NATIONAL INSTITUTE OF TECHNOLOGY AGARTALA.

CURRICULA AND SYLLABI

M. Sc. Course in Chemistry

FIRST SEMESTER

Sl. No.	Subject Code	Subject Name	L – T - P	Credits
1	CY-101	Inorganic Chemistry - I	4 - 0 - 0	4
2	CY-102	Organic Chemistry - I	4 - 0 - 0	4
3	CY -103	Physical Chemistry - I	4 - 0 - 0	4
4	CY -104	Analytical and Environmental Chemistry	3 - 0 - 0	3
5	CY -105	Laboratory – I	0 - 0 - 9	6
		Total	**15 - 0– 6**	21

SECOND SEMESTER

Sl. No.	Subject Code	Subject Name	L – T - P	Credits
1	CY -201	Inorganic Chemistry -II	4 - 0 - 0	4
2	CY -202	Organic Chemistry - II	4 - 0 - 0	4
3	CY -203	Physical Chemistry - II	4 - 0 - 0	4
4	CY -204	Biochemistry	3 - 0 - 0	3
5	CY -205	Laboratory – II	0 - 0 - 9	6
		Total	**15 - 0– 6**	21

THIRD SEMESTER

Sl. No.	Subject Code	Subject Name	L – T - P	Credits
1	CY -301	Inorganic Chemistry - III	4 - 0 - 0	4

2	CY -302	Organic Chemistry - III	4 - 0 - 0	4
3	CY 303	Physical Chemistry - III	4 - 0 - 0	4
4	CY -304	Instrumental Method of Analysis of chemical compounds	3 - 0 - 0	3
5	CY -305	Laboratory – III	0 - 0 - 9	6
		Total	**15 - 0– 6**	21

FOURTH SEMESTER

Sl. No.	**Subject Code**	**Subject Name**	L – T - P	Credits
Inorganic Chemistry specialization				
1	CY -411	Group Theory and Electrochemical Studies	4 - 0 - 0	4
2	CY -412	Inorganic spectroscopy and Supramolecular Chemistry	4 - 0 - 0	4
3	CY -413	Inorganic materials and Bio-Inorganic Chemistry	4 - 0 - 0	4
4	CY - 414	Green Chemistry and Waste reduction	3 - 0 - 0	3
5	CY - 415	Project Work with Seminar and Viva-voce	0 - 0 - 9	6
		Total	**15 - 0– 6**	21
Organic Chemistry specialization				
1	CY -421	Pericyclic and Photochemistry	4 - 0 - 0	4

2	CY -422	Organic name reactions, synthesis, structure and Reactivity	4 - 0 - 0	4
3	CY -423	Natural Products and drug Chemistry	4 - 0 - 0	4
4	CY -424	Bio-Organic Chemistry	3 - 0 - 0	3
5	CY -425	Project Work with Seminar and Viva-voce	0 - 0 - 9	6
		Total	**15 - 0– 6**	21
Physical Chemistry specialization				
1	CY- 431	Electrochemistry and Quantum Chemistry	4 - 0 - 0	4
2	CY- 432	Thermodynamics and Solid State Chemistry	4 - 0 - 0	4
3	CY- 433	Instrumentation and Molecular spectroscopy	4 - 0 - 0	4
4	CY- 434	Biomolecules and Biophysical chemistry	3 - 0 - 0	3
5	CY-435	Project Work with Seminar and Viva-voce	0 - 0 - 9	6
		Total	**15 - 0– 6**	21

Note:

1=Inorganic chemistry

2= Organic chemistry

3= Physical chemistry

FIRST SEMESTER

INORGANIC CHEMISTRY (PCY01B01)

(1) Principle of Inorganic Chemistry (30 marks):

Modern view of atomic structure, wave mechanical description of electron and orbital. Covalent Bond: The natures of covalent bond, resonance, formal charge, overlap of atomic orbital, partial ionic character of a covalent bond, electronegetivity, electron affinity, polarization .VBT/VSEPR, inert pair effect, diagonal relationship. Molecular Orbital Treatment: Hydrogen molecular ion, molecular orbital of diatomic molecules like H_2,N_2,F_2,CO and NO, Hydrogen bond and Vander wall force bond. Acid- base theories, Bronsted, Lewis and Lux -Flood theories, HSAB model

(2) Cage and Cluster Compounds (30 marks):

Bonding in Boranes, styx numbers, synthesis and reaction of boron hydrides, carborane, borazine and boron nitride complexes. Cluster and catalysis, molecular structure of cluster, stereochemical rigidity of clusters, electronic structure of clusters with pi-acid ligands, capping principle, halide cluster, synthesis of metal clusters.

(3) Stereochemistry of Coordination Compounds (40 marks):

Bonding in coordination compounds: Crystal field theory, ligand field theory, molecular orbital theory. Application of bonding theory: thermodynamic properties, variation of ionic radii, lattice energy and hydration energy; magnetic properties, spin cross over, spectral properties, spectrochemical series, nephelauxtic series. Stereochemistry of complexes: Structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, absolute configuration of complexes, stereoselectivity and conformation of chelate ring, structural equilibria. Stability of complexes and its determination (slope ratio and mole ratio methods). Kinetic properties: lability of complexes, elementary idea on reaction mechanism of coordination complexes in solution. Outer sphere and inner sphere reactions, cross rection and Marcus-Hush theory.

ORGANIC CHEMISTRY(PCY01B02)

(1) Reagents and methods (30 marks):

Classification of organic reaction-Oxidation reactions using reagents, reduction- nucleophilic, electrophilic, dissolving metal reductions, catalytic reduction- homo and hetero. Fucntionalization of alkenes-hydroboration,epoxidation and aziridanation.

(2) Stereochemistry (30 marks):

Molecular symmetry and chirality; stereoisomerism, definitions, classifications, configurational nomenclature, configuration and conformation.Relative and absolute configuration; determination of relative configuration: (i) chemical correlation not affecting the chiral atom, (ii) chemical correlation affecting bonds to the chiral atom in a 'known way' (iii) correlation by asymmetric synthesis: Horeaus rule, Prelog's rule, Cram's rule (Felkin modification), and sharpless rule, (iv) Physical methods: NMR, Mass, IR, dipole moment, ORD, CD, Effect of conformation on reactivity in acyclic compounds and cyclohexane derivatives, stereochemistry of poycyclic compounds, allylic straqin (A^{1-2}, A^{1-3}).

(3) Polymer Chemistry (40 marks):

Introductory concepts, definition, common system chemistry and classification of polymer, synthetic and natural polymers, types of polymerization, addition, condensation, co- ordination and ring opening polymerization, Preparation, properties and uses of some important thermoplastic (i.e.PE,PVC,Teflon,PS,PMMA)and thermosetting resins(i.e. Phenolic resin, Amino resin and Epoxy resin),natural and synthetic rubbers,Fibers(i.e.Nylons,PAN,Polyyurethanes).Stereochemistry and Mechanism of Polymerization: free radical, cationic and anionic Polymerization. Polymer degradation and stabilization, biological degradation of polymers. Polymers and environment, environmental pollution by polymers, Zeiler Natta catalyst.

PHYSICAL CHEMISTRY (PCY01B03)

(1) Electrochemistry and Electrode kinetics (30 marks):

Debye-Huckel-Onsagar theory of inter-ionic interaction, Thermodynamic of electrified interface, polarisable and non-polarisable interface, over voltage, exchange current density, derivation of Butler-Volmer equation, Tafel plot, low and high field approximation, mass transfer, charge transfer and Ohmic polarization, some redox reactions, transport property through membrane,cyclic voltametry.

(2) Reaction Dynamics (30 marks):

Molecular basis of chemical reaction, potential energy surfaces and reaction dynamics. Kinetics of different complex reactions. Statistical approach to reaction dynamics, Transition state theory. General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and NMR method. Dynamics of electron transfer and proton transfer processes, photoisomerization. Effect of movement of solvent on reaction dynamics. Diffusion controlled reactions. Kinetic isotope effect,solvent isotopic effect, influence of dielectric constant and ionic strength on reaction rate.

(3) Colloids and Surface Chemistry (40 marks):

The colloidal state Introduction; Classification and colloidal systems; properties of lyophilic and lyophobic colloidal solutions. Structural characteristics ; Preparation and purification of colloidal systems Kinetic properties; The motion of particles in liquid media ,Brownian motion and translation diffusion, Osmotic pressure; Rotary Brownian motion.Light scattering; Tyndall effect- turbidity, Liquid-gas and liquid-liquid interfaces; Surface and interfacial tensions; Adsorption and orientation at interfaces; Association colloids- micelle formation, spreading; Surface films and Langmuir- Blodgett films. Properties and aggregation of surfactants; the solid-gas interface Capillary condensation; Lagmuir adsorption isotherm; BET equation for multi-molecular adsorption. Contact angles and wetting Detergency; Adsorption from solution charged interfaces: The electric double layer Electro-kinetic phenomena; Electro-kinetic theory. Colloid stability; Lyophobic sols; vander Walls forces between colloidal particles; Rheology: Introduction; Viscosity; Non –Newtonian flow; Viscoelasticity Emulsions and foams: Oil –in-water and water-in-oil emulsion; Emulsifying agents and emulsion type; gels and Foams.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY (PCY01B04)

(1) Chemistry of the Environment (30 marks):

Chemical aspects of air, water and soil pollution, chemistry of photochemical and sulphurous smog, stratosphere-chemistry and pollution, chemical specification and organometallic compounds in the environment, priority and water pollutants-their effects, chemical analysis and control. Solid wastes from Industries. Radioactive solid waste disposal. Recovary and recycling. Ecological balance and planning of Industrial complexes. Reactions in living systems. Bioreactors. Biochemical process in industries.

(2) Analysis of air and water pollution (30marks) :

Objectives of chemical analysis of air and water. Analysis of water: colour, turbidity, total solid, conductivity, acidity, alkalinity, hardness, chloride, sulfate, fluoride, phosphates, and different forms of nitrogen. Heavy metal analysis with respect to health significance. Measurement of DO, BOD and COD. Pesticides as water pollutants analysis. Monitoring and analysis of air: Monitoring technique through high volume sampler, SPM and RPM sampler. Measurement and analysis of SPM, RPM, SOX and NOX. Air and water pollution laws and standards.

(3**) Analytical Chemistry (40 marks) :**

Liquid-Liquid extraction: Principle, operation technique, successive extraction, different inorganic extraction systems, various factors, counter-counter distribution.

Chromatography: general principles, methods and applications of column (adsorption and partition), paper chromatography, paper electrophoresis, thin layer chromatography, gas chromatography, high performance liquid chromatography, supercritical fluid chromatography, size-exclusion chromatography and ion chromatography.

Thermal methods: introduction, thermogravimetry, differential thermogravimetry, differential thermal analysis, differential scanning calorimetry and thermometric titration and their applications in numerous chemical systems. Electrochemical methods: introduction, membrane electrodes, diffusion controlled process; polarography, likovic equation, current-voltage diagram and voltametry (CV & DPV).

LABORATARY-1 (CY-105)

Full Marks 100 (Exam 80, Sessional 10, viva 10)

Inorganic:-

Determination of DO, BOD, and COD of water, Estimation of metals ions in the following mixture: (i) Cu^{2+} and Fe^{2+}; (ii) Ag^{+} and Cu^{2+} (iii) Fe^{2+} and Mg^{2+} (iv) Zn^{2+} and Ni^{2+}

Inorganic preparation:

(i) $[Co(NH_3)_6]Cl_3$
(ii) Mohr's salt
(iii) $[Mn(acc)_3]$

Organic:-

Separation of binary mixtures of organic compounds (solid-solid, solid-liquid, liquid-liquid) identification of individual compounds through functional group detection -B.P, M.P. determination.
Estimation of nitrogen by Kjeldhal's method and estimation of methoxy group by Ziesel method.

Physical:

(i) Determination of rate constant of alkaline hydrolysis of ethyl acetate, and determination of activation parameters, effect of ionic strength.
(ii) Determination of Partition coefficient of Iodine between water and organic solvent.
(iii) Determination of distribution coefficient of benzoic acid between water and benzene.
(iv) To study the kinetics of the acid hydrolysis of an Ester.
(v) To determine the concentration of weak acid (CH_3COOH) conductometrically using standard caustic soda solution.
(vi) To determine the concentration of strong acid HCl and a weak acid (CH_3COOH) in a mixture conductometrically using standard NaOH solution.
(vii) To study the adsorption of acetic acid on charcoal and to prove the validity of Frendlich's adsorption isotherm.

SECOND SEMESTER

INORGANIC CHEMISTRY-II (PCY02B05)

(1) Organometallic Chemistry (30 marks):

Historical development, classification, nomenclature, valence electron count, oxidation number, formal ligand charge. Main group and d-block organometallics, structure and bonding of the carbonyls, nitrosyls, and related π-acids, alkyl, alkene, alkyne, π–allyl, polyene and cyclopolyene compounds. Metal-ion catalytic reaction with special reference

to oxidative addition, reductive elimination, insertion, hydrogenation, carbonylation, hydroformylation and polymerization.

(2) Bioinorganic Chemistry (30 marks):

Bioinorganic Chemistry: Biochemistry of iron and copper: Dioxygen binding, transport and storage through Hemoglobin, Myoglobin, Hemerythrin, and Hemocyanin. Blue copper proteins: Type 1, Type 2, and Type 3 copper centers in O_2 activating proteins. Metal-sulfide proteins: Ferredoxin and Nitrogenase. Metalloporphyrins and respiration: Cytochromes. Metals at the center of photosynthesis: Magnesium and Manganese. Metalloenzymes: Carbonic anhydrase, carboxypeptidases, alcohol dehydrogenase and vitamin B_{12}. Ion transport across membrane. Nitrogen fixation.

(3) Chemistry of transition and non-transition elements (40 marks):

Study of d-block elements (a) A general treatment of the d-block elements ,Chemistry of titanium group elements, technetium and rhenium, (b)Metal carbonyls :Preparation, properties, and bonding of Iron ,cobalt and nickel carbonyls,(c)A general treatment of iso poly molybdates and vanadates. A study of f-block Elements: (a) A general treatment of the Chemistry of lanthanides, positioning the periodic table. Electronic configuration ,oxidation states, color pigments , lanthanide contraction general methods of extraction ,(b) Actinides: Electronic structure , ionic radii, oxidation state, spectra and paramagnetic properties of actinides elements, Actinide hypothesis, A brief chemistry of uranium and thorium, isolation of neptunium, plutonium and americium and their aqueous chemistry.

ORGANIC CHEMISTRY –II (PCY02B06)

(1) Heterocyclic chemistry (30marks):

Chemistry of pyrimidines, purines, oxazoles, iso-oxazoles ,thiazoles and iso-thiazoles, pyrazoles, imidazoles and cumarines.

(2) Chemistry of reactive intermediate (30 marks):

Classical and non classical carbocations and carbanions; radicals, radical cations, radical anions, carbenes, arenas and nitrenes. General methods of generation, detection, stability, reactivity and structure of intermediate. Nomenclatural aspect of carbocation and bridged ring system.

(3) Enzyme Chemistry (40 marks):

Enzymes: Chemical and biological catalysts. Nomenclature and classification, concept and identification of active sites by use of inhibitors, catalytic power, specificity and regulation. Examples of some typical enzyme mechanisms for chymotripsin, ribonuclease, lysozyme and carboxypeptidase-A. Different types of enzyme catalyzed reactions, Co-enzyme chemistry. Enzyme models: Host-guest chemistry, chiral recognition, molecular asymmetry and prochirality, crown ether, cryptates, cyclodextrins, calixarin

PHYSICAL CHEMISTRY (PCY02B07)

(1) Quantum Chemistry (30 marks):

Fundamentals of quantum mechanics: operators, functions, basic postulates, Time-independent Schrodinger equation, particle in a box of various dimensions, rigid rotation in a plane, spherical harmonic functions, rotation of diatomic molecule, harmonic oscillator, electronic wave function of hydrogen and hydrogen like atom, magnetic effect on electron movement, many electron theory, raising and lowering operators, Pauli exclusion principle, Time-dependent Schrodinger equation.

(2) Photochemistry (30 marks):

Interaction of electromagnetic radiation and matter, electric and magnetic dipole moment, transition probabilities, selection rules, violation of selection rules, oscillator strength, Jablonski diagram, fluorescence and phosphorescence, excited state lifetime and quantum yields, fluorescence anisotropy, instrumentation for fluorescence spectroscopy, fluorescence polarization, effects of solvents on fluorescence emission spectra, mechanism and dynamics of solvent relaxation, quenching of fluorescence. Determination of excited state dipole moment and pK value. Electron transfer mechanism-Marcus theory.

(3) Equilibrium Thermodynamics (40marks):

The third law of thermodynamics. Calculation of entropy changes in chemical reactions. Mathematical and thermodynamic probability. Entropy and probability. The free energy of a mixture. Dependence of thermodynamic functions on composition . Partial molar quantities.

Analytical form of the chemical potential in ideal solutions. Chemical potential of solute in a binary solution. Application of Gibbs- Duhem equation: The concept of activity: the rational concept and the practical concept. Colligative properties and activity of solute. Activities and reaction equilibria, experimental determination of activity coefficients of non-electrolytes, Numerical problems.

BIOCHEMISTRY: (PCY02B08)

(1) Cell structure and Functions (20 marks) :

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, Overview of metabolic process catabolism and anabolism. ATP – the biological energy currency. Origin of life – chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of biomolecules.

(2) Nucleic acids (20 marks):

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of RNA and DNA, double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis of heredity, an

overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

(3) Lipids: (20 marks):

Fatty acids, essential fatty acids, structure and function of triacyl glycerols,glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins- composition and function, role in atherosclerosis. Properties of lipid aggregates – micelles, bilayers, liposomes and their possible biological functions. Biological membrane. Fluid mosaic model of membrane structure. Lipid metabolism – β oxidation of fatty acids.

(4) Carbohydrates (40 marks):

Conformation of monosaccharides, structure and functions of important monosaccharides like glycosides, deoxy sugars, myoinositol amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose and chitin. Storage polysaccharides - starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism: Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

LABORATARY-2:(CY-205)

Full Marks 100 (Exam 80, Sessional 10, viva 10)

Inorganic:

Quantitative Analysis-Estimation of Cr^{3+} and Fe^{3+}, estimation of $Ca^{2}+$ and Mg^{2+} in dolomite, estimation of silica in sodium silicate.

Organic preparation:

Acylation-Acetyl salicylic acid and acetanilide; condensation-cinnamic acid and benzal acetophenone; nitration- p-nitroacetanilide and nitrobenzene. Hydrolysis-benzoic acid and p-nitro aniline;Esterfication-ethyl benzoate, methyl salicylate and benzyl acetate; Halogenation: Preparation of p-bromoacetanilide, 2,4,6- tribromophenol. Diazotization:

Preparation of methyl orange and methyl red Oxidation: Preparation of benzoic acid from toluene. Reduction: Preparation of aniline from nitrobenzene, Preparation of m-nitroaniline from m-dinitro benzene; rearrangement-benzilic acid; Hofmann reaction-Anthranilic acid,haloform reaction-Iodoform; benzoylation-phenyl benzoate.
Preparation of organic compounds involving multisteps :
Benzil→Benzilic acid→ Diphenyl acetic acid
Phthalic acid→Phthalimide→o-iodobenzoic acid

Isolation of caffine from tea leaves, Isolation of Nicotin-dipicrate from tobacco.

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Physical:-

(i) To determine the heat of neutralization between HCl and NaOH
(ii) Solvent effect and salt effect on the kinetics of alkaline hydrolysis of crystal violet.
(iii) Determination of standard electrode potential of AgCl-Ag electrode and evaluation of mean activity coefficient of HCl.
(iv) Cyclic voltametry for ferrocyanide-ferricyanide system.
(v) Determination of catalytic constant for mutarotation of glucose in presence of perchloric acid.
(vi) To titrate potentiometrically a standard solution of KCl against $AgNO_3$ solution and to determine the concentration of $AgNO_3$ solution and the solubility product of AgCl.

THIRD SEMESTER

INORGANIC CHEMISTRY-III :(PCY03B09)

(1) Inorganic Photochemistry (30 marks):

Fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, substitution, decomposition, fragmentation, isomerisation and redox reactions; photochromism; selective photochemistry using laser beams; chemical actinometry, inorganic photochemistry in biological processes and their model studies; application of photochemical reactions of coordination compounds-synthesis and catalysis.

(2) Industrial Inorganic Chemistry (30 marks):

Introduction to chemical industry, Industrial Gases: carbon dioxide, carbon monoxide, sulphur dioxide, hydrogen, oxygen, nitrogen, rare gases of the atmosphere, coal gas, water gas, manufacture of producer gas. Manufacture of ammonia, urea, nitric acid, calcium ammonium nitrate, cement, glasses, carbon black, abrasives, fertilizers, pulp and paper. Zeolites, Surface active agents, High purity electronic materials, explosives and propellants, extraction of iron, aluminium, copper, tin, lead from ores. Application of catalysis in industry

(3) Solid state chemistry (40 marks):

Introduction to single crystal, unit cell, Bravis lattice, crystal system and symmetry, crystal planes, Miller indices, reciprocal lattice, Lau-equation, Brag's law, scattering of X-ray and X-ray diffraction, fourier series, electron density and structure factor. Various X-ray diffraction method. determination of space group, methods of solving the phase problem, patterson and direct methods for determination of crystal structure.Voids, radiostic, structures of AX, AX_2, AX_3 types and their derived species, sphalite, wurzite, fluorite, perovskite, ilmentite, rutile, silicate and layered structure. Band theory, structure maps; electronic properties of solids, conductors, semiconductors, insulators, superconductors.Optical properties: Refraction, refraction index, bifringence, absorption, luminescence, laser,ionic crystal, lattice energy etc.

ORGANIC CHEMISTRY –III:(PCY03B010)

(1) Organic Photochemistry (20 marks):
Photo-chemical energy, Jablonski-diagram, photo-sensitisation and quenching, Norrish type-I, type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds.

(2) Paints, Agrochemicals and Food Chemicals (20 marks):
Preparation of organic pigments and their applications. Synthesis of pesticides/ herbicides/fungicides. Food chemicals: Flavour, coloring and preservatives. Pheromones: Acyclic and cyclic, chiral and achiral sex attractants, their synthesis.

(3) Industrial Organic Chemistry (20 marks):

Basic products of industrial synthesis, chemicals from natural gases, petrochemicals and coal, chemicals of industrial importance: olefins, di-olefins, acetylenes, halo-compounds, alcohols, aromatics, amides, polyamides, organic reactions in industrial synthesis (oxidation, hydration hydrogenation, dehydroformylation and polymerization) fermentation technology, paints, pigments and coatings.

(4) Pericyclic Reaction (40 marks):
Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Elecctrocyclic reaction – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition – antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 –dipolar cycloadditions abd chelotropic reactions. Sigmatropic rearrangements - suprafcial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements, Fluxional tautomerism. Ene reaction. regioselectivity, periselectivity; aromatic transition state (Huckel-Mobus transition state).

PHYSICAL CHEMISTRY-III: (PCY03B011)

(1) Statistical thermodynamics (40 marks):

Introduction to statistical thermodynamics, probability, ensembles and distribution laws, partition function. Comparison among Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein Statistics.Statistical mechanics of mono, diatomic and polyatomic ideal gas-contribution of rotation, vibration and transition to partition function, electronic contribution to the specific heat of diatomic gases, solids-vibrational contribution to the specific heat of solids, Einstein-Born-Debye model. Dynamics of chemical reaction in solution-transition state theory using partition functions; Adsorption-Langmuir and BET isotherm.

(2) Catalysis-Principles and Application (30marks):

Basic principles of catalysis, adsorption isotherms, surface area, pore size and acid strength measurements. Enthalpy and entropy of adsorption: interpretation of chemisorption based on the structure and the nature if the solid-solid state theories- role of defects in catalysis. Kinetics of surface reactions: rate determining step, various types of reactions, simple, parallel and consecutive reactions. Selection, preparation and evaluation of catalysts-test reactions, promoters, carriers and stabilizers. Mechanisms of selected reactions-hydrogenation and dehydrogenation reaction- dehydration of alcohols-olefin hydrogenation – decomposition of nitrous oxide- oxidation of CO- ketonization of carboxylic acids, cracking of hydrocarbons. Application- petrochemical industry-reforming and refining- value added chemicals- environmental protection –auto exhaust catalysts-Novel catalytic materials- clusters, mesoporous materials. Types of fuel cell and catalyst; Photocatalysis; photocleavage of water; Phase transfer catalysis.

(3)Fundamental of Polymer Chemistry (30marks): Introductory concept, definition, common system chemistry and classification of polymers, resin, rubber, plastics. Characterization: number average, molecular weight average and viscosity average molecular weight. Concept of segment and segment length. Effect of solvents. Thermodynamic of dilute polymer solution. Light scattering method to determine molecular weight and structure of polymers in solution. Kinetics of polymerization. Mechanistic aspect: Addition, ionic, emulsion, aqueous, coordination, condensation polymerization processes. Dendrimers. Crystal structure of polymers: crystalline melting point T_m, glass transition temperature (T_g). Effect of different parameters on T_m and T_g

INSTRUMENTAL METHOD OF ANALYSIS OF CHEMICAL COMPOUNDS (PCY03B012)

(1) ESR Spectroscopy (15 marks):

Hyperfine coupling, Spin polarization for atoms and transition metal ions, Spin-orbit coupling and significance of g-tensors, application to transition metal complexes including free radicals.

(2) NMR Spectroscopy (50 marks):

Long range spin-spin interaction. Interpretation of non-first order NMR; double resonance, Lanthanide shift reagent, spin-tickling, INDOR, NOE, effect of solvents (aliphatic and aromatic), preliminary idea on ^{19}F, ^{31}P, ^{14}N, ^{15}N, ^{17}O. NMR of solids, NMR imaging. C^{13} NMR Spectroscopy: Introduction, theory, instrumentation, chemical shift, coupling constants, application in organic molecules,2D NMR, multidimensional NMR-DEPT, APT and LCNMR.

(3) Mass Spectrometry (35 marks):

Generation of ions and detection; EI, CI, FD, FAB, plasma desorption etc; fragmentation pattern in EI, GC-MS, MS-MS, LC-MS. Application of UV, IR, NMR and MS in structure elucidation, HRMS and Mc Lafferty rearrangement.

LABORATARY-3: (CY-305)

Full Marks 100 (Exam 80, Sessional 10, viva 10)

Inorganic:
Preparation of inorganic and coordination compounds and their characterization: (a) Bi-, tri- and polydentate ligands, (b) Complexetion and purification, (c) spectral studies (IR, UV-VIS), (d) Solution conductivity and electrochemical measurements, (e) Magnetic studies. Kinetics and mechanistic studies of some selected reactions (substitution and redox). Experiments on separation techniques by Ion-exchange, chromatography and solvent extraction processes.

Organic:

Thin Layer Chromatography

Determination of R_f values and identification of organic compounds.
Separation of green leaf pigments (spinach leaves may be used).
Preparation and separation of 2,4-dinitrophenylhydrazones of acetone, 2-butanone, hexan-2- and 3- one using toluene and light petroleum(40:60).
Separation of a mixture of dyes using cyclohexane and ethyl acetate (8.5:1.5).

Paper Chromatography: Ascending and Circular

Determination of R_f values and identification of organic compounds.
Separation of a mixture of phenylalanine and glycine. Alanine and aspertic acid. Leucine and glutamic acid. Spray reagent - ninhydrin.
Separation of a mixture of D, L – alanine, glycine andL – Leucine using n-butanol: acetic acid: water (4:1:5). Spray reagent - ninhydrin.
Separation of monosaccharides – a mixture of D-galactose and D-fructose using n-butanol: acetone: water (4: 5: 1). Spray reagent - aniline hydrogen phthalate.

Column Chromatography:

Separation of Fluorescein and methylene blue
Separation of leaf pigments from spinach leaves
Resolution of racemic mixture of (±) mandelic acid.

Physical:

(i) Determination of specific rotation of cane sugar and determination of composition of a sugar solution of unknown strength.

(ii) Determination of pKa value of a weak acid by pH-metric method.

(iii) To determine the rate constant for the acid catalyzed inversion of cane sugar using the supplied solution and its half diluted solution at the room temperature.

(iv) Solvent and micelle effect on the fluorescence of 1-naphthol and determination of CMC of a surfactant.

(v) To titrate potentiometrically the given ferrous ammonium sulphate using $KMnO_4/K_2Cr_2O_7$ as standard and to find the redox potential of Fe^{3+}/Fe^{2+} system on the hydrogen scale.

(vi) To study kinetics of reaction $I^- + S_2O_8^{2-}$ by Colorimetric method.

(vii) To study the kinetics of saponification of ester by conductometric method.

FOURTH SEMESTER

INORGANIC CHEMISTRY

GROUP THEORY AND ELECTROCHEMICAL STUDIES (PCY01B01)

(1) Chemical Application of Group Theory (50 marks):

Point group, the great orthogonality theorem, character table, representation, projection operator, SALC, direct product; symmetry aspects of MO theory, carbocyclic systems (benzene etc.), electron deficient molecules. Cyclization reactions: thermal and photochemical, symmetry consideration of pericyclic reactions, hybrid and molecular orbitals, sigma- and pi-bonding schemes for AB_n type molecules (n = 6). Treatment of ligand field theory, term splitting, energy level diagram, electronic transitions, vibronic coupling, Tanabe-Sugano diagram, selection rules, polarization. Molecular vibrations,

symmetry of normal vibrations and symmetry types of the normal modes, internal coordinates, selection rules for fundamental vibrations, illustrations.

(2) Electrochemical studies (50 marks):

Preamble, electrochemical cell, electrode, mass transfer, electron transfer, three electrode configuration, supporting electrolyte, solvent, switching and action potentials, electrode potential and factors affecting.Techniques: polarography, cyclic voltammetry, differential pulse voltammetry and coulometry. Electroinduced reactions: electrosynthesis, electrocatalysis, electropolymerization, electrocrystallization, electrochemiluminescence. Conjunctive study: cell design, OTTLE, surface-modified electrode, photoelectrochemistry, spectroelectrochemistry, excimer and it's structure, excited state potential, redox orbital, redox series, redox isomer. Applications: electrochemical reactor, corrosion, fuel cell, electrodialysis, bilayer-liquid membrane and bioelectrochemistry, nerve pulse and cardiovascular electrochemistry, electrochemical sensor.

INORGANIC SPECTROSCOPY AND SUPRAMOLECULAR CHEMISTRY (CY-412)

(1) Applications of spectroscopy (50 marks):

Molecular luminescence spectrometry: theory, instrumentation and applications, light scattering techniques including nephelometry and Raman and IR spectroscopy. Flame spectrometric techniques: atomic absorption, atomic emission and atomic fluorescence - theory, instrumentation and applications of these techniques. Mössbauer and magnetic Mössbauer spectroscopy, Application of NMR in inorganic complexes- ^{31}P, ^{19}F, ^{119}Sn NMR.

(2) Supramolecular chemistry (50 Marks):

Definition, supramolecular building block and spacer, molecular recognition and host-guest interactions, spherical recognition, receptors, co-receptor molecules and multiple recognition, organometallic/macrocyclic receptors, catenane, rotaxane, catenand, catenate, coronand, ferrocene, cobaltocenium and other metallocene receptors, molecular and supramolecular devices, self organization and self assembly of inorganic architectures.

INORGANIC MATERIALS AND BIO-INORGANIC CHEMISTRY(CY-413)

(1) Inorganic material (60 marks)

Solid state reaction: ceramic method, carbothermal reduction, combustion synthesis. Formation of solid from gas phase: chemical vapor transport, chemical vapor deposition, aerosol process. Formation of solid from solution and melt: precipitation method,

solvothermal process, sol-gel process, micelle and reverse micelle method. Preparation and modification of inorganic polymer, porous material, nano-structured material, glasses and ceramic, composites, electronic and magnetic material.

(2) Bio- inorganic chemistry (40)

Metal ions in biology, their vital role in the active-site structure and function of metallo-proteins and enzymes especially those containing Mg, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo and W ions. Both heme and non-heme systems with one-, two- or multi-metal centers (e.g., Fe: Hb, Mb, Hr, P-450, MMO, ferridoxins, Fe-S clusters: Cu: hemocyanin, SOD, Mn: vitamin B12; Zn: CPA, CA, Ni: urease will also be highlighted.

GREEN CHEMISTRY AND WASTE REDUCTION (CY-414)

(1) Medicinal and toxic effect of metals (60 marks):

The elements of life and bioinorganic chemistry, biological functions of the bio-elements, disturbing factors in the metabolic processes and causes of diseases, principles of bioinorganic chemistry in medicine, different classes of drugs.

Evaluation methods for environmental and human health impact, metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs; Metal ions and metal complex interactions with nucleic acid and DNA.

(3) Introduction to Green Chemistry (40 marks):

Definition and strategic of green chemistry. Why Green Chemistry? Prevention, Atom Economy, Less Hazardous Chemical Syntheses, Designing Safer Chemicals, Safer Solvents and Auxiliaries, Design for Energy Efficiency, Use of Renewable, Feedstocks, Reduce Derivatives, Catalysis, Design for Degradation, Real-time analysis for Pollution Prevention, Inherently Safer Chemistry for Accident Prevention, Laboratory pollution prevention with examples.

ORGANIC CHEMISTRY

PERICYCLIC AND PHOTOCHEMISTRY(CY-421)

(1) Pericyclic Reactions (25 marks):

Electrocyclic reactions- 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claisen, cope and aza-cope carbon rearrangements. Fluxional tautomerism, Ene reactions.

(2) Organic Photochemistry (50 marks):

General information, effect of light intensity on the rate of photochemical reactions.
Types of photochemical reactions: Photo-dissociation, gas phase photolysis.
Photochemistry of alkenes: Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes. Photochemistry of Carbonyl compounds: Intramolecular reactions of carbonyl compounds saturated, cyclic

and acyclic, β,γ-unsaturated and α,β-unsaturated compounds. Cycolhexadienones, Intermolecular cycloaddition reactions, dimerisation and oxetane formation. 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, photosubstitution, photoreduction of ketones, photooxidation, di-π methane rearrangement,photochemistry of arenes.organomettalic photochemistry, photochemistry of vision.

Organometallic Chemistry(25 marks): Hake, Suzuki,Sonograsira, nigishi, Kumuda coupling reactions, Olefinic metathesis (RCM, ROM and CROSS)

ORGANIC NAMED REACTIONS ,SYNTHESIS, STRUCTURE AND REACTIVITY(CY-422)

(1) Quantitative relationship between structure and reactivity (20 marks):

HSAB principles and simple illustration of its application in organic synthesis.Linear free energy relations: Hammett equation; equialibria and rates in organic reactions. The separation of polar, steric and resonce effects: Taft equation; Grunwald-Winstein equation.

(2) Organic synthetic Chemistry (30 marks):

Organic synthetic process and uses of Phosphorus, Silicone, tin and Sulphur compounds in synthetic organic chemistry planning a synthetic pathway; molecular characteristics: Retro synthesis; method of formation of carbon skeleton: carbon to carbon bond formations, logistic and stereochemistry. Phospho ylide and sulphur ylide.

(3) Name Reactions and Re-arrangements (50 marks):

Name reaction in organic synthesis: Pinacol-pinacolone rearrangement, Favorski rearrangement, Fries rearrangement, Wagner- Meerwein rearrangement, Benzil-Benzilic

Acid rearrangement, Beckmann Rearrangement, Diels-alder reaction , Claisen rearrangement, Wittig rearrangement, Mc Murry reaction,Mitsunovo reaction,Julia olifination Shapiro reaction, Swern oxidation,Baylis-Hilman reaction, Baeyer Villager reaction, Dienone-phenol rearrangement, Neber rearrangement and Stephen rearrangement.

NATURAL PRODUCTS AND DRUG CHEMISTRY (CY-423)

(1) Natural Pigments (20 marks):

General methods of isolation, structure elucidation and synthesis of anthocyanins, flavones, flavones, isoflavones, aurone, chalcone, xanthone.

(2) Alkaloids, Steroids and terpenoids (40 marks):

Classification, general reactions of alkaloids-biosynthesis, typical reaction conversions and rearrangement of morphine, papaverine, cinchona alkaloids. Reaction and synthesis of steroids, sources of steroid hormones; diosgenin, hecogenin, etc., Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of abietic acid, alpha and beta-carotenoids.

(3) Drug design (40 marks):

Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, structure-activity relationship, mechanism of drug action. Classification of drugs: Based on structure or pharmacological basis with examples. Antineoplastic agents, cardiovascular drugs, local antiinfective drugs, psychoactive drugs, antibiotics. Synthesis: Synthesis of important drugs. Modelling: Molecular modeling, conformational analysis, qualitative and quantitative structure-activity relationship.

BIO-ORGANIC CHEMISTRY (CY-424)

(1) Enzyme Kinetics (30 Marks):

Michaelis Menten and Lineweaver- Burk plots, reversible and irreversible inhibition. Mechanism of enzyme action: Typical enzyme mechanism for ribonuclease, lysozyme. Chemical models and mimics for enzymes, receptors, peptides, carbohydrates and other bioactive molecules, catalytic antibodies- Design, synthesis and evaluation of enzyme inhibitors.

(2) Peptides and proteins (30 marks).

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures. α–helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein – folding and domain structure. Quaternary structure.

(3) Nucleic acids (40 marks):

Introduction, classification, occurrence, nucleosides: Isolation, properties and synthesis of ribosyl and deoxyribosyl nucleosides; biosynthesis of alpha-D- ribose phosphate; nucleotides: Isolation and functions, structure of ribosyl and deoxyribosyl nucleotides, biosynthesis of isosinic acid, adenylic acid, guanylic acids, cystodylic acid and uridylic acid; translation and transcription (general idea), RNA & DNA (structural composition) codon anticodon, genetic code, protein synthesis.

PHYSICAL CHEMISTRY

ELECTROCHEMISTRY AND QUANTUM CHEMISTRY (CY-431)

(1)Interfacial and applied electrochemistry (25marks):

Fundamentals of corrosion science: electrochemical aspects, electrochemical kinetics and phenomena of polarization, E-pH diagram. Different forms of corrosion: mechanism and control. Dry oxidation. Corrosion under various industrial condition and their control. Cathodic and anodic protection. Corrosion inhibitors and passivation, surface coating, corrosion rate expression. Electrochemical methods of corrosion inspection and monitoring.

(2) Interfacial (25 marks):

Double layer across electrified interface. Genesis of DL potential difference,across interface,polarisable and non polarisable interface, electrocapillary thermodynamics, surface excess quantities from electrocapillary and capacitance measurements.Structure of the DL,HB and GC,stern and BDM model, capacitance hump and contact adsorption.specific adsorption and Esin-Mercov coefficient.

(2) Advanced quantum chemistry (50 Marks):

Variation method and time independent perturbation theory: Application to He atom. Antisymmetric and exclusion principle, Slater determinal wave function, spin-orbital interaction: LS and JJ coupling, Term symbol and spectroscopic states, molecules and chemical bonding, Born-Oppenheimer approximation: MO and VB treatment of diatomic molecules. Directed valence and hybridization in simple polyatomic molecules. Idea of self-consistent field theory -Hartree-Fock equation ,Hartree-Fock-Roothaan method. Time dependent perturbation theory: Transition dipole moment. Huckel theory of conjugated systems. Bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene.

THERMODYNAMICS AND SOLID STATE CHEMISTRY(CY-432)

(1) Solid State Chemistry (60 Marks):

Crystal lattices, space groups, Miller indices, crystal morphology and unit cell dimension, crystallization, X-ray data collection: system and procedure, standard deviation (error), laqttice energy, phase determination, scattering, isotropic and anisotropic temperature factors, modeling, refinements, disorder, structural parameters determinations, 3-D structure solution. Bonding of atoms in metals, Band theory. Properties of metal: free electron theory, zone theory. Electrical, magnetic and thermal properties of metals. Properties of semiconductors (n and p type): Band theory, conductivity, optical

properties, junction properties, transistors. Properties of insulators: electrical properties-pyroelectricity and piezoelectricity, optical properties, magnetic properties.

(2) Non equilibrium Thermodynamics (40 marks):

Non-equilibrium thermodynamics, postulates and methodologies, forces and fluxes, linear laws, Gibbs equation, Onsagar reciprocal theory. Curie-Prigogine principle, diffusion, effusion, sedimentation, thermoelectric effect, membrane properties. Stationary states: time variation of entropy production, minimum entropy production, stability of stationary state, fluctuation.

INSTRUMENTATION AND MOLECULAR SPECTROSCOPY(CY-433)

(1) Advanced Spectroscopy (50 Marks):

Fundamentals of 2D-NMR and FT-NMR, Auger spectroscopy, X-ray photoelectron spectroscopy, analytical techniques based on Auger spectroscopy, SEM, TEM, surface enhanced Raman spectroscopy, UV-photoelectron spectroscopy. Single molecule spectroscopy, 3-photon echo spectroscopy. Application of fluorescence spectroscopy to determine the properties of self-organized assemblies. Laser: fundamentals of laser, Q-switched and mode locked laser. Application of ultra fast lasers to determine excited state lifetime and dynamics.

(2)Atomic and Molecular Spectroscopy (50marks) :

Quantum numbers, orbital and spin momentum of electron, Stern-Gerlach experiment, vector model of atom, atomic term symbol, atomic spectra, pure rotational and vibrational spectra of diatomic and polyatomic molecules, vibrational-rotational coupling, Raman spectroscopy of molecules, electronic spectra of molecules, spectroscopic selection rules for vibrational, electronic and Raman spectra, Introduction to resonance spectroscopy-NMR, ESR, EPR, hyperfine interaction, photoelectron spectroscopy, Auger spectroscopy, Mössbauer spectroscopy.

BIOMOLECULES AND BIOPHYSICAL CHEMISTRY: (CY-434)

(1) Biomolecular Structure (40 Marks):

General principle of X-ray diffraction, crystallization of bio-molecules, different methods of crystallization of proteins: vapor diffusion, micro dialysis. reciprocal space and diffraction pattern, structure factor and phase problem, solving the structure by different X-ray methods, nucleic acid structure, protein structure: folding, motif, fibre and collagen structure.

(2) Advanced Biophysical Chemistry (60 marks):

Hydrophobic and hydrophilic interactions in biological systems, biological relevance of chemical potential, protein solvent interactions-binding, hydration and exclusion, protein structure, stability, folding, unfolding and their spectroscopic and calorimetric studies. Protein ligand binding, equillibria across membranes, structure-function relationships Different types of bio-molecules. Complexities in macromolecules, general principles for macromolecular separation: ion exchange, gel filtration chromatography, sedimentation, electrophoresis and isoelectric focusing, solvent effect, structure activity relation, kinetic of enzyme and enzyme-inhibiting complex, cooperative allosteric effect.