of state.

UNIT-4: Gaseous State and Chemical Kinetics

- (a) Gaseous state of matter: Virial theorem, molecular collision, mean free path, viscosity, conductivity and diffusion of gasses, molecular diameter, law of distribution velocity, Brownian motion and determination of Avogadro's number by vertical method.
- (b) Chemical Kinetics: Arrhenius equation, absolute theory of reaction rates, collision theory, application of collision theory to unimolecular and bimolecular reactions.
- (c) Chain reactions with reference to the formation of HBr and pyrolysis of CH₃CHO, chemical reactions in solutions catalysed by acid and base.

Books for Reference:

- 1. Text Book of Physical Chemistry S. Glasstone.
- 2. Thermodynamics for chemists S. Glasstone.
- 3. Physical Chemistry S. Glasstone.
- 4. Theoretical Chemistry S. Glasstone.
- 5. Statistical Thermodynamics M. C. Gupta.

Paper- CHE-104: POLYMER SCIENCE

Full Mark 100- (80+20) Marks)

UNIT-1

- (a) Introduction to Polymer Science: Definition of Polymers, Degree of Polymerization, Nomenclature and classification of polymers, Natural & Synthetic polymers, Homopolymer and Copolymers, Polymerization process, Addition and Condensation polymerization.
- (b) Addition Polymerization: Introduction, Monomers of Addition polymers, Free radical initiators, Polymerization mechanism, Steady-state kinetics of Radical Polymerization, Determination of molecular weight by viscosity method.
- UNIT-2 (a) Condensation Polymerization: Nylon 6, Nylon 6.6, Polyester, Phenol- formaldehyde resins, Epoxy resins, Polysiloxane, Amino resins, Melamine- formaldehyde Polymers.
- (b) Co-polymerization: Classification of copolymer, The copolymer equation, Kinetics of Copolymerization, Mayo and Lewis equation, Determination of Monomer reactivity ratios, Fineman and Ross method, Graft Copolymer.
- UNIT-3 (a) Industrial Polymers: Classification of Industrial Polymers, Polyethylene, Low. Density Polyethylene, HDPE, Natural Rubber, Vulcanization of Rubber.
- (b) Biodegradable Polymers: Introduction, Definition, Types of Biodegradable polymers. Natural Biodegradable Plastics: Starch based plastics, Cellulose based plastics, Proteinbased plastics and protein plastics.

UNIT-4

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. Polymer Processing Plastics, elastomers and fibres. Properties of Commercial Polymers Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers — Fire retarding polymers and electrically conducting polymers. Biomedical polymers — contact lens, dental polymers, artificial heart kidney, skin and blood cells.

BOOKS FOR REFERENCE:

- Principle of Polymer Science Paul J. Flory.
- Text Book of Polymer Science F. W. Billmayer.
- 3. Organic Polymer Chemistry K. J. Saunders.
- 4. A Text Book of Polymer Science P. L. Nayak, Kalyani Publishers.

Paper-CHE-105: ORGANIC PRACTICAL

(100 Marks)

- Identification of organic compounds having at least two functional groups.
- 2. Estimation:
 - (a) Methoxy group
 - (b) Acetyl group
 - (c) Nitrogen
 - (d) Carbon, hydrogen
 - (e) Spectrophotometric and volumetric analysis of keto group.

NOTE: At least three estimations should be performed.

- 3. Preparation:
 - (a) p-toluidine to p-iodotoluine
 - (b) benzaldehyde to benzoin to benzil to benzilic acid
 - (c) benzilic acid to o-benzoyl benzoic acid to anthraquinone to anthrone
 - (d) ethyl acetate to ethyl acetoacetate
 - (e) anisole to phenacetin
- Synthesis of a simple dye and check its purity by paper chromatography or extinction coefficient measurements.

SECOND SEMESTER

Paper - CHE- 201: INORAGANIC

Full Mark 100- (80+20 Marks)

UNIT-1: Organometallics

- (a) Definition, classification transition metal alkyls and aryls, metal carbenes and metal carbynes general methods of preparation, properties, structures, and bonding.
- (b) Transition metal π -complexes, cyclopentadienyl complexes, general methods of preparation, properties, structures, and bonding in ferrocene, η^6 -arene complexes.
- (c) Reactions of organometailic compounds, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack on coordinated ligands.

UNIT -2: Solid state Chemistry-1

Solid State Reactions General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions. Crystal Defects and Non-Stoichiometry Perfect and imperfect crystals, intrinsic and extrinsic defects—point defects, line and plane defects, vacancies—Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect

formation, colour centers, non-stoichiometry and defects. Electronic Properties of solids Metals, insulators and semiconductors, electronic structure of solids- Band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors.

UNIT -3: Solid state Chemistry-II

Optical properties of solids, Optical reflectance, photoconduction, photoelectric effects, refraction, dispersion, polarization. Magnetic Properties of Solids Classification of materials. Quantum theory of paramagnetism – cooperative phenomena – magnetic domains, hysteresis. Organic Solids Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

UNIT-4: Homogeneous Catalysis

General features of catalyst, catalytic steps, hydrogenation of alkenes, Asymmetric hydrogenation, Hydrosilylation, Hydrocyanation, Ziegler-Natta polymerization of alkenes, Alkene Metathesis, hydrocarbonylation of olefenes, Monsanto acetic acid synthesis, water gas-shift reaction, activation of C-H bond, Palladium in homogenous catalysis.

Books for reference:

- Organometallic compounds by Inderjit Kumar.
- 2. Bioorganic Chemistry by Asim K. Das, Books and Allied Pvt Ltd.
- Bioinorganic Chemistry by K Hussain Reddy, New Age International Pvt Ltd.
- Principles of Bioinorganic Chemistry by Lippard SJ and Berg JM, Panima Publ Corp. New Delhi.
- Coordination Chemistry by D. Banerjee.
- 6. Advanced Inorganic Chemistry (6th Edu) by Cotton & Wilkinson.
- 7. Organometallics by R. C. Mehrotra.

Paper - CHE-202: ORGANIC

Full Mark 100- (80+20 Marks)

UNIT-1: Molecular rearrangements

 (a) Rearrangements involving electron deficient carbon: Demjanov, Wolff, Wagner- Meerwein, and Dienone Phenol rearrangement.

- (b) Rearrangement involving electron deficient nitrogen: Curtius, Schmidt and Lossen rearrangement.
- (c) Rearrangement involving electron deficient oxygen: Baeyer-Villiger and hydroperoxide rearrangement.

UNIT-2: Conformation and Reactivity

- (a) Stereochemistry Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis.
- (b) Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus...
- (b) Intramolecular rearrangements and neighbouring group participation reactions. Curtin-Hammett Principle.

UNIT-3: Spectroscopy

 (a) Application of Ultraviolet, IR, NMR and Mass spectros – copy in determination of molecular structure of organic compounds.

UNIT-4: organic photochemistry-1

Photochemistry of Aromatic Compounds Isomerisations, additions and substitutions Miscellaneous Photochemical Reactions Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

BOOKS FOR REFERENCE:

- 1. Stereochemistry of carbon compounds by E. Eliel.
- 2. Organic Reaction mechanism by E. S. Gold.
- Advanced Organic Chemistry Reactions, Mechanisms, and structure by Jerry March. JohnWiley & Sons.
- 4. Spectroscopic Methods in Organic Chemistry by William & Fleming.
- 5. Organic Spectroscopy by Willian Kemp.
- 6. Spectro Scopic identification of organic Compound by Silverstein, Bassler and Morrill.
- Pericyclic Reaction and Organic Photochemistry V. P. Sharma and Rakesh Kumar Pragati Prakashan.

Paper- CHE-203 PHYSICAL

Full Mark 100- (80+20 Marks)

SPECTROSCOPY -1

UNITI

Nuclear Magnetic Resonance Spectroscopy Nuclear spin; nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton—13C, 19 F and 31P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

UNIT 2

Electron Spin Resonance Spectroscopy 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, measurement techniques, applications. Nuclear Quadrupole Resonance Spectroscopy Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings, Applications.

UNIT 3

Vibrational Spectroscopy Infrared Spectroscopy Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibrationrotation spectroscopy, P, Q, R branches. Born-Oppenheimer approximation, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis. Raman Spectroscopy Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrationalrotational Raman spectra, selection rules, Mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectros

UNIT 4

- a. Photoelectron spectroscopy- Principle , application
- b. X-ray absorption spectroscopy- Principle , application
- c. Mass spectroscopy- Principle, application

Reference BOOKS

- Modern Spectroscopy, J.M.Hollas, John Wiley, 4th edition, 2004, Sussex.
- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L.Ho, Wiley Interscience.
- NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood, 1st edition, 1990.
- Physical Methods in Chemistry, R.S.Drago, Sauders College. 4. Introduction to Molecular Spectroscopy, G.M.Barrow, McGraw Hill

Paper - CHE- 204

BIOINORGANIC

Full Mark 100- (80+20 Marks)

UNIT-I

Biomolecules and their Roles in Metal Ions Storage and Transportation Amino acids, peptides and proteins, structures of proteins, lipids, lipid bilayer, biological membranes, chemistry of biologically relevant molecules like ADP, ATP, FAD, NADP, nucleotides. Biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, mechanism of transport of metal ions through biological fluids and membranes, different types of passive and active transport processes and their mechanism, Na+/K+ pump, calcium pump, and ionophores. Storage and transport of iron, copper and zinc, siderophores, structure and function of ferritin, transferrin in regard to Fe-storage and transportation,

UNIT-2

Role of Proteins as Oxygen and Electron Carriers Chemistry of porphyrin, Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobin (Mb) and their behavior as oxygen carrier, O2 affinity, cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. Non-heme oxygen uptake protein (hemerythrin and hemocyanin). Magnesium porphyrins (Chlorophyll): Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

UNIT-3

Biomolecular Catalysis Preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. Enzyme-substrate binding problem, carboxypeptidase, carbonic anhydrase and their biological significance, Interchangeability of zinc and cobalt enzyme. Blue-oxidases (ascorbate oxidase, cerulloplasmin, laccase) and non blue Oxidases (amine oxidase, galactose oxidase, lysyl oxidase, cytochrome c oxidase), structure and biological functions of molybdenum nitrogenase, superoxide dismutase.

UNIT-4

Nitrogen fixation Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems. Photosynthesis Chlorophylls, photo system I and photo system II in cleavage of water

BOOKS: 1. Bio-Inorganic Chemistry by Asim K Das.

- . Bio-Inorganic Chemistry by E. Ochia.
- 3. Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi.
- 4. Inorganic Chemistry (4th Edn) by Huheey, Keiter, Keiter and Medhi.
- 5. Bioinorganic and Suparmolecular Chemistry by A. Bhagi and G. R. Chatwal. CH

Paper - CHE- 206

Nanomaterials and Nanoscience

Full Mark 100- (80+20 Marks)

Nanomaterials and Nanoscience

UNIT-I:

Introduction and concepts of Nanomaterials and nanoscience, Different types of nanomaterials including nonocomposites and nanoporous materials-shapes, structure and properties.

UNIT-2

Quantum Mechanics and Jellium model of nanosystems, electrical and magnetic properties of nanoparticles

UNIT-3

Nanostructured Carbon based materials: Fullerene, Carbon nanotube, graphene. Carbon nanobuds, synthesis and application of carbon nanotubes

UNIT-4

Characterisation Techniques of Nanomaterials- Scanning probe microscopy, Scanning electron microscopy, Transmission electron microscopy, X-ray Diffraction

Books For Reference:

- Shriver and Atkin's Inorganic chemistry, Oxford University press
- 2. Nnomaterials and Nnochemistry- Catherine Brechignac, P. Houdy, M. Lahmani, springer
- 3. An Introduction to Nanomaterials and Nanoscience- Asim K Das

Paper - CHE- 207

SURFACE CHEMISTRY & CATALYSIS

Full Mark 100- (80+20 Marks)

UNIT-I:

Structural Aspects of Organized Molecular Assemblies Surfactants, classification of surfactants, micelles, critical micellar concentration, different methods for determination of critical micellar

concentration, thermodynamics of micellization, aggregation number, shape & size and their determination, shape transition, reverse micelles, emulsion, microemulsion (oil in water and water in oil), effect of cosurfactants, thermodynamics of microemulsion formation.

UNIT-II:

Analytical Applications of Organized Assemblies, Application of micellar systems for UV-Visible/fluorescence spectroscopic detection of ions, micellar enhanced phosphorescence and fluorescence, micellar systems in liquidliquid extraction, surfactant aggregates in flame and plasma atomic spectrometry, micellar systems in chromatography, recent developments in micellar chromatography, application of surfactants in gel electrophoresis.

UNIT-III:

Characterization of Industrial and Model Solid Catalysts Historical development of catalysis, dividing of catalysis to homogeneous and heterogeneous, enzymatic, phase transfer catalysis. Preparation and characterization of catalysts, influence of heat and mass transport on the rate of catalytic process. Evaluation of activity and selectivity of catalysts.

UNIT-IV

Catalysts acido-basic, hydrogenationdehydrogenation, oxidation-reduction, zeolite. Mechanisms of catalyzed reactions. Examples of catalysts applications— cracking, alkylation, hydrogenation, hydration and dehydration processes. Modern sorption and spectral methods of characterization of catalysts.

BOOKS: 1. Introduction to Surface Chemistry and Catalysis by Gábor A. Somorjai (John Wiley & Sons)

2. Physical Chemistry of Macromolecules by C. Tanford CH

Paper - CHE- 208

COMPUTATIONAL CHEMISTRY & MOLECULAR MODELLING

Full Mark 100- (80+20 Marks)

UNIT-i

Molecular mechanics- Vibrational motion, normal modes of vibration, the quantummechanical treatment, the taylor expansion, the morse potential, more advanced empirical potential, molecular mechanics, professional molecular mechanics force fields, a sample MM calculations, General features of potential energy surfaces

UNIT-2

The LCAO procedure, the electronic energy, the Koopmans theorem, open-shell system, unrestricted Hartree-Fock theory, the J^o and K^o operator, Bond lengths and the Huckel model, molecular mechanics and pi-electron systems, alternant hydrocarbons, treatment of heteroatoms, Extended Huckel theory

UNIT-3

Basis Sets- Introduction, the energy calculation from the STO function, the energy calculation of multielecron systems, Gaussian type orbitals, Difference between STOs & GTOs, classifications of basis sets, A comparision of energy caculations of the hydrogen atomsbased on STO-2G, STO-3G & STO-6G basis sets, contracted Gaussian type orbitals, Double and Zeta basis sets and split-Valence basis sets, polarised basis sets.

UNIT-4

- a. Semiempirical methods- Introduction, NDO, CNDO, MNDO, AM1& PM3methods
- Ab Intio Method- Introduction, level of theory, geometry input, An Ab-intio HF-LCAO calculation, computation of the correlation energy
- e. Density Functional Theory-Introduction, electron density, pair density, development of DFT, the kohn and Sham method, density functionals, the Lee, Yang and Parr correlation energy functional and the potential, DFT methods, application of DFT methods

Books recommended

- Modelling Molecular Structures- Alan Hinchliffe, John Wiley& sons, Itd
- 2. Electron Density theory of atoms and molecules-N. H. March, Academic press, London

Paper-CHE-205: INORGANIC PRACTICAL

(100 Marks)

1. QUALITATIVE ANALYSIS (Marks-35)

Qualitative analysis of inorganic mixture containing not more than six radical / six radicals with any one of the following rare metals like tungsten, molybdenum, titanium and vanadium. (Organic radicals are excluded)

2. QUANTITATIVE ANALYSIS (Marks-35)

Estimation major constituents of:-

- (i) chrome iron ore, (ii) white metal, (iii) pyrolusite, (iv) bronze
- (v) Complete 100 percent analysis of (a) dolomite or portland cement and (b) brass
- 3. Viva voce- 20 marks
- 4. Record- 10 marks

THIRD SEMESTER

Paper-CHE-301: INORGANIC

Full Mark 100- (80+20 Marks)

UNIT-1: Theories of metal ligand bonding

- (a) Crystal field theory: Octahedral ligand field, square planner and tetrahedral ligand fields, factors affecting magnitude of crystal fields splitting, tetrahedral distortion in octahedral symmetry. Jahn-Teller effect, crystal field stabilisation energy (CFSE), its uses.
- (b) M. O. theory of metal complexes. Octahedal complexes, MOT for sigma bonding complexes, Effect of π bonding on Δ_0 , relations between bonding ability of ligands and

spectrochemical series.

UNIT-2: Electron Transfer Reactions and Electronic Spectra

a) Crystal field effects on electron transfer reaction, the hydrated electron.

 One and two electron transfer reaction, inner sphere and outer sphere mechanism, complementary and non complementary electron transfer reactions, Kinetic application of crystal field theory.

c) Spectral properties: types of electronic spectra, Laporte selection rule, spin selection rule, charge transfer spectra, d-d-transition spectra, term symbol, Orgel diagram for d¹, d², and d⁵ systems.

UNIT -3

Metal π -Complexes Metal Carbonyls, Structure and bonding, Vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, dinitrogen and dioxygen complexes, tertiary phosphine as ligands. Metal Clusters Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

UNIT-4: Mechanism of inorganic reactions

- (a) Substitution in Octahedral complexes Nature of substitution reactions, Mechanism of substitution reactions of Co (III) and Pt (II) complexes, acid hydrolysis, π-bonding in dissociation reactions of octahedral complexes.
- (b) Base hydrolysis of octahedral Co (III) and Pt (II) complexes, conjugate base and ion pair mechanism.
- (c) Reactions involving replacement of co-ordinated water.
- (d) Substitution reactions without cleavage of metal ligand bond (sigma and pi bonds).

Books For Reference:

- 1. Inorganic Chemistry J. Huheey
- 2. Inorganic Reactions and Mechanism Basolo and Pearson
- 3. Inorganic Reactions and Mechanism M. L. Tobe
- 4. Inorganic Complexes Jorgensen
- Chemistry to Ligand Fields Theory Ballhousen
- Introduction to Ligand Fields Theory Ballhousen.
- 7. Inorganic Co-ordination Compounds D. Banerjee

Paper-CHE 302: ORGANIC

Full Mark 100- (80+20 Marks)

UNIT-1: Natural products

- (a) Alkaloid: quinine (structure, synthesis and biogenesis)
- (b) Vitamin A: structure and synthesis.
- (c) Terpene comphor: structure and synthesis
- (d) Steroid cholesterol structure and synthesis

UNIT-2: Theory of concerted reactions-I

- (a) Molecular orbitals of ethylene, butadine and allyl systems (cation, anion and radical), Assignment of symmetry of the molecular orbitals with respect of mirror plane and C₂ axis.
- (b) Pericylclic reactions: frontier orbital approach, Aromatic transtion state approach (Huckel and Mobilous systems), Woodward - Hofmann rule for pericyclic reactions.

UNIT-3: Theory of concerted reactions- II

- (a) Electrocyclic reactions: conversion of butadiene to cyclobutene (to be discussed on the basis of correlation diagram)
- (b) Cycloadditions: suprafacial and antarafacial cyclo additions, cyclo-additions of butadiene with ethylene, cyclo-addition of ethylene (correlation diagram for superacial additions shall be discussed only antarafacial addition is discussed with frontier orbital approach and aromatic transition state approach)
- (c) Sigmatropic reaction [i,j] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements. Ene

UNIT-4:

Organic photo chemistry -II

Photochemistry of alkenes, Intramolecular reactions of the olefinic bond — geometrical isomerism, cyclization reactions, rearrangement of 1,4— and 1,5— dienes. Photochemistry of Carbonyl Compounds γ , β Intramolecular reactions of carbonyl compounds — saturated, cyclic and acylic, – unsaturated and – unsaturated compounds. Cyclohexadienones. β , α

BOOKS FOR REFERENCE:

- 1. Organic Chemistry Vol. II I. L. Finar
- 2. Chemistry of Natural Products Vol. II Sharma and Agrawal
- 3. Conservation of orbital Symmetry R. B. Wodward and R. Hofmann
- 4. Organic Reactions and Orbital Symmetry T. L. Gilchrist and R. C. Storr.
- Pericyclic Reaction and Organic Photochemistry V. P. Sharma and Rakesh Kumar Pragati Prakashan,
- Frontier Orbital and Symmetry Controlled Pericyclic Reactions by R. K. Kar, Books and Allied Pvt. Ltd.
- 7. Advanced Organic Chemistry by Jagadamba Singh and L. D. S. Yadav, Pragati Prakashan.

Paper-CHE-303: PHYSICAL

Full Mark 100- (80+20 Marks)

UNIT-1

- (a) Interioninc attraction Theory.
- (b) Derivation of Debye-Huckel-Onsagar conductance equation, Its verification and modification, determination of degree of dissociation of electrolytes.
- (c) Theoretical calculation of activity coefficient from ionic strength by Debye-Huckel theory, determination of activity coefficient by Freezing point method, EMF method and solubility method.

UNIT-2

- (a) Ion association, determination of thermodynamic dissociation constant of weak electrolyte by Shedlovsky method, reversible cells, chemical and concentration cells, liquid-junction potential, single electrode potential, oxidation and reduction electrodes.
- (b) Determination of dissociation constant of weak monobasic acid, hydrolysis constant of salts, ionic product of water, solubility product of sparingly soluble salts from EMF measurement.
- (c) Hydrogen ion concentration in ampholytes and isoelectric points.

UNIT-3

- (a) Electrolytic polarization, decomposition potential and over voltage.
- (b) Photochemistry: Laws of light absorption, photoelectric effect, Photochemical equivalence, Fluorescence and Phosphorescence, chemiluminescence, photosensitization, predissociation and quantum efficiency of photo chemical reactions.

UNIT-4

Surface chemistry

Adsorption, Chemisorption, Factors influencing adsorption, Freundich isotherm, Langmuir theory of isotherm, BET theoryof multilayer of adsorption, Derivation of BET equation, Modern trchniques for investigating surfaces

Book for Reference:

- 1. Text Book of Physical Chemistry S. Glasstone.
- 2. Thermodynamics for chemists S. Glasstone.
- 3. Electrochemistry S. Glasstone.
- 4. Advance Physical Chemistry V. K. Gupta & R. G. Sharma.

Paper-CHE-304: SUPRAMOLECULAR CHEMISTRY

Full Mark 100- (80+20 Marks)

UNIT-I:

Fundamentals of Supramolecular Chemistry Terminology and definitions in supramolecular chemistry. Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-pi, anionpi, pi-pi interactions and Van der Waal forces. Solvent and solution properties, solvation and hydrophobic effect. Binding constants; definition and use, determination of binding constant by physical methods.

UNIT-2

Molecular Recognition Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine) as cation and anion binding receptors and receptors for ion-pair recognition. UNIT-3

Supramolecular Reactivity and Catalysis Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-

substrate systems. Influence of organisation (effective molarity) on catalysis, Catalytic acyl transfer, acid-base catalysis, catalysis hydrolysis as ATPase mimic

UNIT-4

Biological supermolecules-supermolecules seen in the biological world,ion channels, information conversion and amplification, energy conversion, material conversion, cleaving genes

Reference books

- Supramolecular Chemistry: from Molecules to Nanomaterials Eds. by P.A. Gale and J.W. Steed (2012).
- 2. Modern Supramolecular Chemistry by F. Diederich, P. J. Stang, R. T. Tykwinski (2008)
- 3. Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace (2007).
- Supramolecular Chemistry by J.W. Steed and J.L. Atwood (2011).
 Supramolecular Chemistry: Concepts and Perspectives by J.-M. Lehn, Wiley VCH, Weinheim (1995).

Paper-CHE-306: ENVIRONMENTAL CHEMISTRY

Full Mark 100- (80+20 Marks)

UNIT I

Environment 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.

Hydrosphere Chemical composition of water bodies-takes, 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, metalsm, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand. Purification and treatment of water.

UNIT 2

Soils Composition, micro and macro nutrients, Pollution –fertilizers, pesticides, plastics and metals. Waste treatment.

Atmosphere Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorophydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

UNIT 3 Industrial Pollution Cement, Sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

UNIT 4

Environmental Toxicology, Chemical solutions to environmental problems, biodegradability, principles of decomposition

Books Recommended

- 1. Environmental Chemistry , S.E. Manahan, Lewis Publishers
- 2. Environmental Chemistry, A.K. De, Wiley Eastern.
- Environmental Chemistry with Green Chemistry, A. K. Das, Books & Allied (P) Ltd., Kolkata, 1st Edn, 2010.
- 4. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication

Paper-CHE-306: INDUSTRIAL PROCESS

Full Mark 100- (80+20 Marks)

UNIT-I:

Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.

LINIT-II:

(a) Oil based industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes. (b) Surface active agents: classification and manufacturing of detergents used for cleansing purpose. (c) Fermentation industries. A general discussion on fermentation conditions, manufacturing of penicillin.

UNIT-III:

Pesticides, Battery and Explosives:

Origin of pesticides and uses, origin of explosive properties in organic compounds, preparation and explosive properties of Lead azide, PETN, cyclonite(RDX),Introduction to rocket propellant, primary and secondary batteries, battery components and their role, characteristics of battery, Fuel cells, solar cells

UNIT-IV

Pharmaceutical industries- Manufacturing of compounds of pharmaceutical importance

BOOKS: 1. Outlines of Chemical Technology by M. Gopala Rao and Marshall Sittig, Affiliated East-

2. Industrial Chemistry by B. K. Sharma

Paper-CHE-306: MATERIAL AND ENERGY BALANCE Full Mark 100- (80+20 Marks)

UNIT-I: Material Balance (a) Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations.

UNIT-II: Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical Reactions, Recycling, Parallel and Bypassing Operations, Metallurgical Applications.

UNIT-III: Energy Balance Energy and Thermo-Chemistry, Energy Balances, Heat Capacity, Heat Capacity of Gases at Constant Pressure, Sensible Heat Changes in Liquids, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfers Accompanied by Sensible Heat Changes, Enthalpy Changes Accompanying Chemical Reactions, Effect of Temperature on Heat of Formation, Heat of Reaction, Adiabatic Reactions, Effect of Pressure on Heat of Reaction, Thermochemistry of Mixing Process, Dissolution of Solids, Liquid-Liquid Mixtures, Heat of Solution by Partial Molal Quantities.

UNIT IV:

Stoichiometry and Unit Operations Distillation, Absorption and Stripping, Extraction and Leaching, Crystallisation, Psychrometry, Drying, Evaporation, Less Conventional Operation

BOOK: Stochiometry by B I Bhatt and S. M. Vora (Tata McGraw Hill, New Delhi)

Paper- CHE-304: PHYSICAL PRACTICAL

(100 Marks)

1. CHEMICAL KINETICS

(a) Kinetics of Ester hydrolysis by acids and alkalis.

2. DISTRIBUTION

- (a) Distribution of lodine in water and any organic solvent.
- (b) Distribution of ammonia in water and any organic solvent.

3. CONDUCTOMETRY

(a) Determination of cell constant and equivalent conductance at infinite dilution.

- (b) Titration (i) NaOH against HCl, (ii) NaOH against mixture of CH₃COOH and HCl.
- (c) Mole ratio of CrO₄²⁻ and Cr₂O₇²⁻.
- (d) Dissociation constant of weak monobasic acid.
- (e) Solubility and solubility product of sparingly soluble salt AgCl.

4. ADSORPTION

(a) Determination of adsorption of acetic acid on activated charcoal in aqueous solution.

5. VICTOR MEYER'S METHOD

Determination of molecular mass of volatile substance.

6. POLARIMETRY

Study of the kinetics of Hydrolysis of cane sugar.

7. POTENTIOMENRY

- (a) Determination of P^H of a given solution using Quinhydrone electrode.
- (b) Determination of dissociation constant of weak monobasic acid.

(Two Experiments 2×35, Viva voce 20, Record 10)

BOOKS FOR REFERENCE:

- 1. Physical Chemistry Practical Behera & Das.
- 2. Physical Chemistry Experiment Palit & Dey.
- 3. Advanced Physical Chemistry Experiment Gurtu & Kapoor.

FOURTH SEMESTER

Paper- CHE-404: GENERAL CHEMISTRY

Full Mark 50- (80+20 Marks)

UNIT-1

 (a) Group theory: groups, subgroups, cosets, classes, symmetry elements and symmetry operations.

- Matrix formulation (idea of matrix multiplication inverse, trace, diagonalisation, eigen (b) (c)
- Classification of point groups, $(H_2O, NH_3, C_6H_6, CH_4$ ferrocene) and Octaheral groups to be discussed. (d)
- Aromaticity, (4n+2) rule, application of group theory to simple MO determinants.

UNIT-2

- Quantum mechanical operators, particle in one and three dimensional box, harmonic (a) oscillator, rigid rotator, the rotational energies of diatomic molecules
- Interaction of radiation with rotating molecules, determination of moment of inertia and bond length from rotational spectra, relative intensities of spectral lines. (b)
- Rotational spectra: linear, molecular symmetric tops, spherical tops, asymmetric tops. UNIT-3

- (a) MO orbital solutions of problems dealing with H_2 , H_2 , and H_2 , ethylene, butadiene, benzene.
- (b) Molecular orbital: Hydrogen like orbitals, M. O. calculations, electronic energy levels, LCAO method, overlap and coulomb integrals, bond order, free value index, charge distribution,

UNIT-4

- Hydrogen atom. The variation theorem,. Perturbation theory Applications of variation method and perturbation theory to the Helium atom.
- Born-oppenheimer approximation, Molecular orbital theory of bonding in H2*, H2, VB treatment

BOOKS FOR REFERENCE:

- Introduction to Molecular spectroscopy Barrow.
- 2. Structure and Molecules Barrow.
- 3. Chemical applications to Group Theory F. A. Cotton.
- 4. M. O. Calculations J. D. Roberts.
- 5. M. O. for Organic Chemistry Stretwieser.
- 6. Introduction to Ligand Field Theory Ballhousen.
- 7. Inorganic Coordination Compounds D. Banerjee.

Paper- CHE-403: PHYSICAL

Full Mark 100- (80+20 Marks)

UNIT-1: Photochemistry

- Light absorption, fluorescence and phosphorescence, light absorption and structure, photo dissociation.
- b) photochemical reduction.
- isomerisation.
- d) flash photolysis, chemistry of vision.

UNIT-2: Spectral method

- (a) ORD: Terminology, Cotton effect, ORD of ketones, axial halo ketone rule.
- (b) Raman spectra, Raleigh and Raman scattering, vibrational and rotational Raman spectra
- (c) Mossbauer Spectroscopy Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting, Magnetic hyperfine interaction

UNIT-3: Thermoanalytical method

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, Differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, Simultaneous study of TGA, DTA with examples. Differential scanning calorimetry (DSC) and thermometric titration

UNIT-4

Electroanalytical methods

Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes

Books For Reference:

- 1. Basic Principles of Organic Chemistry Robert and Casserio
- 2. Spectroscopy Barrow
- 3. Spectroscopy Vol. I & II Walker & Straw
- Instrumental Methods of Chemical Analysis by B. K. Sharma, Goel Publications

Paper-CHE-402

BIOORGANIC

Full Mark 100- (80+20 Marks)

UNIT I

Introduction Basic considerations Proximity effects and molecular adaptation. Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by sitedirected mutagenesis,

UNIT 2

Mechanism of Enzyme Action Kinetics of enzyme action, Michealis Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanism for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

UNIT 3

Reactions Catalyzed by Enzymes and Co-Enzyme Chemistry Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP Cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, Pi-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation. coenzymes, prosthetic groups,

UNIT 4

Organic synthesis

Disconnection Approach An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

Oxidation Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids. Amines, hydrazines, and sulfides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium(III)nitrate.

Reduction Introduction. Different reductive processes. Hydrocarbons - alkanes, alkenes, alkynes. and aromatic rings. Carbonyl compounds - aldehydes, ketones, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups. Hydrogenolysis

Books recommended

- Bioorganic Chemistry, A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
- 2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 3. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.
- 4. Enzyme Mechanisms Ed, M. I. Page and A. Williams, Royal Society of Chemistry
- 5. Designing Organic Synthesis, A programmed introduction to synthon approach, S. Warren, Wiley.
- 6. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, VCH, Weinheim, Germany

Paper-CHE-401

INORGANIC

Full Mark 100- (80+20 Marks)

Unit-1

Magnetochemistry- Magnetic properties of metal complexes, magnetically dilute and concentrated substances, cooperative magnetism, Antiferromagnetism, ferro and ferrimagnetism, Quenching of orbital contribution to magnetic moment by crystal field, comparision of magnetic properties of Fe(II),Co(II), Ni(II), Cu(II) complexes, Temperature dependence of magnetic properties,magnetic properties for the thermal equilibrium between the high spin and low spin states in the cross over region, magnetic exchange interaction.

UNIT II

Organometallics Chemistry of Transitional Element and applications in organic synthesis: Preparative structural and characteristic aspects: oxidative insertion, reductive elimination, ligand migration from metal to carbon. Organo lithium, organo copper compounds, organo boranes, organometallic compounds of Zinc, Cadmium, nickel, palladium, mercury and their utilization in chemical reactions.

. UNIT III

Metal nitrosyls- Coordinating behaviour of the NO, factors forming the linear and bent M-N-O linkage, chemical distinction between the linear and bent M-N-O linkage, relative instability of the pure nitrosyl compounds, requirement electron withdrawing pi-acid ligands to stabilisethe nitrosyl complexes, synthesis of nitrosyl carbonyl and other mixed ligand complexes containing the NO ligand, some important NO complexes

UNIT IV

Application of spectroscopic methods(IR, RAMAN, NMR, ESR, UV-VIS, MOSSBAUER)for the characterisation of inorganic compounds

Books recommended

- 1. Inorganic Chemistry J. Huheey
- Coordination Chemistry by D. Banerjee.
- 3. Advanced Inorganic Chemistry (6th Edu) by Cotton & Wilkinson.

Paper-CHE-405

Analytical practical

- 1. Verification of Beer-Lambert's Law by colorimetry.
- 2. Determination of Na+ / KT ions by flame photometry.
- Determination of ascorbic acid in vitamin C tablets.
- Determination of Dissolved Oxygen (DO) in water samples.
- Measurement of pH of soils by a pH meter.
- 6. Determination of Chemical Oxygen Demand (COD) in water samples.
- 7. Determination of moisture content in soils by gravimetric method.
- 8. Analysis of fat in a butter sample.
- 9. Determination of Biochemical Oxygen Demand (BOD) in water samples.
- 10. Estimation of metal ions by ion-exchange method.
- Adsorption of CH3COOH on activated charcoal and verification of Freundlich's & Langumir's adsorption isotherm.
- 12. Adsorption of CH3COOH on activated charcoal and verification of Freundlich's & Langumir's adsorption isotherm.

Books Recommended.

- Vogel's Text Book of Quantitative Chemical Analysis By J.Mendham, R. C.Denney, J. D.Barnes, M. J. K. Thomas, Pearson Education Publishers, 6th Edition (2007).
 - Hand book of Environmental analysis by Pradyot Patnaik, Lewis Publishers, USA (1997).
- Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington