Corrected Syllabus for M. Sc (Regular) in Chemistry
(Under Choice Based Credit System)

SUMMARY			
Serial Number	Semester	Total Marks	Total Credits
1	1st Semester	400	32
2	2nd Semester	400	32
3	3rd Semester	400	32
4	4th Semester	400	32
Total		**1600**	**128**

1ST SEMESTER

COURSE CODES		Details of Courses	Marks For Theoretical papers: Class Tests plus End Semester Exam.	Credit
Theoretical	CHEM-1101	Organic Chemistry	12 + 38 = 50	4
	CHEM-1102	Inorganic Chemistry	12 + 38 = 50	4
	CHEM-1103	Physical Chemistry	12 + 38 = 50	4
Practical	CHEM-1201	Organic Chemistry	50	4
	CHEM-1202	Inorganic Chemistry	50	4
	CHEM-1203	Physical Chemistry	50	4
Theoretical	¶CHEM-IDC-1	Physical Organic Chemistry	25 + 75 = 100	8
Total Marks &Total Credits			**400**	**32**

¶ IDC = Inter Disciplinary Course

2ND SEMESTER

COURSE CODES		Details of Courses	Marks For Theoretical papers: Class Tests plus End Semester Exam.	Credit
Theoretical	CHEM-2101	Organic Chemistry	12 + 38 = 50	4
	CHEM-2102	Inorganic Chemistry	12 + 38 = 50	4
	CHEM-2103	Physical Chemistry	12 + 38 = 50	4
Practical	CHEM-2201	Organic Chemistry	50	4
	CHEM-2202	Inorganic Chemistry	50	4
	CHEM-2203	Physical Chemistry	50	4
	CHEM-IDC-2	Bioorganic, Supramolecular and Medicinal Chemistry	25 + 75 = 100	8
Total Marks & Total Credits			**400**	**32**

3RD SEMESTER

COURSE CODES		Details of Courses	Marks For Theoretical papers: Class Test plus End Semester Exam.	Credit
Theoretical	CHEM-3101	Organic Chemistry	12 + 38 = 50	4
	CHEM-3102	Inorganic Chemistry	12 + 38 = 50	4
	CHEM-3103	Physical Chemistry	12 + 38 = 50	4
Practical	CHEM-3201	Organic Chemistry	50	4
	CHEM-3202	Inorganic Chemistry	50	4
	CHEM-3203	Physical Chemistry	50	4
Group Discussion & Viva-voce	CHEM-3304	Advanced General Chemistry	50	4
Seminar	CHEM-3404	Advanced General Chemistry	50	4
Total Marks &Total Credits			**400**	**32**

4TH SEMESTER

COURSE CODES*		Details of Courses	Marks For Theoretical papers: Class Test plus End Semester Exam.	Credit
Theoretical	CHEM-4101	Organic Chemistry Special-I	25 + 75 = 100	8
	CHEM-4102	Organic Chemistry Special-II	25 + 75 = 100	8
	CHEM-4103	Inorganic Chemistry Special-I	25 + 75 = 100	8
	CHEM-4104	Inorganic Chemistry Special-II	25 + 75 = 100	8
	CHEM-4105	Physical Chemistry Special-I	25 + 75 = 100	8
	CHEM-4106	Physical Chemistry Special-II	25 + 75 = 100	8
	CHEM-4107	Environmental Science	50	4
Project	CHEM-4501	Organic Chemistry	150	12
	CHEM-4502	Inorganic Chemistry	150	12
	CHEM-4503	Physical Chemistry	150	12
Total Marks & Total Credits			**400**	**32**

*COURSE CODES	SPECIALIZATION
CHEM-4101, CHEM-4102 & CHEM-4501	FOR ORGANIC CHEMISTRY SPECIALIZATION
CHEM-4103, CHEM-4104 & CHEM-4502	FOR INORGANIC CHEMISTRY SPECIALIZATION
CHEM-4105, CHEM-4106	FOR PHYSICAL CHEMISTRY SPECIALIZATION

& CHEM-4503	
CHEM-4107	COMPULSORY PAPER

Organic Chemistry

Semester – I

Paper: **Organic Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-1101** (Full Marks: 50/4 Credits)

Unit-I: Structure Activity Relationship

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

Unit-II: Stereochemistry – I

Acyclic systems up to 4 chiral centers, compounds with asymmetric carbons in branched chains, symmetry, point groups, correlation of axial dissymmetry and centro-dissymmetry. 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, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

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

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

The E_1, E_2 and E1cB mechanisms and their spectrum, mechanism and orientation in pyrolytic *syn* elimination reaction.

Unit-IV: Pericyclic Reaction

Classification and stereochemical modes. Thermal and photo-pericyclic reactions, selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheleotropic reactions. Rationalization based on Frontier Molecular Orbital (FMO) approach, correlation diagram, Dewar-Zimmermann approach, Möbius and Hückel systems, Sommelet-Hauser, Cope, Aza Cope and Claisen rearrangements, Ene Reaction. Wittig

rearrangement, suitable examples of [(2π+2π), (4π +2π), (4π +4π), (2π +2π +2π)] and metal-catalyzed 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 of sesqui-, di- and tri-terpenoids.

Unit-VII: Aromatic Electrophilic and Nucleophilic substitution

Orientation & reactivity, the *ortho-para* ratio, *ipso* attack, Vilsmeier reaction, S_NAr1, S_NAr2. Benzyne mechanism, reactivity-effect of substrate, structure, leaving group and attacking nucleophile. Von Richter and Smiles rearrangements.

Course ID: **CHEM-1201** (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 (UV, IR, NMR etc.).

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

Semester – II

Paper: **Organic Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-2101** (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 functionalization in organic molecules involving Barton reaction, *Cis-trans* isomeriation, stereo mutation, Paterno-Büchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-π-methane rearrangement, photochemistry of arenes, photoreaction in solid state. Method of generation and detection (ESR, CIDNP etc.) of radicals, radical initiators, reactivity pattern of

radicals, substitution and addition reactions involving radicals, cyclization of radicals, allylic halogenations and auto-oxidation.

Unit-II: Synthetic Strategy

Retrosynthetic analysis, disconnection approach, typical examples to illustrate the disconnection approach, functional group interconversion, umpolung (1,3-dithiane), convergent synthesis, C-C bond formation reactions ylide method, silicon 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 etc.

Unit-III: Synthetic Methodology

Chemistry of organoboron compounds, carboranes, hydroboration reaction, reactions of organoboranes, unsaturated hydrocarbon synthesis, allylboranes, boron enolates.

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig, Stobbe condensation, hydrolysis of esters and amides, ammonolysis 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 dissymmetry and centro-dissymmetry, nomenclature of compounds involving axial and planar chirality, dynamic stereochemistry.

Unit-VI: Reaction Kinetics & Mechanism

Labelling and Kinetic isotope effects, (Hammett, Hansch, Taft equation, Sigma-Rho relationship, Marcus Theory, Baldwin's ring closure rule, Hammett scale, Hammond's postulates, law of microscopic reversibility.

Unit-VII: Natural Products – II

Familiarity with methods of structure elucidation (chemical & spectroscopic methods), biosynthesis, synthesis and biological activity of the alkaloids: Nicotine, Atropine, Coniine and Papavarine etc.

Course ID: **CHEM-2201** (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

Paper: **Organic Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-3101** (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 uinactivated), alcohols, diols, aldehydes ketones, ketals and carboxylic 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, nitro, nitroso, azo and oxime groups, hydrogenolysis etc.

Unit-IV: Rearrangements / selective organic name 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 mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction: Mizoroki–Heck, Suzuki–Miyaura, Stille, Hiyama, Negishi, Castro-Stephens, Corriu-Kumada, Fukuyama, Sonogashia, Buchwald-Hartwig couplings, Ziegler Natta catalysis, Walker Process, Alkene metathesis reactions, Tebbe's reagent, Pauson-Khand reaction, Vollhardt co-trimerization, C–H activation, Cross dehydrogenative coupling (CDC), Tsuji-Trost reactions,

Organosilicon chemistry, functional organometallic compounds, asymmetric hydrogenations, π-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-dithiane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Lawesson's reagent, Wilkinson's catalyst, Baker Yeast, hypervalent organoiodine (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

Course ID: **CHEM-3201** (Full Marks: 50/4 Credits)

Practical

Extraction of natural products & their purification (thin layer and column chromatography) and partial characterization by UV, IR and NMR techniques.

Separation and identification of the components of a binary mixture of organic solids, chromatographic separation, purification and identification of individual components (use of UV, IR, NMR), derivatization of individual component and analytical establishment of their identity.

Semester – IV

Paper: **Organic Chemistry Special-I** **120L**

(Optional Paper)

Course ID: **CHEM-4101** (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 rule, sector rule, helicity rule.

Unit-II: Advanced Heterocyclic Chemistry – II

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

Unit-III: Medicinal Chemistry

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

Group B **4 Credits**

Unit-IV: Supramolecular Chemistry

Metallocenes, non-benzenoid aromatics and polycyclic aromatic compounds, bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Unit-V: Hemoglobin, chlorophyll and phthalocyanines

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

Unit-VI: **Steroids**

Occurrence, nomenclature, basic skeleton and stereochemistry, synthetic principles and chemical reactions.

Semester – IV

Paper: **Organic Chemistry Special-II** **120L**

(Optional Paper)

Course ID: **CHEM-4102** (Full Marks: 100/8 Credits)

Group A **4 Credits**

Unit-I: Spectroscopy – IV

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

Unit-II: Bio-Organic Chemistry

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

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions 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, 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, auteolin, querecetin, myrcene, quercetin-3-glucoside, vitexin, diadzein, butein, aureusin, cyanidine-7-arabinoside, cyanidin, hirsutidin etc. Biosynthesis of flavonoids: acetate pathway and shikimic acid pathway.

Unit-VI: Green Chemistry

Green Chemistry – Introduction and overview, Principles of Green Chemistry, atom economy, Catalysis: Homogeneous and heterogeneous catalysts, photocatalysts, biocatalysts, Green synthetic methods with examples of industrial applications, organic synthesis in aqueous media, on-water and in-water reactions, room temperature reactions, uses of ionic liquids, supercritical fluids and applications of microwave, flow reactor, ball milling apparatus. Solvent-free organic reactions, Merrifield resins and 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.

Course – ID**: CHEM-4501** (Full Marks: 150/12 Credits)

Project work/Review work

Project work/review work is to be carried out under the supervision and guidance of a teacher.

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Inorganic Chemistry

Semester-I

Paper: **Inorganic Chemistry** **60L**

(Core paper)

Course ID**: CHEM-1102** (Full Marks: 50/4 Credits)

Unit-I: 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.

Unit-II: Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds.

Unit-III: 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-Eigene equation, linear free energy relation (LFER) etc., conjugate base formation, anation reaction and base hydrolysis, reactions without metal-ligand cleavage.

Unit-IV: Magnetic Properties and Spectra-I

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

Paper: **Inorganic Chemistry**

Practical

Course ID: **1202** (Full Marks: 50/4 Credits)

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

Semester-II

Paper: **Inorganic Chemistry** **60L**

(Core paper)

Course ID: **CHEM-2102** (Full Marks: 50/4 Credits)

Unit-I: Organometallic Compounds of Main Group Elements-II

Synthesis, properties and structures of organometallic compounds of group-IV & V elements of the periodic table.

Unit-II: 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.

Unit-III: Isopoly and Heteropoly Acids and Their Salts.

Unit-IV: 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).

Unit-V: Molecular Term Symbol.

Course ID: **CHEM-2202** (Full Marks: 50/4 Credits)

Practical

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

Semester-III

Paper: **Inorganic Chemistry** **60L**

(Core paper)

Course ID: **CHEM-3102** (Full Marks: 50/4 Credits)

Unit-I: Molecular Symmetry and Group Theory

Applications: SALC & MO's, formation of hybrid orbitals, irreducible representations of vibrational motions, predicting probability of a spectral transition, correlation diagrams for a d^2 ion in an octahedral and tetrahedral environments.

Unit-II: Application of Spectroscopy in Inorganic Chemistry-I

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

Unit-III: 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. Hückel MO treatment for simple and conjugated polyenes such as molecule such as ethylene, butadiene, benzene etc.

Unit-I: 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. Organometallic catalysts.
f. Fluxional organometallic compounds

Course ID: **CHEM-3202** (Full Marks: 50/4 Credits)

Practical

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.

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 hexachlorostannate, ammonium hexachloroplumbate.
7. Hexa-bis (4-nitropheoxy) cyclotriphosphazene.
8. Synthesis of trichloro diphenyl antimony (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 (III) chloride.
20. Reaction of Cr (III) with a multi-dentate 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-xylene to terephthalic acid catalyzed by $CoBr_2$ (Homogeneous catalysis).
26. Preparation of tetraphenyltin.
27. Preparation of lithiated reagents.

Semester-IV

Paper: Inorganic Chemistry Special-I **120L**

(Optional paper)

Course ID: **CHEM-4103** (Full Marks: 100/8 Credits)

Group: A 4 Credit

Unit-I: 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-sulfur proteins, cytochromes. Photosynthesis: PS-I & PS-II, nitrogenase, metal ion storage and transport, metalloenzymes, Na^+/K^+ pumps, metal-nucleic interactions.

Unit-II: Chemistry of non-transitional elements
Compounds with B–N, P–N and S–N bonds.

Unit-III: Solid state chemistry
Electronic properties and band theory. Solid state reactions, general principles, crystal defects and non-stoichiometry, colour centre, photographic process, phosphors.

Unit-IV: Crystal morphology
Important minerals and different types of silicates, structural and physical properties.

Group: B **4 Credit**

Unit-V: Chemistry of Materials
Glasses, ceramics, composites, liquid crystals, ionic conductors, molecular devices, thin films, semi conductor and super conductor.

Unit-VI: Nanomaterials
General introduction to nanomaterials, nanowires, nanotubes and nanorods, techniques of synthesis, characterization of nanomaterials, applications of nanoparticles.

Unit-VII: 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

Semester-IV

Paper: **Inorganic Chemistry Special-II** **120L**

(Optional paper)

Course ID: **CHEM-4104** (Full Marks: 100/8 Credits)

Group: A **4 Credit**

Unit-I: 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-atomic emission spectroscopy
e) Transmission electron microscopy (TEM), scanning electron microscopy (SEM), scanning & transmission electron microscopy (STEM), atomic force microscopy (AFM)
f) Photoacoustic spectroscopy.

Unit-II: Application of Spectroscopy in Inorganic Chemistry-II

Nuclear Magnetic Resonance (NMR) Spectroscopy and its applications to inorganic compounds, Optical Rotatory Dispersion and Circular Dichroism (ORD/CD) for inorganic compounds & XPS or ESCA (electron spectroscopy for chemical analysis).

Unit-III: X–ray diffraction, Electron diffraction and Neutron diffraction: Application of scattering experiments to determine the atomic and/or magnetic structure of a material with interpretations.

Unit-IV: 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 **4 Credit**

Unit-V: Chemistry of Actinides: Introduction, spectral properties of actinide complexes, f-f transitions, f-d transitions and their sensitivity to ligand environment.

Unit-VI: Chemistry of missing elements: History, background and chemical properties.

Unit-VII: 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, cyclophanes as synthetic receptors, catenanes and rotaxanes, dendrimer, molecular switch.

Unit-VIII: 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.

Course ID: **CHEM-4502** (Full Marks: 150/12 Credits)

Project/Review work

Project work/review work is to be carried out under the supervision and guidance of a teacher.

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Physical Chemistry

Semester – I

Paper: **Physical Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-1103** (Full Marks: 50/4 Credits)

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, Schrödinger 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 Eigen value 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 Schrödinger 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 interactions and its calculation, structural treatment of ion-solvent interactions, ion-dipole and ion-quadruple model of ion-solvent interactions, dielectric constant of solution.

Ion-ion interaction

Ion-ion interaction, ionic atmosphere, Debye-Hückel theory (detail calculation), asymmetry and electrophoretic effect, Debye-Hückel-Onsagar conductance equation, activity coefficient of electrolytes, extended Debye-Hückel 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 of Li-ion battery.

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: **CHEM-1203** (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 partially miscible system.
9. Determination of molecular property of a molecule by semi-empirical method.

Semester – II

Paper: **Physical Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-2103** (Full marks: 50/4 Credits)

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: Quantum Mechanical Formalisms

Operator algebra and operator related theorem, Hermitian 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 and 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: 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 precession, 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, FT-NMR (Fourier Transform NMR) qualitative idea and its advantages.

Unit VII: Photochemistry

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

Course ID: **CHEM-2203**

(Full marks: 50/4 Credits)

Practical

1. Studies on alkalis hydrolysis of ethyl acetate conductometrically.
2. Determination of pK_1 and pK_2 of phosphoric acid pH metrically.
3. Verification of Debye-Hückel-Onsager equation.
4. Kinetics study of the reaction between $K_2S_2O_8$ and KI by spectrophotometric 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/QH_2 electrode.
7. Kinetics of oxidation of alcohol by potassium dichromate-spectrophotometry.
8. Evaluation of HOMO, LUMO and dipole moment of a molecule by quantum chemical (DFT, semiempirical) methods 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 and Linear Sweep Voltammetry (CV & LSV) etc.

Semester – III

Paper: **Physical Chemistry** **60L**

(Core Paper)

Course ID: **CHEM-3103** (Full marks: 50/4 Credits)

Unit-I: Classical Thermodynamics

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, μ-space and γ-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 wave function, relation among principal, azimuthal and magnetic quantum number, nodal properties of angular part as well as the radial part of the hydrogen atom wave function, shape of the orbitals, space quantization, selection rules for hydrogen atom.

Unit- IV: Approximate Methods in Quantum Chemistry

Basic concept of variation and perturbation methods and application to simple systems, introduction to computational chemistry.

Unit-V: Advance Electrochemistry-1

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 Reactions: luminescence and energy transfer processes, study of kinetics by stopped–flow and relaxation methods, flash photolysis and magnetic resonance method.

Course ID: **CHEM-3203** (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.
3. Determination of the activation energy of the reaction between $KBrO_3$ and KBr of the ester hydrolysis reaction.
4. 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.
5. Conductometric titration of sodium sulphate by barium chloride.
6. 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.
7. Effect of ionic strength on the rate of persulphate iodide reaction.
8. Determination of activity solubility product of calcium sulphate by complexometric titration.
9. Evaluation of quantum chemical property of a molecule and spectra by ab initio method using software Gaussian and GaussView.
10. 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

Paper: **Physical chemistry Special-I** **120L**

(Optional paper)

Course ID: **CHEM-4105** (Full marks: 100/8 Credits)

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 systems, 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 systems, helium atom by variational method, the Wentzel–Kramers–Brillouin (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 orbitals in hydrogen atoms. Many electron systems: 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-Fock method for molecules, Roothaan's 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 (molecular orbital) calculations using single configuration wave function, configuration interaction calculation.

Unit-IV: **Molecular Orbital Theory**

Hückel's molecular orbital theory with application to polyatomic carbonaceous molecules, outlines of the Hückel molecular orbital theory, the Hückel approximations, the Hückel parameters, the secular determinant, linear chain molecule butadiene and closed ring benzene, working formula for linear chain and closed molecules.

Unit-V: *Ab initio* and Density Functional Methods and Semi Empirical Methods

Ab initio methods and density functional theory, Basis functions, RHF, ROHF and UHF wave functions, Slater type orbitals, Gaussian type functions, minimal basis set, self-consistent field (SCF) MO treatment of methane, ethane and ethylene, semiempirical MO treatments of planar conjugated molecules, the free electron MO method, The Hückel MO method, molecular mechanics methods, molecular docking.

Unit-VI: Computational Chemistry

The Pariser-Parr-Pople (PPP) method and parameters, the zero differential overlap (ZDO) approximation for integrals, CNDO, INDO, NDDO , MINDO, MNDO, AM1, MNDO, PM3, PM7 methods; introduction to software like MOPAC, Gamess, Gaussian, Autodock etc.

Unit-VII: **Advance electrochemistry-2**

Electrode kinetics

Electrified interface, polarizable and nonpolarizable interfaces, structure of electrified interfaces, Guoy-Chapman, Stern etc. models, electrical double layer theory, over potential, exchange current density, Butler-Volmer equation, Tafel plot, multistep reactions, relation between current density and over potential, 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.

Electrocatalysts

Electrocatalysis-comparison of electrocatalytic activity, fuel cell: Uses of fuel cell, cell reactions in a fuel cell, choice of fuels, cell efficiency, cell performance, different kind of fuel cells-merits and

demerits, alcohol fuel cell and different anode materials (emphasis on nanomaterials), 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, photo-electochemistry.

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 models, conditions for oscillation, chemistry of BZ reaction (Brusselator model).

Unit-IX: Macromolecules

Fundamentals of polymer, electrically conducting polymers, electrochemical synthesis 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 synthesis of polymers (polyaniline).

Semester-IV

Paper: **Physical Chemistry Special-II** **120L**

(Optional paper)

Course ID: **CHEM-4106** (Full marks: 100/8 Credits)

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, Planck's formula for blackbody radiation from Bose-Einstein statistics, Bose-Einstein statistics and consequences, superfluidity and superconductivity, Bose-Einstein 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 (SALC), 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, Donnan effect and Donnan 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 modeling, 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, Paschen-Back 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 poly-electronic 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.

Electron spin resonance (ESR) spectroscopy, Mossbauer spectroscopy: principle of Mossbauer spectroscopy, instrumentation, spectral 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 photo-physical processes, Fluorescence quenching, collisional quenching, Stern-Volmer equation, static and dynamic quenching, solvent effect, Lippert-Mataga equation.

General principles of nuclear magnetic resonance epectroscopy, multiplets in NMR spectra spin-spin interaction treatment by perturbation theory, spin-spin coupling between chemically equivalent protons.

Unit VIII: **Light Amplification by Stimulated Emission of Radiation** (**LASER**)

Spontaneous and stimulated emission, Einstein coefficients, creation 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 (X-ray diffraction), SEM (Scanning Electron Microscopy), TEM (Transmission Electron Microscopy), AFM (Atomic Force Microscopy), STM (Scanning Tunneling Microscopy), EDAX (Energy Dispersive Analysis of X-ray), application of nanomateials, fundamentals of liquid crystals.

Unit-X: Surfactant Chemistry

Different kinds of surfactants, micelles reverse micelles, thermodynamics of micellization, revision of adsorption and transport properties.

Unit-XI: 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 Schottky and Frenkel defects, F-centers/color-centers in ionic crystals, band theory of solids, semiconductors (extrinsic and intrinsic), hopping semi-conductors, rectifiers, transistors, superconductivity, organic conducting solids, solid state reactions.

Course ID: **CHEM-4503** (Full marks: 150/12 Credits)

Project/Review work

Project work/review work is to be carried out under the supervision and guidance of a teacher.

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Inter Disciplinary Courses (IDC)

In Semester - I

Paper: **Physical Organic Chemistry** **120L**

Course ID: **CHEM-IDC-I** (Full Marks: 100/8 Credits)

Unit-I: Thermodynamics

Classical thermodynamics and statistical basis of thermodynamics, Probability, Thermodynamic probability, Boltzmann distribution law, partition function, thermodynamic functions from partition function, thermodynamics of biological system and biological redox reactions, ion channels, voltage gates.

Unit-II: Chemical kinetics

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

Unit-III: Symmetry and Group Theory-I

Introduction to symmetry, symmetry elements and symmetry operations, definition of a group, point symmetry groups, quantum theory and elementary quantum mechanics, operators, particle in a box and its application, tunneling, emission of α–particle, computational chemistry and molecular modeling.

Unit-IV: Electrochemistry

Conductance, hydrogen and hydroxyl ion conductance, ion-solvent interactions, quantitative treatment of ion-solvent interaction, Born model, ion-ion interaction, ionic atmosphere, Debye-Hückel theory, asymmetry and elctrophoretic effect, applications in biological systems, energy storage devices: lithium ion battery, cathode and anode materials, electrolytes.

Unit-V: **Spectroscopy**

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 Spectroscopy: 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 Spectroscopy: 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.

In Semester - II

Paper: **Bioinorganic, Supra-molecular and Medicinal Chemistry** **120L**

Course ID: **CHEM-IDC-II** (Full Marks: 100/8 Credits)

Group A: Bioinorganic and Supra-molecular Chemistry

Unit-I: Metal Storage Transport and Biomineralization
Ferritin, transferrin and siderophores

Unit-II: Calcium in Biology
Calcium in living cells, transport and regulation, molecular aspects of intramolecular process, extracellular binding proteins.

Unit-III: Metalloenzymes
Zinc enzymes-carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzymes-superoxide dismutase. Molybdenum oxtransferase enzymes-xanthine oxidase. Coenzyme vitamin B_{12}.

Unit-IV: Metal-Nucleic Acid Interactions
Metal ion and metal complex interactions. Metal Complexes-nucleic acid.

Unit-V: Metals in Medicine
Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Unit-VI: Supramolecular Chemistry
Concepts and language

(A) Molecular recognition: Molecular receptors for different type of molecules including arisonic substrates, design and synthesis of co-receptors molecules and multiple recognition.
(B) Supramolecular reactivity and catalysis.
(C) Transport process and carrier design.
(D) Supramolecular devises. Supramolecular photochemistry, supramolecular electronic, ionic and switching devises.

Some example of self-assembly in supramolecular chemistry.

Group B: Medicinal Chemistry

Unit-I: Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compounds and lead modification, concepts of pro-drugs 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 constant, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relation between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

Unit-II: Pharmacokinetics
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.

Unit-III: Pharmacodynamics
Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

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

Unit-V: Cardiovascular Drugs
Introduction, cardiovascular diseases, drug inhibitors, of peripheral sympathetic function, center intervertion of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

Unit-VI: Local Antiinfective Drugs
Introduction and general mode of action, synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, griseofulvin, chloroquin and primaquin.

Unit-VII: Phychoactive Drugs: The chemotherapy of mind
Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental disesses. Antipsychotic drugs-the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, phenytoin, ethosuximde, trimethadione, barbiturates, thiopental sodium, glutethimide.

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

In Semester - IV

Paper: **Environmental Science** **60L**

(Compulsory paper)

Course ID: **CHEM-4107** (Full Marks: 50/4 Credits)

Unit-I: Environment

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

Unit-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 method for measuring BOD, DO, COD, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

Unit-III: Soils

Composition, micro and macro nutrients. Pollution: fertilizers, pesticides, plastics and metals, waste treatment.

Unit-IV: Atmosphere

Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reaction in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical method of measuring air pollutants. Continuous monitoring instruments.

Unit-V: Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear plants, metallurgy, polymers etc. Radionuclide analysis. Disposal of wastes and their managements.

Unit-VI: Environmental Toxicology

Chemicals 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: Introduction to Green Chemistry, Needs, goals and limitations in the pursuit of Green Chemistry in reference to environment, the twelve set of principles of Green Chemistry, Simple examples of Green Synthesis/ Reactions; catalysis, and future trends in green chemistry.

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

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