New Syllabus for M. Sc (Regular) in Chemistry

Total Marks=1600 (128 credit)

Semester	Course ID	Theory (T)	Course ID	Practical (P)		Total
First Semester: 400 Marks/32 Credits						
I	Organic Chemistry (ORG)				**IDC-I**	
	S1/ORG/I-T	50	S1/ORG/I-P	50		
	Inorganic Chemistry (ING)					
	S1/ING/I-T	50	S1/ING/I-P	50		
	Physical Chemistry (PHY)					
	S1/PHY/I-T	50	S1/PHY/I-P	50		
	Marks	**150 (12 credit)**		**150 (12 credit)**	**100 (8 credit)**	**400 (32 credit)**
Second Semester: 400 Marks/32 Credits						
II	Organic Chemistry (ORG)				**IDC-II**	
	S2/ORG/II-T	50	S2/ORG/II-P	50		
	Inorganic Chemistry (ING)					
	S2/ING/II-T	50	S2/ING/II-P	50		
	Physical Chemistry (PHY)					
	S2/PHY/II-T	50	S2/PHY/II-P	50		
	Marks	**150 (12 credit)**		**150 (12 credit)**	**100 (8 credit)**	**400 (32 credit)**
Third Semester: 400 Marks/32 Credits						
III	Organic Chemistry (ORG)				**Group Discussion and Viva-voce: 50** (4 credit) **Seminar: 50** (4 credit)	
	S3/ORG/III-T	50	S3/ORG/III-P	50		
	Inorganic Chemistry (ING)					
	S3/ING/III-T	50	S3/ING/III-P	50		
	Physical Chemistry (PHY)					
	S3/PHY/III-T	50	S3/PHY/III-P	50		
	Marks	**150 (12 credit)**		**150 (12 credit)**	**100 (8 credit)**	**400 (32 credit)**
Fourth Semester: 400 Marks/32 Credits						
IV	Organic Chemistry (ORG)					

	S4/ORG/IV-T1 (Spl.) S4/ORG/IV-T2 (Spl.) Environmental Science (S4/Comp/Envs/T)	100 100 50			**Project:** **S4/ORG/IV-Project 150** (12 credit)	
	Inorganic Chemistry (ING)					
	S4/ING/IV-T1 (Spl.) S4/ING/IV-T2 (Spl.) Environmental Science (S4/Comp/Envs/T)	100 100 50			**Project:** **S4/ING/IV-Project 150** (12 credit)	
	Physical Chemistry (PHY)					
	S4/PHY/IV-T1 (Spl.) S4/PHY/IV-T2 (Spl.) Environmental Science (S4/Comp/Envs/T)	100 100 50			**Project:** **S4/PHY/IV-Project 150** (12 credit)	
	Marks	**250 (20 credit)**			**150 (12 credit)**	**400 (32 credit)**
Total Marks		**700 (56 credit)**		**450 (36 credit)**	**450 (36 credit)**	**1600/128 Credits**

Organic Chemistry

Semester – I

General Organic Chemistry-I **60L**

(Core Paper)

Course ID- S1/ORG/I-T **(Full marks: 50/4 Credits)**

Unit-I: Structure Activity Relationship

MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes (C_{60}), alternante and non-alternante hydrocarbons, anti-aromaticity, pseudoaromaticity, homo-aromaticity; graphical methods – Frost diagram, Huckel treatment - applications to ethylene, allyl cyclopropenyl, butadiene, cyclobutadiene, Hammett equation and its modifications.

Unit-II: Stereochemistry – I

Acyclic systems upto 4 chiral centers: Comnpounds with asymmetric carbons in branched chains, symmetry; point groups, correlation of axial dissymmetry and centrodissymmestry, Nomenclature of compounds involving axial and planar chirality, Winstein-Holness equation, Curtin Hammett principle; Conformational analysis of cyclohexene, decalins and their derivatives; Effects of conformation on reactivity in acyclic compounds and cyclohexanes.

Interconversion of Fisher, Newman and Sawhorse projections; effects of conformation on reactivity of acyclic compounds and cyclohexanes: E-Z isomerization.

Elements of Symmetry and Chirality, Optical purity, enantrotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

Unit-III: Substitution (aliphatic electrophilic & nucleophilic) & Elimination reactions

S_E1, S_E2 & S_Ei mechanism, electrophilic substitution accompanied by double bond shifts; Reactivity – effects of substrate, leaving group and the solvent polarity. Mixed S_N1 & S_N2 and SET mechanism; Reactivity effects on S_N reaction – substrate structure, attacking nucleophilic, leaving group and reaction medium; phase transfer catalysis; ultrasound, ambient nucelophile, regioselectivity.

The E_2, E_1 and E1cB mechanisms and their spectrum, Mechanism and orientation in pyrolytic elimination reaction.

Unit-IV: Pericyclic Reaction

Classification and stereochemical modes. Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheleotropic reactions. Rationalization

based on Frontier M.O. approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems, Sommelet-Hauser, Cope, aza Cope and Claisen rearrangements, Ene Reaction. Wittig rearrangement, suitable examples of [(2Π +2 Π), (4Π +2 Π), (4Π + 4Π), (2Π +2 Π +2Π)] and metal catalysed cycloaddition reactions

Unit-V: Spectroscopy – I

Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin decoupling, spin tickling, classification of ABX, AMX, ABC, A_2B_2 in proton NMR. Elementary principles of ESR, EPR and mass spectral techniques.

Unit-VI: Natural Products – I

Isoprene rule, Structure elucidation (by chemical and spectroscopic methods), Synthesis, Biogenesis and Biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes, Structural types; general introduction is sesqui, di- and tri-terpenoids.

Unit-VII: Aromatic Electrophilic and Nucleophilic substitution

Orientation & reactivity, the ortho – para ratio, ipso attack, Vielsmeyer reaction. S_NAr 1, S_NAr2, Benzyne mechanism ; Reactivity – effect of substrate, structure, leaving group and attacking nucleophile ; Von Richter and Smiles rearrangement.

Course ID- S1/ORG/I-P (Full marks: 50/4 Credits)

Practical

Identification of single organic liquid with one or more functional groups : purification of organic sample by distillation / vacuum distillation / fractional vacuum distillation, determination of boiling point, solubility analysis and classification, functional group analysis, derivatization and complete identification, use of spectroscopic techniques (IR, UV, NMR).

Organic preparation involving Aldol condensation, aromatic substitution reaction, Sandmeyer reaction, Friedel-Crafts reaction etc.

Semester – II

General Organic Chemistry-II **60L**

(Core Paper)

Course ID- S2/ORG/II-T (Full marks: 50/4 Credits)

Unit-I: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Excited states (S1 and T1) of some photo excited organic molecules; mechanism of photo excitation; photo-induced reactivity of olefins, ketones, unsaturated ketones and various conjugated systems; photo-induced functionalisation in organic molecules involving Barton reaction,Cis-trans isomeriation, stereo mutation Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection (ESR) of radicals, radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, autooxidation.

Unit-II: Synthetic Strategy

Retrosynthetic analysis, disconnection approach, Typical examples to illustrate the disconnection approach, Functional group interconversion, Umpolung (1,3-dithlane), Convergent synthesis, C-C bond formation reactions; ylide method, Si in C-C bond formation, organometallic; acetylides and nitriles, logistic and stereochemistry.

Structure, transformations, synthesis of simple and monoterpenoid derived indole alkaloids - reserpine, strychaine, ellipticins, lysergic acid.

Unit-III: Synthetic Methodology

Organoboron – Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates.

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig, stobbe reaction, hydrolysis of esters and amides, ammonysis of esters, addition to C - C & C - N multiple bonds.

Unit-IV: Spectroscopy – II

Introduction to ^{13}C NMR spectroscopy; theoretical treatment of rotational, vibrational and electronic spectroscopy, principles of photoelectron spectroscopy. Application of electronic, vibrational, NMR, ESR, EPR and mass spectral techniques to simple structure and mechanistic problems.

Unit-V: Stereochemistry – II

Correlation of axial disymmetry and centrodissymetry, nomenclature of compounds involving axial and planar chirality, dynamic stereochemistry.

Unit-VI: Reaction Kinetics & Mechanism

Labelling and Kinetic isotope effects, (Hamette, Hanch, Taft equation, sigma-rho relationship, Marcus Theory, Baldwin's ring closure rule, hamette scale, Hammond's postulates, Law of microscopic reversibility.

Unit-VII: Natural Products – II

Familiarity with methods of structure elucidation (chemical & spectroscopical method), biosynthesis, synthesis and biological activity of the alkaloids - nicotine, atropine, coniine and papavarine.

Course ID- S2/ORG/II-P (Full marks: 50/4 Credits)

Practical

Organic preparation involving Aldol condensation, aromatic substitution reaction, Sandmeyer reaction, Friedel-Crafts reaction. Organic multi-step preparations by the use of organic reagents and purification of the products by chromatographic techniques.

Quantitative analysis - Estimation of Phenol, Glucose & Sucrose, Determination of pk_a of benzoic acid.

Semester III

Advanced Organic Chemistry **60L**

(Core Paper)

Course ID - S3/ORG/III-T **(Full marks: 50/4 Credits)**

Unit-I: Spectroscopy-III

Applications of electronic, vibrational, ESR/EPR and Mass spectral techniques.

Unit-II: Heterocyclic Chemistry – I

Synthesis and reactions of aziridines, azetidines, oxazoles, thiazoles, imidazoles, isoxazoles, isothiazoles, pyrazoles and higher azoles and corresponding fused systems ; Nomenclature of bicyclic and tricyclic fused systems ; Introduction to the chemistry of azerins, oxepines, thiopins and their aza analogues; Phosphorus and selenium containing heterocycles, Cyclazines.

Unit-III: Oxidative processes and Reactive processes

Introduction to 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 sulphides

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

Introduction to different reductive processes: Hydrocarbons - alkanes, alkenes, alkynes and aromatic rings.
Carbonyl compounds: aldehydes, ketones, acids and their derivatives, Epoxides.Nistro, nitroso, azo and oxime groups, Hydrogenolysis.

Unit-IV: Rearrangement / Selective Organic reactions
Wagner-Meerwein, Favorskii, Neber, Baeyer – Villiger, Shapiro, Sharpless asymmetric epoxidation, Ene reaction, Barton reaction, Hofmann - Loffler – Freytag reaction.

Unit-V: Organometallic Reagents
Principle, preparations, properties and application of organometallic compounds of transition elements – Cu, Pd, Ni, Fe, Co, Rh, Ru, Cr and Ti in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization) – , structure and machinistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction – Heck, Stille, Suzuki coupling, Sonogashia, Buchwald-Hartwig , Ziegler Natta catalysis, Walker Process, Olefin metathesis, Tebbe's reagent, Pauson-khand reaction, functional organometallic compounds, pi-acid metal complexes, activation of small molecules by coordination.

Unit-VI: Reagents in organic synthesis
Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, 1,3 - Dithane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Laweson's reagent. Wilkinson's catalyst, Bakeryeast., hypervalent organo iodines (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

Course ID- S3/ORG/III-P **(Full marks: 50/4 Credits)**

Practical

Extraction of Natural products & their purification (Thin layer and Column Chromatography) and partial characterization by IR, UV and NMR.
Separation and identification of the components of a binary mixture of organic solids: chromatographic separation, purification and identification of individual components (use of IR, UV, NMR), derivatization of individual component and analytical establishment of their identity.

Semester IV

Organic Chemistry Special-I **120L**

(Optional Paper)

Course ID- S4/ORG/IV-T1(Spl.) **(Full marks: 100/8 Credits)**

Group A **4 Credits**

Unit-I: Stereochemistry – III

Chiroptical properties of Organic Molecules: Origin, Theory. CD, ORD, VCD- principles and applications, haloketone rules, sector rules, helicity rules.

Unit-II: Advanced Heterocyclic Chemistry – II

Indoles, pyrimidines, pyridazines, pyrazines, purines, pteridines, compounds. Role of heterocyclic compounds in biological systems.

Unit-III: Metallocenes, non benzenoid aromatics and polycyclic aromatic compounds, **Bonds** weaker than covalent – addition compounds, crown ether, complexes and cryptands, inclusion compounds, cyclodextins, catenanes and rotaxanes.

Unit-IV: Medicinal Chemistry

Introduction to chemotherapy, sulfonamides, arsenical drugs, antibiotics, penicillins, antimalerials, cephalosporin, streoptomycin, chloramphenicol, polypeptide antibiotics, polyacetylene antibiotics, macrolide group of antibiotics.

Group B **4 Credits**

Unit-V: Supramolecular Chemistry:

Unit-VI: Hemoglobin, chlorophyll and phthalocyanines

Introduction, Haemoglobin, porphyrin, bile pigments, chlorophyll, phalocyanines.

Unit-VII: **Steroids:** Occurrence, nomenclature, basic skeleton, and stereochemistry; Synthetic principles and chemical reactions.

Semester IV

Organic Chemistry Special-II **120L**

(Optional Paper)

Course ID- S4/ORG/IV-T2 (Spl.) **(Full marks: 100/8 Credits)**

Group A **4 Credits**

Unit-I: Spectroscopy – IV

Application of Dept, 1H- ^{1}H COSY, HETCOR, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, reaction monitoring etc. q - NMR & DOSY.

Unit-II: Bio-Organic Chemistry

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, Cyclodestrins, cyclodextrin-based models, calizazerenes, ionophores, micelles, synthetic enzymes or synzymes.

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structurecand Biologicalfunctions of coenzymes A, thiamine pyrophosphate, pyrodoxal phosphate, NAD+, NADP+, EMN, FAD, lipoic, vitamin B_{12}. Mechanisms of reactions catalyzed by the above cofactors.

Unit-III: Spectroscopy - V

Modern techniques of mass spectroscopy FAB, MIKE LCMS / MS, ES / MS.

Unit-IV: Natural Products –III

Structure and Chemistry of quinine alkaloids with special reference to cinchona group; isoquinoline alkaloids – morphine group.

Group B **4 Credits**

Unit-V: Plant Pigments: Synthesis and reactions of Coumarin and Chromones; occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Querectin, Mycetin, Quercetin 3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cynanidine-7-arabinoside, Cynidin, Hirsutidin.

Biosynthesis of flavonoids: Acetate pathway and shikimic and pathway.

Unit-VI: Green Chemistry

Green Chemistry – Overview, Set of Principles of Green Chemistry, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, solid phase organic synthesis.

Unit-VII: Nucleoside & Nucleotide

Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Replication, transcription, protein biosynthesis, Covalent interactions of nucleic acids with small molecules, Structural features of DNA and RNA.

Unit-VIII: Compounds of non metals

Chemistry of Organo sulphur, Organo phospohorus and organo silicon compounds.

<u>Course – ID</u> – S4/ORG/IV-Project (Full marks: 150/12 Credits)

Project Work/Review Work

Project work/Review work as given by guide teacher.

N.B: Teacher may teach any other relevant topic(s) which is (are) not mentioned in the Organic chemistry syllabus.

Syllabus: Inorganic Chemistry

Semester-I

Paper: General Inorganic Chemistry-I

Course ID- **S1/ING/I-T** **Theory (Core paper)** **60 L**
Full Marks: 50 (38+12) : **Credit point: 4**

A: Organometallic compounds of main group elements-**I**

Synthesis, properties and structures of organometallic compounds of group-I to group-III elements of the periodic table.

B: Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes.

Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds.

C: Reaction mechanism of transition metal complexes-**I**

Classification of reactions of complex compounds, inert and labile complexes, consideration of octahedral substitution reactions in the light of VBT and CFT, energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ($\Delta S^{\#}, \Delta H^{\#}, \Delta V^{\#}$), substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc., conjugate base formation, anation reaction and base hydrolysis, reactions without metal-ligand cleavage.

D: Magnetic properties and spectra **-I**

Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, determination of magnetic susceptibility, magnetic properties of first transition series metal ions and lanthanides.

N.B: List of recommended books will be given shortly.

Paper: Qualitative Inorganic Analysis

Course ID- **S1/ING/I-P** **Practical (Core paper)**
Full Marks: 50 **Credit point: 4**

Less common metals – Be, Mo, W, Ti, Zr, Th, V, U, Ce and all the radicals included in the U.G Chemistry(H) syllabus.

N.B: List of recommended books will be given shortly.

Semester-II
Paper: General Inorganic Chemistry-II

Course ID- **S2/ING/II-T** **Theory (Core paper)** **60 L**
Full Marks: 50(38+12) **Credit point: 4**

A: Organometallic compounds of main group elements-**II**
Synthesis, properties and structures of organometallic compounds of group-IV & V elements of the periodic table.
B: Reaction mechanism of transition metal complexes-**II**
Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter, etc.
Redox reactions- complementary and non-complementary reactions, mechanisms of outer sphere and inner sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross relation.
C: Isopoly and heteropoly acids and their salts.
D: Magnetic properties and spectra-**II**
Orgel diagrams and spectra, calculations of Dq , B and β - parameters, charge transfer spectra, anomalous magnetic moment, magnetic exchange coupling and spin crossover.site preference in mixed metal oxides (Spinel and inverse spinel structures),

E. Molecular term symbol.

N.B: List of recommended books will be given shortly.

Paper: Quantitative Inorganic Analysis

Course ID- **S2/ING/II-P** **Practical (Core paper)**
Full Marks: 50 **Credit point: 4**

Separation and estimation of two metal ions from minerals, alloys or solutions.

N.B: List of recommended books will be given shortly.

Semester-III

Paper: Advanced Inorganic Chemistry

Course ID- **S3/ING/III-T** **Theory (Core paper)** **60 L**

Full Marks: 50(38+12)

Credit point: 4

A: Molecular symmetry and group theory - Applications:

SALC & MO's, formation of Hybrid orbitals. Irreducible representations of vibrational motions,predidcting probability of a spectral transition, correlation diagrams for a d^2 ion in an octahedral and tetrahedral environments.

B: Application of spectroscopy in inorganic chemistry-**I**

Introduction to vibrational & rotational spectroscopy, ESR, Mössbaur & EXAFS.

C: Chemical bonding

Adjusted crystal field theory, Nephelauxetic series, experimental evidence for metal-ligand overlap,

MOT for bonding in complex compounds including σ- and π-bonding.

Huckel MO treatment for simple and conjugated polyenes such as molecule such as ethylene, butadiene.benzene

D : Organotransition metal chemistry

a. Alkyls and aryls of transition metals.
b. Compounds of transition metal –carbon multiple bonds.
c. Transition metal-π-complexes.
d.Transition metal compounds with bonds to hydrogen.
e. Organometalic catalysts
f.Fluxional organometallic compounds

N.B: List of recommended books will be given shortly.

Paper: Preparation, separation and Characterisation Inorganic Compounds.

Course ID- S3/ING/III-P **Practical (Core paper)**

Full Marks: 50 **Credit point: 4**

Preparation of inorganic compounds and their study by IR, electronic, Mössbaur, ESR spectra and magnetic susceptibility measurements, handling of air and moisture sensitive compounds involving vacuum lines.

Selection can be made from the following or any other compound as selected by the teacher concerned:

1. Sodium amide.
2. Synthesis and thermal analysis of group II metal oxalate hydrate, atomic absorption analysis of Mg and Ca.
3. Trialkoxyboranes- Preparation, IR and NMR spectra.
4. Dichlorophenylborane-synthesis in vacuum line.
5. Preparation of Tin (IV) iodide, Tin (IV) chloride and Tin (II) iodide.
6. Relative stability of Tin (IV) and Pb (IV): Preparation of ammonium hexachlorosttanate, ammonium hexachloroplumbate.
7. Hexa-bis (4-nitropheoxy) cyclotriphosphazene.
8. Synthesis of trichlorodiphenylantimony (V) hydrate.
9. Sodium tetrathionate.
10. Metal complexes of dimethyl sulphoxide- $CuCl_2$.2DMSO, $PdCl_2$.2DMSO, $RuCl_2$.4DMSO.
11. Synthesis of metal acetylacetonate: Magnetic moment, IR, NMR.
12. Bromination of $Cr(acac)_3$.
13. Magnetic moment of $Cu(acac)_2.H_2O$.
14. Cis and Trans $[Co(en)_2Cl_2]^+$.
15. Separation of optical isomer of cis-$[Co(en)_2Cl_2]Cl$.
16. Ion-exchange separation of oxidation state of vanadium.
17. Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), determination of O_2 absorption by Co(salen), reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
18. Preparation of Fe (II) chloride.
19. Preparation of Fe (II) chloride.
20. Reaction of Cr (III) with a multidentate ligand: a kinetics experiment (visible spectra Cr-EDTA complex).
21. Preparation of [Co(phenonthroline-5,6-quinone].
22. Preparation and use of Ferrocene.
23. Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
24. Preparation of phosphine and its transition metal complexes.
25. Any other experiment such as conversion of p-xylent to terephthalic acid catalysed by $CoBr_2$ (Homogeneous catalysis).
26. Preparation of tetraphenyltin.
27. Preparation of lithiated reagents.

Experiments will be set depending upon the availability of instruments and material

N.B: List of recommended books will be given shortly.

Semester-IV

(Optional paper)

Paper: Inorganic Chemistry special-I

Course ID- **S4/ING/IV/T1** **Theory (Optional paper)** **120 L**

Full Marks: 100(75+25) **Credit point: 8**

Group: A Credit Point: 4 60L

A: Bio-inorganic Chemistry

Metal ions in biological systems, essential and trace elements, Transport and storage of dioxygen: hemoglobin, myoglobin, hemerythrin and hemocyanine.Electron transfer in biology:Structure and functions of metalloproteins in electron transfer process: iron-sulfer proteins, cytochromes. Photosynthesis: PS-I & PS-II, nitrogenase, metal ion storage and transport, metalloenzymes, Na^+/K^+ pumps, metal-nucleic interactions.

B: Chemistry of non-transitional elements

Compounds with B-N bonds, P-N bonds and S-N bonds.

C: Solid state chemistry

Electronic properties and Band theory. Solid state reactions, general principles, crystal defects and non-stoichiometry, colour centre, photographic process, phosphors.

D: Crystal morphology:

Important minerals and different types of silicates: structural and physical properties.

Group: B **Credit Point: 4** **60L**

E: Chemistry of materials

Glasses, ceramics, composites, liquid crystals, ionic conductors, molecular devices, thin films. Semi conductor and super conductor.

F. **Nanomaterials**

General introduction to nanomaterials; nanowires,nanotubes.and nanorods; Techniques of synthesis: characterisation of nanomaterials, Applications of nanoparticles.

G: Analytical Chemistry-I

Role of analytical chemistry, Classification of analytical methods- classical and instrumental, types of instrumental analysis, selection of an analytical method, neatness and cleanliness, laboratory operations and practices.

Analytical balance-techniques of weighing and errors, volumetric glassware cleaning and calibration, Sample preparations- dissolution and decompositions, gravimetric techniques, selection and handling of reagents, laboratory notebooks, safety in analytical laboratory.

Selected analytical techniques-**I**

i. Solvent extraction.
ii. High performance liquid chromatography (Brief ideas).
iii. Ion exchange chromatography.
iv. Polarography & amperometry.

v. Analysis of water.
vi. Analysis of drugs.
vii. Analysis of soil
viii. Management & reutilization of industrial effluents and wastes

N.B: List of recommended books will be given shortly.

Paper: Inorganic Chemistry special-II

Course ID- S4/ING/IV/T2 Theory (Optional paper)

Full Marks: 100(75+25) ; Credit point: 8
120L

Group: A Credit Point: 4 60L

A: Analytical Chemistry-II

Selected analytical techniques -II

a) Spectrophotometry
b) Thermal methods of analysis
c) Radioactive methods of analysis
d) Fluorimetry,phosphorimetry, nephelometry, turbidometry and atomic absorption spectroscopy,ICP
e) TEM,SEM,STM,AFM
f) Photoacoustic spectroscopy.

B: Application of spectroscopy in inorganic chemistry-**II**
NMR, ORD/CD & ESCA.

C: X-ray, electron diffraction and neutron diffraction.

D: Molecular spectroscopy.

Electronic absorption spectroscopy- potential energy curves, Franck-Condon principle, oscillator strength, selection rules and intensity of electronic transitions, charge transfer spectra.

Group: B Credit Point: 4 60L

E: Chemistry of Actinides.

F: Chemistry of missing elements

G: Supramolecular chemistry

Basic concepts and principles, host-guest interactions,classification of macrocyclic systems: podand, cyrptand etc, crown ethers ,molecular recognition, spherical recognition, application of macrocyclic crown ethers, calixarenes as receptors, cyclodextrins as receptors ,cylophanes as synthetic receptors, ,catenanes and rotaxanes, Dendrimer, Molecular switch.

H: Photoinorganic chemistry

Basics of Photochemistry properties of excited states, excited states of metal complexes, ligand field photochemistry, redox reactions by excited metal complexes, metal complex sensitizers.

N.B: List of recommended books will be given shortly.

Paper: Project/Review

Course ID- S4/ING/IV/Project **(Optional paper)**

Full Marks:150 **Credit point: 12**

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Project :

Student will select topic for review/ project work in consultation with sectional teachers. Student will submit typed written-up with abstract, methods, findings with proper tables, structures, figures and references. Student will deliver his/her seminar lecture on his/her topic in presence of external expert and sectional teachers.

*** Project to be selected and executed from Semester III and it will be evaluated in Semester IV.**

N.B: Teacher may teach any other relevant topic(s) which is (are) not mentioned in the inorganic chemistry syllabus.

Syllabus: Physical Chemistry
Semester – I

General Physical Chemistry-I
(Core paper)

Course ID- S1/P/I-T **(Full marks: 50/4 Credits)**
60L

Unit-I: Symmetry and Group Theory-I

Introduction to symmetry. Symmetry elements and Symmetry operations. Definition of a Group. Point symmetry groups. Group multiplication tables. Theorems of groups. Conjugate elements and class. Matrix representation of groups

Unit- II Introduction to Classical mechanics

Newton's equation of motion, Lagrange's equation of motion, Hamilton's equation of motion, Poisson Bracket.

Unit-III: Introduction to Quantum Mechanics

Postulates of Quantum Mechanics. Schrodinger wave equation and its solution. Wave function and its probabilistic interpretation. Orthogonality and normalization of wave functions, schwarzs inequality. Operator and related theorems. Linear operators. Hermitian operators. Kinetic energy operator. Eigenvalue equation. Commutation relation. Heisenberg uncertainty relation (derivation of general form).

Unit-IV: Quantum mechanics of translational motion

Particle-in-a Box and energy quantization. Selection Rules. Discussion on Bohr's correspondence principle. Checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg's Uncertainty principle. Quantum Mechanical Tunneling.

Unit-V: **Fundamental electrochemistry**:

Ion Solvent interactions

Introduction, quantitative treatment of ion solvent interaction, Born model, enthalpy and entropy of ion-solvent interaction and its calculation, structuural treatment of the ion-solvent intractions, ion-dipole and ion-quadruple model of ion-solvent interactions, dielectric constant of solution.

Ion ion interaction:

Ion-Ion interaction, Ionic atmosphere, Debye-Huckel theory (Detail calculation),asymmetry and elctrophoretic effect,Debye Huckel onsagar conductance equation. Activity coefficient of electrolytes, Extended Debye-Huckel theory, Pitzer equation for activity coefficient, Experimental determination of mean ionic activity coefficient.

Energy storage device:

Lithium ion battery, cathode and anode materials, electrolytes, working mechanism.

Unit VI:**Chemical kinetics:**

Basic revisionary problems on order, rate constant, collision theory, theories of reaction rates: applications to uni-, bi- and termolecular reactions, Lindemann theory.

Course ID- S1/P/I-P **(Full marks: 50/4 Credits)**

Practical

1.`Studies on the kinetics of iodination of acetone.

2.Determination of solubility product of PbI_2 by titrimetric method.

3 Determination of solubility product of potassium hydrogen tartarate in water and in presence of different concentrations of a common ion at room temperature.

4. Determination of ionic product(K_w) of water at room temperature pH metrically

5.Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.

6. Conductometric titration of a mixture of acids/dibasic acids.

7.Potentiometric titration of Mohr salt solution with standard potassium dichromate solution.

8. Determination of CST of of partially miscible system.

10. Determination of molecular property of a molecule by semiemperical method.

Semester – II

General Physical Chemistry-II

(Core paper)

Course ID- S2/P/II-T **(Full marks: 50/4 Credits)**

60L

Unit-I:Group Theory

Symmetry Operators and their Matrix Representation. Reducible and irreducible representations. Equivalent representations. Characters of representations.

Great Orthogonality Theorem- statement and interpretation. Proof of its corollaries. Character table and its construction. Number of times an irreducible representation occurs in a reducible one. The reduction of reducible representations. Notation of irreducible representations.

Unit-II:

Operator algebra and operator related theorem. Hermition operator, Angular momentum operators and their commutation relations. Heisenberg's equation of motion. Ladder operators. Projection operator, Parity operator, Permutation operator.

Virial theorem, Ehrenfest theorem.

Unit-III: Harmonic Oscillator

Solution of Schrodinger equation of a Harmonic oscillator using the operator method as well as the technique for solution of differential equation. Selection rules for Harmonic oscillator. Checking the validity of Schrodinger wave equation based on correspondence principle Heisenberg's Uncertainty principle.

Unit-IV: Quantum Mechanics of Rotational Motion

Solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation. Quantum Mechanics of rigid rotor and its application.

Unit V: Molecular Spectroscopy:

Principles: Transition probability, transition moment, selection rules, intensity of spectral lines, width of spectral lines and its various causes.

Rotational spectra**:** classification of molecules into spherical, symmetric and asymmetric tops; diatomic molecules as rigid rotors – energy levels, selection rules and spectral features, isotope effect, intensity distribution, effect of non-rigidity on spectral features;

vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches;

Raman spectra: Raman spectra: origin, selection rules, Raman and Rayleigh scattering rotational and vibrational Raman spectra of diatomics, exclusion principle.

Unit VI: Nuclear Magnetic Resonance (NMR)Spectroscopy*:*

Basic instrumentation, principles, nuclear spin, energy levels, Larmor precision, nuclear resonance, shielding of magnetic nuclei, chemical shift, and its measurements, spin-spin interactions, high and low resolution spectrum and splitting of energy levels, coupling constant, relaxation process. FTNMR (qualitative idea) and its advantages.

Unit VII:Photochemistry:

Flurescence and phosphorescence emission, mirror image rule, phosphorescence and heavy atom effect.

Course ID- S2/P/II-P

(Full marks: 50/4 Credits)

Practical

1. Studies on alkalis hydrolysis of ethyl acetate conductometrical
2. Determination of pK_1 and pK_2 of phosphoric acid pH metrically.
3. Verification of Debye Huckel Onsager-equation.

4.. Kinetics study of the reaction between $K_2S_2O_8$ and KI by sphectrophotometric method/ any other method /Studies on the kinetics of reaction between $KBrO_3$ and KBr titrimetrically.

5 Effect of electrolytes on the critical solution temperature.
6 Determination of standard reduction potential of Ag/Ag+, Q/QH2 electrode.
7 Kinetics of oxidation of alcohol by potassium dichromate-Spectrophotometry

8. Evaluation of HOMO, LUMO and dipole moment of a molecule by DFT method using the software Gaussian and Gaussview.
9. Experiments based on cyclic voltammetry instrument:
Study of electrochemical reversibility, effect of concentration and scan rate on potassium ferro-ferri cyanide system./Corrosion study of Steel by polarization study (Cyclic voltammetry,LSV etc).

Semester – III

Advance Physical Chemistry
(Core paper)

Course ID- S3/P/III-T **(Full marks: 50/4 Credits)**
60L

Unit-I: Classical Thermodynamics (Revision)
Brief review of 1st, 2nd and 3rd laws of thermodynamics, Nernst heat theorem and 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.

Unit-II: Connection between Thermodynamics and Statistical Mechanics: Probability, Principal of Equal a priory probability, permutation, combination, Microstates and Macrostates. Thermodynamic probability. Ensemble and average properties. Degrees of freedom, Position space, momentum space, phase space, mu-space and gamma space. Fundamental postulates of statistical mechanics. Statistical ensemble. Microcanonical, canonical and grand canonical ensemble. Boltzman Canonical distribution law, partition function and its relation with thermodynamic quantities. Gibbs paradox.

Unit-III : Hydrogen Atom: Energy levels and atomic orbitals
Separation of translational and internal motion of a two-body problem. Determination of radial part of the wavefunction. Relation among principal, azimuthal and magnetic quantum number. Nodal properties of angular part as well as the radial part of the Hydrogen atom wavefunction. Shape of the orbitals, Space quantization. Selection rules for Hydrogen atom.

Unit- IV: Basic concept of variation and perturbation methods and application to simple system. Introduction to computational Chemistry.

Unit-V: Advance electrochemistry:

Solvation number and methods for determination of solvation number, Ion-solvent-non-electrolyte interactions: Salting-in and salting-out phenomena. Ion association, ion-pair formation, Bjerrum and Fuoss treatment, The fraction of ion-pair, Triple ion formation, Determination of ion-association constant.

Unit-VI: Chemical kinetics:

Thermodynamic formulation of reaction rate, Statistical formulation of chemical kinetics reaction dynamics, Activation energy, potential energy surface.

Reactions in solution –single sphere and double sphere model, cage effect, diffusion and activation controlled reactions (elementary idea), dielectric effect on ion-ion reaction, electrostriction, volume of activation, effect of pressure on reaction rate, classification of reactions on the basis of volume of activation, primary and secondary salt effects, Curtin-Hammett principle, Influence of substituents on reaction rates, electronic theory of organic reactivity, linear free energy relationship, Hammett and Taft equation.

Fast Ractions: Luminescence and energy transfer processes. Study of kinetics by stopped–flow and relaxation methods, flash photolysis and magnetic resonance method.

Course ID- S3/P/III-P **(Full marks: 50/4 Credits)**

Practical

1. Determination of CMC and micellization parameters of surfactant
2. Determination of the activation energy of the reaction between $K_2S_2O_8$ and KI.

Determination of the activation energy of the reaction between $KBrO_3$ and KBr/ of the ester hydrolysis reaction.

3. Determination of the hydrolytic constant of aniline hydrochloride using a pH meter/Determination of strength of HCl and acetic acid and their mixture pH metrically.

4. Conductometric titration of sodium sulphate by barium chloride.
5. Determination of standard reduction potential of ferricyanide-ferrocyanide ion system/ Potentiometric titration of Zn(II) solution by potassium ferrocyanide solution and also determination of the composition of the complex/ Redox titration: ferrous ammonium sulphate and ceric sulphate.
6. Effect of ionic strength on the rate of persulphate iodide reaction
7. Determination of activity solubility product of calcium sulphate by complexometric titration.
8. Evaluation of quantum chemical property of a molecule and spectra by ab initio method using software Gaussian and Gaussview.
9. Experiments based on cyclic voltammetry instrument:
   Study of effect of concentration and scan rate on potassium ferro-ferri cyanide system. Different kinds of Electrode preparation and their cyclic voltammetry study in different systems.

Semester IV
(Physical Chemistry special)
(Optional paper)

Course ID- S4/**PHY/IV-T 1** **(Full marks: 100/8 Credits)**

Physical chemistry Special-I

120L

Unit-I : **Approximation Methods and their applications:**

Time independent and dependent Perturbation theory. First Order Perturbation, Second Order Perturbation. Application of perturbation theory to simple system. Atoms in External Magnetic Field. Normal Zeeman Effect and Anomalous Zeeman Effect . Degenerate Perturbation theory: The Stark Effect. Helium atom by Perturbation theory

The Variation Theorem. Proof of the Variation Theorem. Application of variation theorem to simple system. Helium atom by Variational Method. The WKB approximation. Application of WKB method to Bound States.

Unit –II: The Electron Spin Related Phenomena and Many Electron atoms:

Spin operators and Pauli spin matrices. Magnetic Moment and the Bohr Magneton. Spin Orbit Interaction. Relativistic Energy and Spin Orbit Coupling Effects. Spin orbital's in hydrogen atoms. Many Electron System: The slater Determinant. The Hartree-Fock Self- Consistent-Field method. Orbitals and periodic table. Electron Correlation.

Unit-III :Quantum mechanical treatment of diatomic molecule:

The Hartree Folk method for molecules, Roothans' equation

LCAO approximation, Hydrogen molecule ion, Hydrogen molecule, Improved valence bond calculation of hydrogen, the molecular orbital theory, molecular orbital calculation of hydrogen molecule, MO calculations using single configuration wave function, configuration interaction calculation.

Unit-IV: Huckel's Molecular Orbital Theory with application to polyatomic carbon molec

ules. Outlines of the Huckel molecular orbital theory. The Huckel approximations, The Huckel Parameters. The secular determinant. Linear chain molecule butadiene and closed ring benzene. Working formula for linear chain and closed molecules.

Unit-V: Abinitio and Density functional methods and semi empirical methods

Abinitio methods and Density functional theory. Basis functions. RHF, ROHF and UHF wave function Slater type orbital. Gaussian type function. Minimal Basis set. SCF MO treatment of methane, ethane and ethylene. Semiempirical MO treatments of Planar Conjugated Molecules, The Free Electron MO method., The Huckel MO Methods, Molecular mechanics methods. Molecular Docking

Unit-VI:
Computational Chemistry

The PPP Method and parameters. molecules. The ZDO approximation for integrals. CNDO, INDO, NDDO , MINDO, MNDO, AM1, MNDO, PM3, PM7 methods. Introduction software to like MOPAC, Gamess, Goussian, Autodock.

Unit-VII: **Advance electrochemistry-3**
Electrode kinetics:
Electrified interface, polarizable and nonpolarizable interfaces, Structure of electrified interfaces, Guoy-Chapman, Stern etc. models; Electrical double layer theory, overpotential, exchange current density, Butler-volmer equation, Tafel plot. Multistep reactions –relation between current density and overpotential, concept of rate determining step, reaction order
Quantum aspect of charge transfer at the electrode – solution interfaces, Electrocapillarity (EC), nature of EC curves, Lipmann equation,. Electrochemistry at semiconductor interfaces. Fundamentals of simple ionic liquids.
Electrocatalyst:
Electrocatalysis-comparison of electrocatalytic activity, Fuel cell: Uses of fuel cell, cell reactions in a fuel cell, choice of fuels fuel, cell efficiency, cell performance, Different kind of fuel cells- merits and demerits. Alcohol fuel cell and different anode materials (emphasis on nano materials)
Oxygen reduction reaction and different electrocatalysts.
Corrosion:
Causes, electrochemical theories of corrosion, kinetics of corrosion(corrosion current and corrosion potential) corrosion measurements, passivity, corrosion prevention. Photoelectochemistry.
Electrochemical techniques:
Polarography, Cyclic voltammetry: Instrumentation, principle, interpretation of cyclic voltammograms and parameters obtainable from voltammagram. Principle and applications of amperometry, coulometry, electrogavimetry.
Unit VIII: **Chemical Kinetics:**
Kinetics and matrix representation, theories of unimolecular reactions: Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK) and Rice-Ramsperger- Kassel-Marcus (RRKM) theories. Homogeneous catalysis, acid-base catalysis.
Autocatalysis, chain reactions: branched and non-branched kinetic rate equations, Semenov treatment for branched chain reactions; explosion: population explosion, upper and lower ignition/explosion limits; thermal ignition and ignition temperature; chemical oscillation: some models (Lotka, Oregonater and Brusselator); analysis of Lotka and Brusselator model, conditions for oscillation, chemistry of BZ reaction (Brusselator

model

Unit-VIII: Macromolecules:

Fundamentals of polymer, electrically conducting, Electrochemical sysnthesis of polymers (polyaniline), kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, different molecular mass determination methods, chain configuration of macromolecules, and calculation of average dimensions of various chain structures, Electrochemical sysnthesis of polymers (polyaniline).

Course ID- S4/PHY/IV-T2 **(Full marks: 100/8 Credits)**

(Optional paper)

Physical chemistry Special-II

120L

Unit-I: **Equilibrium statistical mechanics:**

Partition Function and ideal monoatomic gas, diatomic gas, polyatomic gas.

Quantum statistics. Failure of classical statistics, Fermi Dirac and Bose Einstein Statistics, Fermi energy, Plancks formula for blackbody radiation from Bose Einstein statistics. Bose-Einstein statistics and consequences. Super fluidity and super conductivity. Bose Condensation.

Unit-II Non-equilibrium Statistical Mechanics:

Random processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker- Planck equation

Unit- III Group theory and Spectroscopy:

Symmetry adapted linear combination, projection operator. Symmetry aspect of molecular orbital theory, symmetry of hybrid orbitals.

Symmetry aspects of molecular vibrations – infrared and Raman activity Normal modes of vibration, G and F matrices, internal and symmetry coordinates. Raman spectroscopy, polarizability and selection rules for rotation and vibrational Raman spectra.

Unit-IV Biophysical Chemistry :

Structure of Protein, nucleic acid, carbohydrate, lipid domain structure of protein. Inter and intra molecular forces, non covalent interactions. Thermodynamics of protein

folding. Enzyme kinetics, protein DNA interactions. Spectra of protein and nucleic acids. Protein structure prediction.

Biochemical application of thermodynamics, membranes and transport, equilibrium dialysis, donan effect and Donan potential. Active and passive transport. Biological redox reactions. Ion channels, Voltage gates.

Binding of small molecule by polymers. Identical and independent site model. Nearest neighbor interaction. Cooperative, anti cooperative and extended site binding. Protein ligand interaction.

Protein structure prediction, Ramachandran plot. Binding site of protein, protein drug interaction, drug design, molecular mechanics and molecular modelling. Molecular dynamics simulation, Monte carlo simulation & Molecular docking etc.

Unit-V: Irreversible Thermodynamics

Thermodynamic criteria for Non-equilibrium states. Entropy production and Entropy balance equations. Generalized flux and forces. Stationary states. Phenomenological equations. Microscopic reversibility and Onsager equation. Applications in physico-chemical and biological phenomena. Coupled reactions.

Unit- VI: Atomic spectra:

Vector representation of momenta and vector coupling approximation, normal and anomalous Zeeman effect, Paschenback effect.Stern-Gerlach experiment, angular momenta, magnetic moments, coupling of angular momenta, R-S coupling, term symbol, Non-equivalent electrons, equivalent electrons, spectra of alkali metal atoms, Helium, alkaline earth metal atoms and other polyelectronic atoms.

Unit-VII: Spectroscopy and photochemistry:

Interaction of electromagnetic radiation with matter, time dependent perturbation theory, Violation of Franck Condon principle, oscillator strength. Nature of transitions (e.g., *n*–*π**, *π*–*π**, d–d, charge transfer transition) solvent effect on absorption and emission spectra, Stoke's shift. Electronic spectra of polyatomic molecules. $n \rightarrow \pi^*$, $\pi \rightarrow \pi^*$, CT transition ,

Electron Spin Resonance (ESR) Spectroscopy**.**Mossbauer spectroscopy: Principle of Mossbauer Spectroscopy, instrumentation,spectal parameters and spectrum display, Chemical Shift, Quadruple effect,effect of Magnetic Field, Application of Mossbauer Spectroscopy-elucidation of structure and bonding of Fe(III) and Fe(II).Photoelectron spectroscopy, Auger spectroscopy: Principle and application.

Properties of electronically excited molecules-life time, redox potential, dipole moment, pK values (Forster-Weller thermodynamic scheme), photophysical kinetics, Delayed fluorescence, quantum yield, mirror image rule, flurescence anisotropy,Mechanism and decay kinetics of photophysical processes. Fluorescence quenching-collisional quenching

Stern -Volmer equation, static and dynamic quenching, solvent effect, Lippert-Mataga equation.

NMR:

Multiplets in NMR spectra-spin-spin interaction treatment by perturbation theory, spin-spin coupling between chemically equivalent protons.

Unit VIII: **Laser:**

Spontaneous and stimulated emission, Einsteins coefficients, creration of population inversion, two and three level system, characteristics of LASER beam,Inside of a LASER,solid state lasers, applications of LASERs.

Unit-IX: Nanochemistry and liquid crystal:

Nanomaterials, effect of nano dimensions on materials behaviour,Synthesis routes: Bottom-up approach, top-down approach;Nanomaterials characterization: XRD, SEM, TEM,AFM, STM etc and EDAX; Application of nanomateials. Fundamentals of liquid crystals.

Unit-X Surfactant chemistry:

Different kinds of surfactant, micelles reverse micelles, Thermodynamics of micellization, Revision of adsorption and transport properties.

Unit-VII X-ray diffraction and Solid State:

Bragg-Miller indices, X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Defects in solids: point, line and plane defects, Determination of equilibrium concentration of Scottky and Frenkel defects, F-centres/color-centres in ionic crystals, Band theory of solids, Semiconductors (extrinsic and intrinsic), hopping semi-conductors, rectifiers, transitors, Super conductivity, Oraganic conducting solids, solid state reactions.

<u>Course – ID</u> – S4/PHY/IV-Project (Full marks: 150/12 Credits)

Project Work/Review Work

Project work/Review work as given by guide teacher.

N.B: Teacher may teach any other relevant topic(s) which is (are) not mentioned in the Physical chemistry syllabus.

IDC-I:

Physical Organic Chemistry

Marks: 100 **Credit: 8** **120hrs**

Unit-I: Thermodynamics **[24 hours]**

Classical thermodynamics and Statistical basis of thermodynamics. Probability, thermodynamic probability. Boltzmann distribution Law. Partition Function. Thermodynamic functions from partion function. Thermodynamics of biological system and Biological redox reactions. Ion channels, Voltage gates.

Unit-II:Chemical kinetics **[20 hours]**

Order, determination of rate constant, collision theory, Lindemann theory, fast reactions, application to bio systems.

Unit-III: Symmetry and Group Theory-I **[20 hours]**

Introduction to symmetry. Symmetry elements and Symmetry operations. Definition of a Group. Point symmetry groups.

Unit –II Quantum theory and elementary quantum mechanics, Operators, particle in a box and its application, tunnelling, mutation of DNA, emission of alpha particle. Computational chemistry and molecular modelling.

Unit-IV: Electrochemistry **[20 hours]**

Conductance, hydrogen and hydroxyl ion conductance, Ion Solvent interactions, quantitative treatment of ion solvent interaction, Born model, Ion-Ion interaction, Ionic atmosphere, Debye-Huckel theory, asymmetry and elctrophoretic effect, applications in biological systems.

Energy storage devices: Lithium ion battery, cathode and anode materials, electrolyte, mechanism.

Unit- V: **Spectroscopy** **[36 hours]**

Principles, Transition probability, transition moment, selection rules, intensity of spectral lines, width of spectral lines and its various causes.

Rotational spectra**:** diatomic molecules as rigid rotors – energy levels, selection rules and spectral features, isotope effect, intensity distribution.

vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands.

IR Spectra: Modes of molecular vibrations, application of Hooke's law, characteristic stretching frequencies of O-H, N-H, C-H, C-D, C=C, C=N, C=O functions; factors

effecting stretching frequencies (H-bonding, mass effect, electronic factors, bond multiplicity, ring size).

UV Spectra: Electronic transition (σ-σ*, n-σ*, π-π* and n-π*), Selection rules for electronic transition, Lambert's Beer's Law, Determination of λ_{max} by Woodward-Fieser rule for conjugative dienes, polyenes and α,β-unsaturated compounds, relative positions of λ_{max} considering conjugative effect, steric effect, solvent effect, red shift (bathochromic shift), blue shift (hypsochromic shift), hyperchromic effect, hypochromic effect (typical examples), photosensitizers and its role in photochemical reactions, charge transfer spectra.

IDC-II

Bioinorganic, Supramolecular and Medicinal Chemistry

Marks: 100 Credit: 8

Group A

Bioinorganic and Supramolecular Chemistry F.M:50 60hrs

I Metal Storage Transport and Biomineralization **5 Hrs**

Ferritin, transferrin, and siderophores

II Calcium in Biology **6 Hrs**

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins

III Metalloenzymes **20 Hrs**

Zinc enzymes – carboxypeptidase and carbonic anhydrase. Iron enzymes – catalase, peroxidase and cytochrome P-450. Copper enzymes – superoxide dismutase. Molybdenum oxatransferase enzymes – xanthine oxidase. Coenzyme vitamin B_{12}

IV Metal–Nucleic Acid Interactions **8 Hrs**

Metal ions and metal complex interactions. Metal complexes - nucleic acids

V Metals In Medicine **5 Hrs**

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

VI Supramolecular Chemistry **18 Hrs**

Concepts and language.

(A) Molecular recognition : Molecular receptors for different types of molecules including anionic substrates, design and synthesis of coreceptor molecules and multiple recognition.

(B) Supramolecular reactivity and catalysis.

(C) Transport processes and carrier design.

(D) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Some example of self-assembly in supramolecular chemistry

Group B

Medicinal Chemistry F.M:50 60Hrs

I Drug Design 15 Hrs

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

II Pharmacokinetics 5 Hrs

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

III Pharmacodynamics 5 Hrs

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

IV Antineoplastic Agents 5 Hrs

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.

Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

V Cardiovascular Drugs 5 Hrs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators.

Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

VI Local Antiinfective Drugs **10 Hrs**

Introduction and general mode of action.

Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin.

VII Psychoactive Drugs- The Chemotherapy of Mind **7 Hrs**

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs.

Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximde, trimethadione, barbiturates, thiopental sodium, glutethimide

VIII Antibiotics **8 Hrs**

Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

Semester-IV

Environmental chemistry Course ID- S4/Comp/Envs/T

(Compulsory paper)

Full Marks: 50 **Credit point: 4** **60 L**

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.

II Hydrosphere

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

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

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.

III Soils

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

IV 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, chlorofluorohydrocarbons.

Green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments.

V 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.

VI Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Bhopal gas tragedy, Chernobyl, Three mile island, Sewozo and Minamata disasters.

VII Green Chemistry: The 12 principles of green chemistry.

VIII Pollution Regulation status in West Bengal: List of industries under different (red, orange, green) categories.

Books Suggested

Environmental Chemistry, S. E. Manahan, Lewis Publishers.

Environmental Chemistry, Sharma & Kaur, Krishna Publishers.

Environmental Chemistry, A. K. De, Wiley Eastern.

Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern

Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.

Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.

Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.

Environmental Chemistry, C. Baird, W. H. Freeman.