University of Gour Banga

(Established under West Bengal Act XXVI of 2007)

N.H.-34(Near Rabindra Bhawan), P.O.:Mokdumpur Dist.: Malda, West Bengal, Pin-732103

M.Sc. in Chemistry
Two Years (Four Semesters) Syllabus

Main Feature of the Syllabus

M.Sc. in Chemistry

Semester	*Theory*			*Practical*			*Internal Assessment*		*Total Marks*
	Paper Code	*Marks*	*Time*	*Paper*	*Marks*	*Time*	*Marks*	*Time*	
Semester I	PC-T/01 OC-T/02 IC-T/03	40 40 40	2.00 Hr 2.00 Hr 2.00 Hr	PC-P/01 OC-P/02	50 50	3.00 Hr 3.00 Hr 3.00 Hr	10 10 10	30.00 Min 30.00 Min 30.00 Min	**250**
Semester II	PC-T/04 OC-T/05 IC-T/06	40 40 40	2.00 Hr 2.00 Hr 2.00 Hr	OC-P/03 IC-P/04	50 50	3.00 Hr 3.00 Hr	10 10 10	30.00 Min 30.00 Min 30.00 Min	**250**
Semester III	PC-T/07 OC-T/08 IC-T/09	40 40 40	2.00 Hr 2.00 Hr 2.00 Hr	IC-P/05 PC-P/06	50 50	3.00 Hr 3.00 Hr	10 10 10	30.00 Min 30.00 Min 30.00 Min	**250**
Semester IV	PC-T/10 OC-T/11 IC-T/12	40 40 40	2.00 Hr 2.00 Hr 2.00 Hr	PC-Pro/07 or OC-Pro/07 or IC-Pro/07	100	6.00 Hr	10 10 10	30.00 Min 30.00 Min 30.00 Min	**250**
Grand Total		**480**			**400**		**120**		**1000**

N.B.: PC = Physical Chemistry; OC= Organic Chemistry; IC = Inorganic Chemistry; P = Practical; Pro = Project

Specialization will be designated as per Project Work

Detailed Syllabus

Semester I

Theory: ***Paper: PC-T/01***

Unit-I: Introduction to Quantum Mechanics

Wave-particle duality. Uncertainty principle. Postulates of Quantum Mechanics. Schrodinger wave equation and its solution. Wavefunction and its probabilistic interpretation. Orthogonality and normalization of wavefunctions. Operator and related theorems. Linear operators. Hermitian operators. Kinetic energy operator. Eigenvalue equation. Commutation relation. Operators and observables. Heisenberg uncertainty relation (derivation of general form). Heisenberg's equation of motion. Virial theorem.

Unit-II: Free particle and Particle-in-Box

Free Particle. Particle-in-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-III: 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. Symmetry Operators and their Matrix Representation. Reducible and irreducible representations. Equivalent representations. Characters of representations.

Unit-IV: Electrochemistry

Ion association, symmetric and asymmetric ion-pair formation, Bjerrum theory, The fraction of ion-pair, Triple ion formation, Determination of ion-association constant, Activity coefficient of electrolytes, Extended Debye-Huckel theory, Pitzer equation for activity coefficient, Experimental determination of mean ionic activity coefficient. Solvation of ions, Solvation number, Frank-Wien model of ionic solvation, Born model, Thermodynamics of ionic solvation, Enthalpy and free energy of solvation of ions, Experimental determination of solvation of ion.

Unit-V: Surface Chemistry and Biophysical Chemistry

Surface tension, curved surfaces, Young-Laplace and Kelvin equations. Adsorption on solids, micelles reverse micelles, microemulsion, Thermodynamics of micellization, Application of micelles and microemulsion. Hydrophobic hydration, micelle formation, hydrophobic interaction, stabilization and denaturation of protein. Water structure alternation theory of denaturation of protein, protein–lipid interaction, Transport of ions and small molecules through membranes. Ion channels.

Theory: ***Paper: OC-T/02***

Unit I : Structure Activity Relationship

MO treatment of acyclic and cyclic conjugated systems. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Graphical methods: Frost diagram. Huckel's rule and concept of

aromaticity, annulenes, heteroannulenes, fullerenes (C_{60}), alternate and non alternate hydrocarbons, anti aromaticity, pseudoaromaticity, homo-aromaticity.

Hammett equation and its modifications.

Unit II: Stereochemistry

Acyclic systems upto 4 chiral centers. Compounds with asymmetric carbons in branched chains, symmetry, point groups. Correlation of axial dissymmetry and centrodissymmetry. Nomenclature of compounds involving axial and planar chirality. Winstein-Holness equation. Curtin Hammett principle. Conformational analysis of cyclohexane, cyclohexene, decalins and their derivatives. Effect of conformation on reactivity in acyclic compounds and cyclohexanes. Cram's rule, Felkin modification.

Unit III: Pericyclic Reactions

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 +2Π+2Π)] and metal catalysed cycloaddition reactions

Unit-IV: NMR Spectroscopy

Principles, instrumentation and different techniques (CW and FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J); Jablonski diagram, spin-decoupling. First order and second order spectra, spin system notations.

Introduction to ^{13}C: proton decoupled ^{13}C spectra, NOE, cross polarization, peak integration, off resonance ^{13}C.

Unit V: Mass Spectroscopy Principles, instrumentation and applications of mass spectrometry – methods of generation of ions in EI, CI, FD and FAB, MALDI-TOF. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotope, ion-molecule interaction and analysis of fragmentation patterns. Calculation MF from mass.

Applications of Mass, UV-VIS, IR and NMR spectroscopy to structural and mechanistic problems.

Theory: *Paper: IC-T/03*

Unit-I: Coordination Chemistry

Experimental evidence of metal-ligand overlap, spin orbit coupling constant and interelectronic coupling parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect, adjusted CFT, hole formalism, Tetrahedral distortion and Jahn Teller effect, Static and Dynamic Jahn-Teller effect, Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of complexes (Irving Williams order). Colour and spectra, Kinetic aspects of crystal field stabilization. Crystal field activation energy, Limitations of CFT, Labile and inert complexes. ***Electronic spectra of transition metal complexes***: Microstates, Russell-sander's terms, determination of ground and excited state terms of d^n ions; Orgel diagrams (qualitative approach), selection rules for spectral transitions, *d-d* spectra of d^n ions and crystal field parameters, nephelauxetic series. MOT to rationalize σ and π interactions in octahedral, square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams.

Unit-II: Theories of bonding

Heitler – London theory of hydrogen molecule. Molecular Orbital theory. Salient features of valence bond theory (VBT) and molecular orbital theory (MOT). Bonding in homonuclear and heteronuclear diatomic molecules of 2nd period. Bonding in triatomic (H_3^+, BeH_2, H_2O), tetraatomic (BH_3, NH_3) and CH_4. MO diagrams, Walsh diagrams. Model of structure predictions: VSEPR and hybridization models, Bent's rule. Application to H2 molecule by Valance bond theory.

Unit-III: Metal – ligand equilibria in solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and template effect. Spectrophotometric and pH metric determination of binary formation constants.

Unit-IV: Organometallics I

Organotransition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification ligands, kinetic and thermodynamic stability of organometallic compounds. Compounds with metal carbon σ and multiple bond: Heptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Unit-V: Electrochemical analyses

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, current – voltage relationship during electrolysis. Principles and applications of Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry.

Practical: Paper: PC-P/01

1. Studies on the kinetics of iodination of acetone (iodine effect /acetone effect/acid effect).
2. To determine the formal potential of Fe^{III}/ Fe^{II} couple by potentiometry.
3. To determine the rate constant and salt effect on the rate constant of decomposition of $K_2S_2O_8$ by KI.
4. Studies on alkaline hydrolysis of ethyl acetate conductometrically.
5. To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry
6. To study the titration of H_3PO_4 by NaOH using potentiometry.
7. Estimation of strong and a weak acid in a given mixture by pH metrically.
8. To determine the pH of a given solution through matching its colour developed by an indicator.

Practical *Paper: OC-P/02*

Separation (chromatography, chemical method or any other methods) of components from a mixture of organic compounds followed by their characterization.

Semester II

Theory: *Paper: PC-T/04*

Unit-I: 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-II: Quantum Mechanics of Rotational Motion

Angular momentum operators and their commutation relations. Operator algebra and Ladder operators for 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-III: Hydrogen Atom

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: Solid State Chemistry

Crystalline and amorphous structures. Lattice vector and reciprocal lattice vector. Defects in the solid state. Band theory of solids. Band theory – Quantum mechanical aspect. Brillouin zone. Free electron gas theory of metal. Fermi energy. Electrical and thermal conductivity of metals. Semiconductor Hall effect and Hall co-efficient. Bloch's Theorem.

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.

Theory: *Paper: OC-T/05*

Unit I: Substitution and Elimination reactions.

Mechanism of aliphatic nucleophilic Substitution (S_N): Borderline Mechanism, Structural and solvent effect on reactivity, Neighboring Group Participation. Role of phase transfer catalyst. Aromatic and aliphatic electrophilic substitution.

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

Unit II: Organic reactive intermediates

Generation, stability and reactivity of carbocations, carbenes, benzynes and nitrenes. Sulfur and nitrogen Ylides.

Unit III: Common name reactions and rearrangements

Robinson annulation, Peterson elimination, Wittig reactions and various modifications, Sharpless asymmetric epoxidation and dihydroxylation, Barton reaction, Hofmann-Loffler-Freytag reaction, Shapiro reaction, Baeyer-Villiger reaction, Favorskii, Fragmantation reactions; Grob fragmentation, Von Richter and Smiles rearrangement, Mitsunibu Reaction, Yamaguchi and Mukayama esterifications, Ohira-bestmann reagents, Corey-Fuchs Reaction, Olefin metathesis, Nazarov cyclization, Transition metal catalyzed organic reactions involving pd, Ni, Cu, Rh, Ru etc.

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

Unit IV: **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 V: **Photochemistry**

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomeriation stereomutation 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, auto-oxidation.

Theory: *Paper: IC-T/06*

Unit-I: **Organometallics 2**

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkens and alkynes, Zieglar- Natta catalysis, photo dehydrogenation catalyst (platinum POP).

Unit-II: Magneto Chemistry

Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, Russell-sander's terms, determination of magnetic susceptibility, application of Van Vleck susceptibility equation, Magnetic properties and coordination compounds Spin and orbital moments, spin – orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments and spin crossover. Magnetic properties of first transition series metal ions, lanthanides and actinides, Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples). magnetic exchange interactions. Basic concept of Single Molecule Magnets (SMM), properties and examples of SMMs.

Unit-III: Material Chemistry

Theory of crystalline solids, free electron model and its limitations, Kronig Penny model, Band theory, band gap, metals, Insulators, Semiconductors, P-N junction semi-conductors (intrinsic and extrinsic) materials, Superconductors, rectifiers and transistors, point defects – Schottky and Frenkel defects. History of Nanoscience, Nano-world definitions, Properties of Nanomaterials, Typical synthetic strategies for nanomaterials, Modern characterization and Applications of nanomaterials in different areas.

Unit IV: Chemistry of Elements:

d-Block Elements: Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr- Hf , V-Nb-Ta, Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of V, Mo, W, Re, Pt. Iso-and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, metal-metal bonded dinuclear d-metal complexes (examples), Bonding in dirhenium complexes.

Unit V: Bioinorganic Chemistry 1

Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes. Chelato theraphy. Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (ferredoxines). Respiratory electron transport chain, cytochrome c oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems, model study.

Practical: *Paper: OC-P/03*

Single stage and or multistep organic preparation, Quantitative estimation of phenol, carbohydrates, anilines and others organic materials.

Practical: *Paper: IC-P/04*

Group-A

Synthesis of some metal complexes:

- bis(ethylene)nickel(II)thiosulphate,
- tris(acetylacetonato)manganese(III),tris(acetylacetonato)Aluminium(III), tris(acetylacetonato)iron(II), tris(acetylacetonato)copper(II),
- Hexaminecobalt(III)chloride,
- Mercury tetrathiocyanatocobaltate(II),
- Reineki salt,
- Copper(II) biguanide
- Mn_{12} Acetate Single Molecule Magnet
- Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
- Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), Mn(salen), determination of O_2 absorption by Co(salen), reaction of oxygen adduct with $CHCl_3$ (deoxygenation).

Group-B

Semi-Micro Qualitative Inorganic Analysis:

Semi-Micro Qualitative Inorganic Analysis of complex inorganic mixtures containing not more than six (6) inorganic radicals from the lists ***(a), (b), (c),*** and ***(d),***of which two (2) radicals must be derived from the rare elements ***(d)***, and the mixture should not contain more than one insoluble material from the lists ***(c),*** and ***(d),*** :

(a) Cation Radicals derived from:

Ag, Hg, Pb, Bi, Cd, Cu, As, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Zn, Ba, Sr, Ca,

Mg, Na, K and NH_4^+ ion.

(b) Anion Radicals:

F^-, Cl^-, Br^-, I^-, BrO_3^- , IO_3^-, SCN^-, S^{2-}, $S_2O_3^{2-}$,SO_3^{2-}, SO_4^{2-}, NO_2^-, NO_3^-, PO_4^{3-},

AsO_3^{3-}, AsO_4^{3-}, BO_3^{3-}, H_3BO_3, SiO^{2-},CrO_4^{2-}, $Cr_2O_7^{2-}$, $[Fe(CN)_6^{4-}]$, $[Fe(CN)_6^{3-}]$.

(c) Insoluble Materials:

$PbSO_4$, $BaSO_4$, $SrSO_4$, $PbCrO_4$, CaF_2, SiO_2 and various silicates, SnO_2,

Al_2O_3, Fe_2O_3, Cr_2O_3, AgCl, AgBr, AgI.

(d) Cation radicals, anion radicals and insoluble materials derived from the following rare Elements: V, Mo, W, U, Ti, Zr, Ce, Th and Be.

Semester III

Theory: *Paper: PC-T/07*

Unit-I: Approximate Methods and their Applications

Variation theorem, Linear variation method, Applicability of variation method to excited states. Time-independent perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and their applications, Eckert's Theorem. Hydrogen and Helium atoms. Hellman-Feynman and Virial Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum, Radiation-matter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

Unit-II: Spin and Many Electron Wavefunctions

Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, Eigenvalues and eigenfunctions of spin operators. Non-relativistic wavefunction for Hydrogen atom. Many-electron wavefunctions- examples with 2 and 3 electron systems, Slater determinants. Projection Operators. Parity Operator and Pauli Principle, The Pauli exclusion principle. Introduction of core, Coulomb, and exchange integrals with their properties- example of He atom.

Unit-III: Theory of Many-electron Systems and their Applications

The Born-Oppenheimer approximation, Hartree self consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules.

Unit-IV: Density- Functional and Semiempirical Methods in Quantum Chemistry

Introduction to density functional, Hohenberg-Kohn variation theorem, Kohn-Sham equations, Exhange-correlation energy, Local density approximation, Generalized gradient approximation. Semiempirical MO treatments of Planar Conjugated Molecules, The Free-electron MO method, The Huckel and Extended Huckel MO method, The Pariser-Parr-Pople method, General semiempirical MO methods.

Unit-V:Group Theory-II

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. Representations and quantum mechanics. The invariance of Hamiltonian operator under symmetry transformations. Direct product representation. Molecular vibrations. Symmetry species of the vibrational mode. Selection rules for Infra-red and Raman spectra. Crystal field splitting.

Theory: *Paper: OC-T/08*

Unit I: Oxidations in Organic Chemistry

Different oxidative processes based on one-electron and two-electron oxidants, oxidations with Cr(VI) oxidants; Collin oxidation, PCC, PDC and others, DMSO-based oxidations: Swern, Moffat, DMSO-SO3 complex, DMSO-Ac_2O, Hypervalent iodine oxidations: Dess-Martin periodinane, IBX, iodobenzene diacetate, Oxidations with MnO2, $Tl(NO_3)_3$, Ag2O, RuO4, Ag(RCOO) and OsO4.

Unit II: **Reductions in Organic Chemistry:**

Different reductive processes, catalytic hydrogenation; homogenous and heterogeneous, reduction with metal hydrides of B, Al, Sn and Si, catalytic and transfer hydrogenations, dissolving metal reductions, diimide reduction, synthetically useful hydrogenolysis reactions, samarium and indium-based reducing agents, enzymatic and microbial reductions.

Unit III: Carbohydrate Chemistry

Basic structure and type of sugars; Conformational analysis of monosaccharides (pentoses and hexoses). Protection and deprotection. *O*-glycosylation, *C*-glycosilation. Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools in organic synthesis.

Unit IV: Synthetic Strategy

Retrosynthetic analysis, disconnection approach, Typical examples to illustrate the disconnection approach, Functional group interconversion, Umpolung (1,3-dithlane), protecting groups, Linear and Convergent synthesis.

Unit V: Natural Products; Part-I

Terpenoids : Introduction, Classification (with proper structural examples of each category), isolation and structure elucidation of some representative compounds. Biogenesis and biosynthesis of terpenoids.

Steroids: Introduction, classification, source of occurrence, brief chemistry of cholesterol, importance and role of steroids in our body, conversion of cholesterol into other bioactive steroids and chemistry of estrone.

Theory: *Paper: IC-T/09*

Unit-I: Inorganic Rings, Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds- Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Unit-II: Electron spin resonance spectroscopy

Basic principles, zero field splitting, and Kramer`s degeneracy, factors affecting the `g` value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship. Basic instrumentation, measurement techniques and simple applications. Applications of ESR in inorganic complex system and simple SMMs clusters.

NMR spectroscopy: Principles, ^{1}H NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, magnetic susceptibility and resonance shifts. ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P, ^{51}V – NMR spectra. Pascal

triangle, Contact shifts. Factors contributing the magnitude of chemical shift. NMR shift reagent and MRI reagent. Applications of NMR spectroscopy in inorganic systems.

Unit-III: Mossbauer spectroscopy

Principles, experiment, line-width center shift, quadrupole interaction, magnetic interaction, information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in varieties of environments, Application of Mossbauer spectroscopy in inorganic complex chemistry.

Photoelectron spectroscopy: Photo excitation and photoionization, core level photo ionization (XPS, ESCA.) and valence level (UPS) experiments, detection of atoms in molecules, chemical shift, differentiating same element in different environments. Application of TG, DTA and DSC spectroscopy in different inorganic systems.

Unit IV: Nuclear Chemistry & Radiochemical Analysis

Nuclear models: **N**uclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry; Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. *Nuclear reactions:* Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.

Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

Unit-V: Advanced Bioinorganic Chemistry 2

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.

Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase; molybdo enzymes: xanthene oxidase, nitrate reductase, sulfite oxidase including some model study.

Vitamins and coenzymes: Vitamin B_6 and vitamin B_{12} coenzymes, model systems: Supramolecular chemistry:

Practical: *Paper: IC-P/05*

Group-A: **Analysis of Complex Materials**

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and or instrumental methods as applicable.

Model Samples

Ores, Minerals , Concentrates: Dolomite ($CaCO_3$, Mg CO_3, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys: Brass (Cu, Zn); Soldier / Type metal (Pb, Sb, Sn); Bronze(Cu, Zn, Sn), Aluminium bronze(Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P).

Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

Group-B: FT-IR and UV assignment of synthesized metal complexes

Practical: *Paper: PC-P/06*

1. Determination of Hydrolytic Constant (K_h) of Ammonium Chloride solution pH -metrically.
2. Determination of pKa values of phoshphoric acid of any dibasic acid pH- metrically at laboratory temperature.
3. Potentiometric titration of Zn(II) solution by Potassium Ferrocyanide solution and also determination of the composition of Zn(II) Ferrocyanide complex.
4. Determination of E^o of Ag^+/Ag electrode and solubility product of AgCl.
5. Estimation of Cl^-, Br^- and I^- in a mixture potetiometrically.
6. Study the kinetics of inversion of cane sugar polarimetrically.
7. Determination of activity solubility product of Calsium Sulphate by complexometric titration.
8. To Determine the composition and stability constant of Fe(III)-Salicylic acid complex colorimetrically.

Semester IV

Theory: *Paper: PC-T/10*

Unit-I: Connection between Thermodynamics and Statistical Mechanics

Definition of Microstates and Macrostates. Boltzmann's definition of entropy. Formula for calculation of thermodynamic properties in terms of number of microstates. Determination of number of microstates for classical ideal gas. Connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.

Unit-II: Ensemble Method and its Application

Definition of ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open). Partition function. Calculation of thermodynamic properties in terms of partition function. Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.

Unit-III: Boltzmann, Fermi-Dirac and Bose-Einstein Statistics

Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behavior. Ideal monoatomic gas. The translational partition function. The electric partition function. Ideal diatomic gases. The vibrational partition function. The rotational partition function of a heteronuclear molecule. The rotational partition function of a homonuclear diatomic molecule. The classical partition function. Equipartition of energy. Ideal polyatomic gas. The vibrational and the rotational partition functions. An ideal gas of photons.

Unit-IV: Excitation of Molecules, Motion in Excited State and Photoexcited Processes

Theory of Electromagnetic Radiation. Interaction between Matter and Electromagnetic Radiation – Semiclassical treatment using Time-dependent perturbation Theory. Fermi golden rule, Transition probabilities and rates, Spectral shapes. Decoupling of the nuclear and electronic motions in a molecule: Born-Oppenheimer approximation. Excitation of molecules – Singlet and Triplet states. Radiative and Non-radiative relaxations. Franck-Condon principle. Absorption, emission and excitation spectra - mirror symmetry. Quenching of Fluorescence. Excited state processes – proton transfer, electron transfer and energy transfer. Marcus Theory. Solvent effect in spectroscopy. Solvation dynamics. Non-linear optical processes. Stimulated emission of radiation. Principles of Laser action. Applications of Lasers.

Unit-V: Molecular Spectroscopy:- Rotational, Vibrational, Raman , Electronic, Mossbauer and Spin Spectroscopy (NMR and ESR) :

Rigid & Non-rigid Rotors. Vibrational spectroscopy – Harmonic and Anharmonic Oscillators. Normal coordinates. Effects of Anharmonicity. Vibration-rotation transitions. Raman and Rayleigh scattering – Classical and Quantum Mechanical treatments. Polarization of scattered light. Rotational and Vibrational Raman spectroscopy. Resonance

Raman effect. Selection rules of rotational, vibrational and Raman spectroscopy. Atomic structure: vector model, spin-orbit coupling, atomic states and term symbols. Many-electron atoms Hund's rules. Selection rules for atomic electronic transitions. Diatomic molecules – Hund's coupling cases. Rotational and vibrational structures of diatomic electronic transitions. Franck-Condon principle. Dissociation, Photodissociation and Predissociation. Chromophores. Vibronic transitions. Spin-orbit coupling and singlet – triplet transitions. Selection rules for molecular electronic transitions. Photoelectron spectroscopy.

Principal of Mossbauer Spectroscopy. Application of Mossbauer Spectroscopy- Chemical Shift, Quadruple effect, effect of Magnetic Field.

Nuclear magnetic moment and response in an external magnetic field. Classical and Quantum Mechanical perspectives of nuclear magnetic resonance (NMR). Spin-spin and spin-lattice relaxation and spectral shapes. Chemical shift and nuclear shielding. Spin magnetic moment of electrons and electron spin resonance signal (ESR). The g-factor and hyperfine splitting – interaction between nuclear spin and electron spin. Nuclear quadrupole resonance.

Theory: *Paper: OC-T/11*

Unit I: NMR Spectroscopy II

Theory and Applications of DEPT, ^{1}H-^{1}H COSY, HMBC, HMQC, NOESY and other techniques such as Mosher ester analysis in structure elucidation of organic compounds, reaction monitoring.

Unit II: Asymmetric synthesis

Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

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

Unit III: 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 IV: Natural Products; Part-II

Alkaloids: Introduction, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, nicotine and papaverine. Structure and stereochemistry and medicinal importance of alkaloids of quinine and morphine group (cinchona and opium alkaloids).

Natural Antioxidants: Chemistry of naturally occurring oxygen heterocycles, polyphenolics and other antioxidants.

Unit V: Heterocyclic Chemistry

Synthesis, reactivity and uses of the following compounds and their derivatives: imidazole, pyrazole, oxazole, iso-oxazole, thiazole, iso-thiazole and 5, 6-membered rings containing two heteroatoms, pyrimidines and purines.

Theory: *Paper: IC-T/12*

Unit-I: Inorganic Reaction Mechanism

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. 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 ($\Delta S^{\#}$, $\Delta H^{\#}$, $\Delta V^{\#}$), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.

Unit-II: Inorganic Photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process. Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing, quantum yield, decay fluorescence. Fluorence quenching, Stern-Volmer equation. Photochemical process: photo substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes.

Unit-III: Symmetry and Group Theory

Group and their properties-concept of groups, subgroups, classes and related theorems, commutative (abelian) groups and cyclic groups and their examples. Symmetry elements and operations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry in platonic solids, identification of point groups.

Effect of lowering of symmetry on the orbitals and energy levels, correlation table, Correlation diagrams, Tanabe-Sugano diagram, Justification of Laporte selection rule, vibronic coupling and vibronic polarization, polarization of electronically allowed transitions. Symmetry adapted linear combinations (SALCs) and the M.O. Description of organic and organometallic molecules.

Unit-IV: Crystallography

Fundamentals of X-ray crystallography, crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their properties, Diffraction of X-ray, lattice planes, indices, Brag's condition, reciprocal lattice, Brag's law in reciprocal, Geometric data collection (simple examples), structure factor, systematic absence, heavy atom method. Fourier synthesis, Patterson function, experimental diffraction methods (Laue method, rotating crystal method). Methods of growing single crystals: data collection, structure solution, structure refinement and R value.

Unit-V: Supramolecular Chemistry

Basic concepts and principles, molecular recognition and host-guest interactions, anion coordination and recognition of anionic substrates, organometallic receptors and their host-guest complexes, spherical recognition, podand, podate, cyrptand, cryptate, crownethers, molecular devices and supramolecular assemblies, supramolecular orbital, supramolecular arrays: ribbon. Ladder, rack, braded, grid; harnessing noncovalent forces to design functional materials. Receptors and receptor-substrate complexes, Drendrimer.

Course ID- PC-Pro/07 or OC-Pro/07 or IC-Pro/07

Project:

Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and sectional teachers

Specialization will be designated as per Project Work.

The framework of the syllabus is O.K. however the contents may be modified as and when required.