

**PROPOSED SYLLABUS
FOR
M. Sc. COURSE IN CHEMISTRY
2020
(CBCS SYSTEM)**



**Department of Chemistry
Diamond Harbour Women's University
Sarisha, West Bengal
743368**

(Effective from the Academic Session 2020-21)

Syllabus for Two-Year Four-Semester PG Course in Chemistry
DHWU
COURSE STRUCTURE
Two – Year, 4 – Semester PG Course in Chemistry:
Grand Total Marks – 1050
SEMESTER WISE

DIVISION OF MARKS AND CREDITS

SEMESTER	Theoretical (Core)	Practical (Core)	Discipline Centric Elective		Open Elective (Theory)	Total Marks	Total Credits
			Theory	Practical			
SEMESTER-I	150	100	-	-	-	250	25
SEMESTER-II	150	100	-	-	-	250	25
SEMESTER-III	50	-	50	100	100	300	28
SEMESTER-IV	-	-	150	100		250	22
Total	350	200	200	300	100	1050	100

First Year (First Semester)

Paper	Subject/Topics	Marks		Total Marks in End semester	Credits		Total Credits End semester	Class hours /week	Total Class hours
		Internal	Semester exam		Intern al	Semester exam			
Chem/ThG/ 101	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/ThG/ 102	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/ThG/ 103	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/LG/ 104	Chemistry Laboratory General	20	30	50	2	3	5	9	135
Chem/LG/ 105	Chemistry Laboratory General	20	30	50	2	3	5	6	90
Total		70	180	250	7	18	25	30	450

First Year (Second Semester)

Paper	Subject/Topics	Marks		Total Marks in End semester	Credits		Total Credits End semester	Class hours /week	Total Class hours
		Internal	Semester exam		Internal	Semester exam			
Chem/ThG/201	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/ThG/202	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/ThG/203	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/LG/204	Chemistry Laboratory General	20	30	50	2	3	5	9	135
Chem/LG/205	Chemistry Laboratory General	20	30	50	2	3	5	6	90
Total		70	180	250	7	18	25	30	450

ThG: Theory General; LG: Laboratory General

Second Year (Third Semester)

Paper	Subject/Topics	Marks		Total Marks in End semester	Credits		Total Credits End semester	Class hours /week	Total Class hours
		Internal	Semester exam		Internal	Semester exam			
Chem/ThG/301	Chemistry Theory General	10	40	50	1	4	5	4	60
Chem/ThS/302	Chemistry Theory Special	10	40	50	1	4	5	4	60
Chem/LS/303	Chemistry Laboratory Special	10	40	50	1	3	4	6	90
Chem/LS/304	Chemistry Laboratory Special	20	30	50	1	3	4	6	90
Chem/ThEP/305	Open Elective paper# Basic Concepts of Modern Chemistry-1 [CBCS]	-	50	50	-	5	5	5	75
Chem/ThEP/306	Open Elective paper# Basic Concepts of Modern Chemistry-2 [CBCS]	-	50	50	-	5	5	5	75
Total		70	180	300	4	24	28	30	450

Second Year (Fourth Semester)

Paper	Subject/Topics	Marks		Total Marks in End semester	Credits		Total Credits End semester	Class hours /week	Total Class hours
		Internal	Semester exam		Internal	Semester exam			
Chem/ThG/401	Chemistry Theory General	10	40	50	1	4	5	4+1	75
Chem/ThS/402	Chemistry Theory Special	10	40	50	1	4	5	4+1	75
Chem/ThS/403	Chemistry Theory Special	10	40	50	1	4	5	4+1	75
Chem/LS/404	Chemistry Laboratory Special	-	50	50	-	3	3	6	90
Chem/LS/405	Chemistry Laboratory Special	-	50	50	-	4	4	8	120
Total		70	180	250	3	19	22	29	435

ThS: Theory Special; LS: Laboratory Special

Notes:

- (i) Full marks for each paper is 50.
- (ii) For each theoretical paper (Th), there will be 5 units; each unit will carry 8 marks; two questions per unit are to be set and any one is to be answered; 10 marks are reserved for sessional/internal/continuous assessment.
- (iii) For each practical paper up to the third semester, 20 marks will be reserved for sessional/internal/ continuous assessment. The assessment should include regularity and periodic viva-voce/quiz tests.
- (iv) Chem/ThS and Chem/LS are distributed over the special papers (S) in the three branches of Chemistry: Inorganic, Organic & Physical e.g. Chem/ThSI/302-303, Chem/ThSI/401-403 for Inorganic special theory and Chem/LSI/304-305, Chem/LSI/404-405 for Inorganic Special Laboratory. Any one special course is to be opted and continued systematically.
- (v) Papers Chem/LS/404 and Chem/LS/405 will generally contain the following components for any specialization, as outlined here.

Course ID	Components	Marks	Total Marks

Chem/LS/404	\$Write-up of Review/Literature Survey	15	50
	\$Continuous Assessment	15	
	#Grand Viva-voce	20	
Chem/LS/405	\$Write-up of Project Report	25	50
	#Oral Presentation and discussion	25	

\$To be assessed by the guide

#To be assessed by an external examiner in presence of all teachers of the department

Acronyms

Chem/ThG : Chemistry Theory General

Chem/LG : Chemistry Laboratory General

Chem/ThS : Chemistry Theory Special

Chem/LS : Chemistry Laboratory Special

Chem/ThSI: Chemistry Theory Special Inorganic

Chem/LSI : Chemistry Laboratory Special Inorganic

Chem/ThSO: Chemistry Theory Special Organic

Chem/LSO : Chemistry Laboratory Special Organic

Chem/ThSP: Chemistry Theory Special Physical

Chem/LSP : Chemistry Laboratory Special Physical

- (vi) Students will choose one special paper subject before the beginning of the 3rd Semester. Option once exercised is final and binding. No change shall be permitted. **Special papers will be offered as per the existing infrastructure.**

This course will be offered for students of all other Departments of University.

Semester – I

Course ID: Chem/ThG/101

Unit-1: Coordination Chemistry 1

Crystal field theory, Splitting of d orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal, octahedral and pentagonal bipyramidal fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environments, octahedral site preference energy, tetragonal distortion and Jahn Teller effect. Shapes of complexes. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stability of complexes (Irving Williams order). Kinetic aspects of crystal field stabilization, crystal field activation energy, labile and inert complexes.

Unit-2: Organometallics 1

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, isolobal and isoelectronic relationships with examples. Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and -cyclopentadienyl complexes. Structure and bonding in η^2 -ethylenic and η^3 -allylic compounds with typical examples; structure and bonding of $K[Pt(C_4H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph-C\equiv C-Ph)]$ and $[Co_2(CO)_6(Ph-C\equiv C-Ph)]$. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination; electrophilic and nucleophilic reactions of coordinated ligands.

Unit-3: Bioinorganic Chemistry 1

Elements of life: basic reactions in biological systems and roles of metal ions. Bioenergetic principle and role of ATP. Transport across biological membrane: Na⁺ -K⁺ -ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxypeptidase, urease. Metal dependent diseases: Wilson's disease, Alzheimer disease, Metal complexes as drugs: Pt, Rh, Ru and Au drugs. Toxic effects of metal ions, detoxification by chelation therapy.

Unit-4: Inorganic Reaction Mechanisms 1

Mechanistic labels A, D, Ia, Id: compare with SN1 and SN2; Crystal field activation energy. Labile and inert complexes. Rate laws, activation parameters. Studies on Octahedral complexes of common metal ions: anation, aquation, acid- and base-catalyzed reactions, hydrolysis, pseudo-substitution, isomerization, racemization; Ray-Dutt and Bailar twist mechanisms (octahedral and square-planer complexes). Square-planer complexes of Pt(II): the trans-effect.

Unit-5: Statistical Error and Radiochemical Analyses

Errors in quantitative analyses, types of errors, handling of systematic errors. Random errors: distribution, standard deviation, confidential limits of the mean, presentation of results, propagation of random errors. Radiochemical methods of analysis: Introduction to chemical effects of nuclear transformations, Szilard-Chalmer's effect, Use of Szilard-Chalmer's effect in the syntheses of labeled compounds; enrichment factors, enrichment of radio isotopes; retention, mechanism of retention, nuclear reasons for retention.

Course ID: Chem/ThG/102

Unit-1: Structure-Activity Relationship

MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes (C₆₀), alternant and non-alternant hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods-Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Hammett equation and its modifications.

Unit-2: Stereochemistry 1

Concept of centre and plane of chirality, axial chirality and point groups. Winstein-Holness equation, Curtin-Hammett principle; Conformational analysis of cyclohexane, cyclohexene, cyclohexanone, decalin and their derivatives; perhydroanthracene, perhydrophenanthrene etc., Felkin-Anh, Cieplak and Zimmerman-Traxler Models; Addition Reactions to Carbonyl Compounds.

Unit-3: Pericyclic Reactions

Classification and stereochemical modes. Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, 2-component cycloadditions, sigmatropic rearrangements. Rationalization based on Frontier M.O. approach, correlation diagrams, DewarZimmermann approach (concept of aromaticity in the transition states), Mobius and Huckel systems. Reactivity, regioselectivity and periselectivity in cycloaddition reactions (Diels Alder reaction), Intramolecular Diels alder reaction, Sommelet, Hauser, Cope and Claisen rearrangements, Ene reactions including the reaction of allylic metal reagents (derived from Mg, Zn, Li, Ni, Pd, Pt), Wittig rearrangement. Cheletropic reactions involving neutral molecules and reactive species, 1,3 dipolar cycloadditions.

Unit-4: NMR Spectroscopy 1

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, A₂B₂ in proton NMR. Introduction to ¹³C. Application of NMR spectroscopy and other spectroscopical techniques to simple structural and mechanistic problems.

Unit-5: Natural Products-1

Terpenoids: Introduction, Classification (with proper structural examples of each category viz., sesqui-, di- and tri-terpenes, carotenoids etc.). Isolation, structure elucidation, synthesis of some representative members of acyclic, monocyclic and bicyclic mono- and sesqui-terpenes. Biogenesis and biosynthesis of terpenoids.

Steroids: Introduction, classification, sources of occurrence and role of steroids (including steroidal hormones) in human body. Chemistry of oestrone. Brief chemistry of cholesterol and conversion of cholesterol into other bioactive steroids. Biosynthesis of cholesterol.

Course ID: Chem/ThG/103

Unit-1: Thermodynamics and Statistical Mechanics 1

State functions. Legendre transformations. Entropy and probability. MB distribution. Partition function. Relevance to thermodynamics. PF for atoms and diatomics. Application to chemical equilibrium. Equipartition principle. Gibbs paradox. Sackur-Tetrode equation.

Unit-2: Atomic Structure and Spectra

Atomic spectra; orbital and spin angular momentum; Stern-Gerlach experiment. Zeeman and anomalous Zeeman effects; fine structure; spin-orbit interaction (vector model). Lande-g factor. Atomic and molecular terms.

Unit-3: Quantum Mechanics 1

Postulates and their analysis. Properties of operators and commutators. Uncertainty principle. Schrodinger equation: Equation of motion, constant of motion, stationary states, energy and norm conservation. Ehrenfest's theorems. Step potential; rectangular barrier problem, tunneling; alpha decay.

Unit-4: Kinetics 1

Fast reactions: relaxation method. Oscillatory reactions: observations and mechanisms. Electrode kinetics: Special features; Nernst, Butler-Volmer and Tafel equations.

Unit-5: Polymer chemistry

Classification of polymers; kinetics of polymerization. Mean molar masses of polymers and the various methods of determinations; nature of distributions about the mean. Thermodynamics of polymer solution: Polymer conformation.

Course ID: Chem/LG/104

1. Use of free software for chemically relevant information of molecules.

Course ID: Chem/LG/105

1. Semi-micro qualitative analysis for selected uncommon elements.
2. Stability constants of coordination complexes and analysis of drugs

Semester – II

Course ID: Chem/ThG/201

Unit-1: Coordination Chemistry 2

Electronic spectra of transition metal complexes – determination of free ion terms of $d1$ to $d9$, microstates, determination of ground and all excited state terms of d_n terms in octahedral and tetrahedral fields, Orgel diagrams (qualitative approach), hole formalism, inversion and equivalence relations, selection rules for spectral transitions, d-d spectra and crystal field parameters, Nephelauxetic series, qualitative idea of Tanabe–Sugano diagrams, charge transfer spectra. Magnetic properties – elementary idea.

Unit-2: Chemical Bonding

Different types of bonding including weak interactions. Variation method. LCAO method. Molecular orbital of H_2^+ , H_2 ; homo- and hetero-diatomics, triatomic and polyatomic molecules/ions (including T_d , O_h , and D_{4h} coordination complexes). Molecular term symbols. Electron-pair wave function; VB theory and its application to H_2 molecule. Comparison of VB and MO theories.

Unit-3: Clusters and Boranes

Clusters: Definition, clusters compounds of heavier transition elements, in particular their halides and carbonyls (including bridged carbonyls) – preparation, properties and structures (inorganic ring, cages, Keggin and clusters); metal-metal bonds in metal atom clusters including quadrupole bonds in binuclear complexes, Bonding in metal atom clusters – qualitative MO theory/Hoffman's isolobal concept.

Boranes – Boron hydrides: Structure and bonding, Lipscomb topology, 'styx' system of numbering, nomenclature. Carboranes, metalloboranes, and metallocarboranes: preparation, properties, structures; Wade's rules.

Unit-4: Complex Equilibria

Thermodynamic and stoichiometric stability constants of metal-ligand complexes. Determination of composition and stability constants of complexes by pH-metric, spectrophotometric and polarographic methods. Conditional stability constants and their importance in complexometric EDTA titration of metal ions. Solubility equilibria: Quantitative precipitation criteria of metal hydroxides, sulphides, chelate complexes, etc.

Unit-5: Solid-state Chemistry

Defects in solids, point, line and plane defects, determination of equilibrium concentration of Schottky and Frenkel defects, stoichiometric imbalance in crystals and non-stoichiometric phases, colour centres in ionic crystals, band theory, band gap, metals, insulators, semiconductors (intrinsic and extrinsic), hopping semiconductors, rectifiers and transistors, bonding in metal crystals, free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, superconductivity, Meissner effect, basic concept of BCS (Bardeen-Copper-Schriffer) theory.

Course ID: Chem/ThG/202

Unit-1: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di- π -methane, oxo di- π methane and aza di- π methane rearrangements, Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, SRN1 reaction, photooxidation, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications: cyclisation of radicals including various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction.

Unit-2: Synthetic Methodology 1

Organoboron: Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes (oxidation, protonolysis, halogenolysis, amination, isomerisation, carbonylation, cyanidation etc.), organoborane route to unsaturated hydrocarbons, allyl boranes, boron enolates. Organophosphorus: Chemistry of phosphorus ylides (Wittig reaction, Horner- WordsworthEmmons modification, Schlosser' modification) and chiral phosphines. Organosulphur: Sulphur stabilised anions and cations, sulphonium salts, chemistry of sulphur ylids. Chemistry of nitrogen ylids and oxonium ylids.

Unit-3: Heterocyclic Chemistry 1

Synthesis and reactivity of quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole, isooxazole, isothiazole, coumarines and flavanoids and their applications in organic synthesis.

Unit-4: Synthetic Methodology 2

Methods of conversion of carbonyl group to methylene group and 1,2- ketone transposition. Reduction using electrophilic and nucleophilic reagents, Dissolving metal reductions. Oxidation using Cr, Mn, Se, Ru, Tl derived reagents, Fremy's salt, peracids, hypervalent iodine reagents, Swern oxidation and related reactions.

Unit-5: Natural Products -II

Alkaloids: Introduction, classification (with examples), general methods of isolation and familiarity with methods of structure elucidation (chemical & spectroscopic methods). Structure, synthesis and bio-synthesis of ephedrine, nicotine, coniine and papaverine. Structure, stereochemistry, biogenetic precursors and medicinal importance of alkaloids from terrestrial and marine sources with special reference to morphine, quinine, reserpine, yohimbine and lysergic acid.

Course ID: Chem/ThG/203

Unit-1: Quantum Mechanics 2

Bound-states and their properties. Box with finite walls; Harmonic oscillator (wavefunction and operator methods). Ideas of variational method and perturbation theory for stationary states.

Unit-2: The H-atom Problem

Cartesian and polar coordinates. Centre of mass and relative coordinates. General forms of solutions for stationary states with orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constants of motion like L^2 , L_z , etc.

Unit-3: Group theory 1

Reducible and irreducible representations; classes and characters; the great orthogonality theorem and related theorems; projection operators; direct product representation; construction of SALC; selection rules in spectroscopy; study of normal modes.

Unit-4: Interfacial Chemistry

Curved surfaces: Young-Laplace and Kelvin equations. Adsorption on solids: BET equation. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; emulsions.

Unit-5: Kinetics 2

PE surface, reaction coordinates and reaction paths. Idea of the BEBO method. Absolute rate theory. Sample case-studies using partition functions. Comparison with collision theory. Ionic reactions in solutions.

Course ID: Chem/LG/204

1. Identification of single organic compounds (solid/liquid).
2. Organic preparations, including methods of purification.

Course ID: Chem/LG/205

1. Selected equilibrium/kinetics experiments (analytical).
2. Selected equilibrium/kinetics experiments (instrumental).

Semester – III

Course ID: Chem/ThG/301

Unit-1: EPR and Mössbauer Spectra

Principle of EPR and spin Hamiltonian (comparison to NMR spectra), spectrometer, external standard, line-width, nuclear hyperfine interactions, anisotropy in Lande g factor and hyperfine interaction, magnetically equivalent and nonequivalent set of nuclei, intensity, structural information of organic radicals and inorganic molecules from EPR spectra.

Mössbauer activity: principle, experiment, line-width, center shift, quadrupole interaction, magnetic interaction; information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mössbauer active nuclei in varieties of environments.

Unit-2: PES and Diffraction Methods

Photoelectron spectroscopy: Photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about the nature of molecular orbital from UPS, UPS of simple diatomic molecules e.g. N₂, O₂, CO, HCl, etc.. Principles of electron, neutron and X-ray diffraction methods in determining the structure of molecules – a comparative approach.

Unit-3: Mass Spectroscopy

Principles, instrumentation and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD and FAB and other techniques. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, ion-molecule interaction and analysis of fragmentation patterns. Modern techniques: MALDI-TOF, ESI-MS, Principles of HRMS.

Applications of mass spectroscopy to simple structural and mechanistic problems.

Unit-4: Absorption Spectroscopy and Molecular Interactions

$\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and $d \rightarrow d$ transitions. Solvent effects on spectra. Weak and CT interactions.

Vibronic and spin-orbit coupling: detection from spectral data.

Unit-5: Emission Spectroscopy

FC principle. Mirror-image symmetry and its violation. Radiative and radiationless deactivation. Polarization characteristics of emission. Quenchers and lifetime variations.

Course ID: Chem/ThSI/302

Unit-1: Bioinorganic Chemistry 2

Dioxygen transport/storage proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin. Electron transport proteins: cytochromes, Fe-S proteins. Other electron carriers in biosystems. Respiratory electron transport chain. Photosynthesis, chlorophyll, PS-I, PS-II, photosynthetic electron transport chain and water oxidation mechanism. Protective metalloenzymes such as cytochrome P-450, catecholase, peroxidase.

Unit-2: Supramolecular Chemistry

Origin of supramolecular chemistry (why chemistry beyond the molecules?), concepts and terminology; nature and types of weak supramolecular interactions like hydrogen bonding, pi pi, CH-pi, electron deficient/rich pi interactions, etc. Molecular recognition, self-assembly and crystal engineering: Applications to real systems like drug design, material science, molecular machines, etc.

Unit-3: Organometallics 2

Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples. Catalysis by organometallic compounds: Hydrogenation of unsaturated compounds, Wilkinson's catalyst, Tolman catalytic loop; Syntheses 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 reaction of alkenes and alkynes; Ziegler-Natta catalysis, photodehydrogenation catalyst (platinum POP).

Unit-4: Magnetochemistry 1

Definition of magnetic properties, types of magnetic bodies, experimental arrangements for determination of magnetic susceptibility: Gouy method, Faraday method, vibrating sample magnetometer, SQUID, NMR method. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic systems, Pascal's constants. Two sources of paramagnetism: spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, Curie equation, Curie's law and Curie-Weiss law.

Unit-5: Comparative study of d and f block elements

Electronic configuration and chemistry in different oxidation states with comparison; properties and structures of lower halides of Nb-Ta, Mo-W, Tc-Re with special emphasis on the metalatom clusters present, Polyoxometallates, blue oxides of Mo and W, Tungsten bronze, sulphides of Mo. Extraction of lanthanides, separation and purification of lanthanides, chemical properties of lanthanides in their common oxidation states, spectral and magnetic properties of d- and fblock elements with comparison, lanthanide shift reagents and uses of lanthanides.

Course ID: Chem/ThSO/302

Unit-1: Stereochemistry 2

Advanced course involving conformation and reactivity- acyclic system, monocyclic systems- 3 to 10 member rings, 6-6, 6-5, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-5, 5-5-5 tricyclic systems. Introductory course on molecular mechanics computations.

Unit-2: NMR Spectroscopy 2

Advanced Techniques and Applications of NMR: ^1H and ^{13}C NMR principles, rules for carbon ^{13}C calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation

processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.

Unit 3: Synthetic Methodology 3

Chemistry of organosilicon compounds, Synthetic uses of silyl ethers, silylenol ethers, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon BaeyerVilliger rearrangement. Ionic hydrogenation, synthetic use of TMSiCN, TMSiNCO, TMSi, TMSiNHCOMe, TMSiN₃ etc. Organotin reagents for selective reactions.

Unit-4 : Medicinal Chemistry 1

Chemical basis of disease states, definition and classification of drugs. Concept of pharmacokinetics and pharmacodynamics. Methods of drug administration, drug metabolism and drug excretion, enzyme inhibitors, receptors, chemical messengers, agonists and antagonists. Drug dosing and drug half-life, drug tolerance and physical dependence, drug potency, drug efficacy, dose response curves and therapeutic index (LD-50 & CD-50). Development of new drugs, concepts of prodrugs and soft drugs, pharmacophores, lead compounds and molecular modification, qualitative and quantitative structure activity relationship. Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B1, B6 and folic acid, etc.

Unit 5: Name reactions and Methods of Ring Formation

Name reactions: Baylis –Hillman reaction, Shapiro reaction, Mitsunobu reaction, Julia olefination, McMurry reaction etc.

Methods of Ring formation: Nazarov cyclisation, Annelation methods (Robinson annelation, Wickterle annelation, Halo ketal annelation – cation effect on this reaction, Woodward annelation and Danishefsky's modification with phosphoranes), Dieckmann, Ruzicka, Thorpe cyclisation, Acyloin condensation, and other miscellaneous cyclisations. Ring formation via polyene cyclisation. Cation Olefin Cyclization, Anionic Cyclization, Divinylcyclopropane Rearrangement, Oxy Ene Reaction (Conia Reaction), Carbonylation Cyclization, Olefin Ring Closing Metathesis.

Course ID: Chem/ThSP/302

Unit-1: Valency

Born-Oppenheimer approximation and beyond. Avoided crossings. Virial theorem and chemical bonding. Theories of valence: VB and MO. Discussion on H₂⁺ and H₂; dissociation limits

Unit-2: Reaction Dynamics

Properties of electronically excited molecules; potential energy diagram for donor-acceptor system. Nonradiative intramolecular electronic transition; crossing of potential energy surfaces (Franck-Condon factor). Adiabatic-nonadiabatic cross-over. Kasha's rule. Study of molecular energy transfer and state-to-state reactions. Macroscopic rate from microscopic rate coefficients.

Unit 3: Rotational and vibrational spectroscopy: Rigid and non-rigid rotors, selection rule for rotational spectra; nuclear spin and rotational energy levels. Stark effect. Linear harmonic oscillator, Ro-vibrational selection rule for diatomic and polyatomic molecules, anharmonic correction by perturbation – appearance of overtones; Raman scattering, selection rule for rotational-vibrational Raman effect. Non-linear scattering phenomena.

Unit-4: Biophysical chemistry

Structure and function of Biomolecules: Protein, nucleic acid, carbohydrates and lipids. Membrane structure. Biomolecular complexes: Protein–ligand, Enzyme–substrate and Drug–DNA. Examples. Techniques for study of biomolecular structure and function.

Unit-5: Electrochemistry

Debye-Huckel theory, Debye-Huckel-Onsager theory, Electrophoretic and relaxation effects, Wien effect, Debye–Fulkenhagen effect. Electrocapillarity (EC): nature of EC curves, Lipmann equation. Helmholtz, Guoy-Chapman and Stern double layer models.

Course ID: Chem/LSI/303

1. Instrumental analysis.
2. Preparation and characterization of some coordination complexes.

Course ID: Chem/LSI/304

1. Magnetic, electrochemical and CD experiments.
2. Kinetics and ion-exchange studies.

Course ID: Chem/LSO/303

1. Multistep organic preparations.
2. Extraction and purification of selected natural products.

Course ID: Chem/LSO/304

1. Chromatographic separation of the components of a mixture of organic solids.
2. Identification of the said components by (A) chemical and (B) spectroscopic methods.

Course ID: Chem/LSP/303

1. Numerical analysis and programming.
2. Selected quantum-chemical and statistical applications of programs.

Course ID: Chem/LSP/304

1. Selected equilibrium/kinetics experiments (analytical).
2. Selected equilibrium/kinetics experiments (instrumental).

Semester – IV

Course ID: Chem/ThSI/401

Unit-1: X-ray Crystallography

Crystal and lattice, process of crystallizations, crystal form, habit, defect, lattice planes, indices, crystal systems and symmetry, primitive and nonprimitive lattice, diffraction of X-ray, Bragg's condition, reciprocal lattice, Bragg's law in reciprocal lattice, Ewald sphere, X-ray Crystallography Instrumentation, goniometer, geometric data collection, lunes, crystal mosaicity and beam divergence, completeness of data collection, crystal to detector distance vs resolution, atomic scattering factor, structure factor, intensity of diffracted beam, Friedel's Law, systematic absences, temperature factor on the intensity of diffracted beam.

Unit-2: Redox reaction mechanisms

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

electron transfer reactions, applications of Marcus expression (simple form); redox-catalysed substitution reactions.

Unit-3: Inorganic nanomaterials

Chemical designing of inorganic nanomaterials. Hybrid organic-inorganic nanomaterials, self-assembly of nanoscale materials; fundamental aspects of self-assembly, control of morphology and nanostructure, compositional control, structural properties and different techniques of synthesis. Top-down and bottom-up approach; SEM, TEM analysis.

Unit-4: Inorganic Photochemistry

Introduction to Inorganic photochemistry: Photophysical and photochemical processes, characteristics of electronic excited states of inorganic compounds, ligand field states, charge transfer states, Frank-Condon and Thexi states. Kinetics of photochemical processes, reactivity of transition metal complexes in the ligand field and charge transfer excited states. Excited-state redox reactions – photoelectrochemistry, selective inorganic photochemistry using laser beams; relevance of Ruthenium polypyridine complexes in solar energy conversion and storage, photosplitting of water; inorganic photochemistry of biological processes and their model studies.

Unit-5: Materials Chemistry

Syntheses, structures and bonding features and technical applications in respect of polymeric inorganic materials: polysilanes, polyoxysilanes, polyphosphazenes, polyphosphates, silicates, aluminosilicates with special reference to talc, mica, asbestos, zeolite, coordination polymers, dendritic macromolecules based on inorganic elements, Zintl phases, halogen X_n^+ ions and their compounds, charge transfer complexes with halogens and halogen bridges or as ligands. Clathrates. Perxenic acid and its salts. Metal alkoxides and aryl oxides; metal complexes with oxo anions as ligands. One dimensional solids, solid state extended arrays, chevrel phases.

Course ID: Chem/ThSO/401

Unit-1: Stereochemistry-III

Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules. Chiral analysis by Polarimeter, NMR, GC, HPLC and Capillary Electrophoresis (CE) methods. Baldwin's Rules-applications, hydrolytic kinetic resolution.

Unit-2, Asymmetric Synthesis

Principles and newer method of asymmetric synthesis (including enzymatic and catalytic nexus), enantio- and diastereoselective synthesis. Reactions of enolates (substitution), Addition to $C=C$ double bonds (electrophile induced cyclisation, iodolactonisation, Asymmetric hydroboration, Conjugate additions. Reduction of $C=C$ double bonds, Aldol Reaction, Diels-Alder cycloaddition, cyclopropanation, oxidation, epoxidation, dihydroxylation and aminohydroxylation. Rearrangement: [3,3] Sigmatropic, (2,3)-Wittig, alkene isomerisation. Organo-catalytic reactions leading to chiral molecules.

Unit-3: Heterocyclic Chemistry-II

Nomenclature of fused heterocycles. Reactivity and synthesis of pyrimidine, pyridazines, pyrazines, purines, pteridines with and without oxygen and/or sulfur atoms, and their role in biological systems. Introduction to the chemistry of seven-membered heterocyclic compounds: azepines, oxepines, thiepinines and their aza-analogues.

Unit-4: Organometallic Chemistry of Transitional Elements

Application of organotransition metals in organic synthesis-preparative, structural and mechanistic aspects. Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction-Heck, Stille, Suzuki, Kumada, Negishi and Sonogashira coupling ZieglerNatta reaction, Olefin metathesis. Tebbe's reagent, Pauson-Khand reactions, Volhsrdt co-trimerisation, functional organometallic compounds. Use of nontransition metal Indium, tin, zinc. Chemistry of arene – chromium tricarbonyl complexes, Reaction of Fieser and Schrock type carbene complexes.

Unit-5: Supramolecular Chemistry

From molecular to supramolecular chemistry: factors leading to strong binding (non-covalent interactions). New molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin, calixarenes, dendrimers and their application in specific recognition processes. Supramolecular reactivity and catalysis, switching devices. Self-assembly of supramolecular aggregates, crystal engineering.

Course ID: Chem/ThSP/401

Unit-1: Angular Momentum

Constants of motion: parity and angular momentum. General rules for representations. Commutation relations; step-up/step-down operators; spin-1/2 case. Quantization. Spin and Pauli matrices. Matrix representations of total angular momentum operators ($J = 1, 3/2$, etc). Addition of angular momenta.

Unit-2: Quantum Chemistry 1

Variation method: Basis and applicability. Limitations of non-linear variations. Linear variation method: secular determinant. Properties of states. Sigma-pi separability. Pi electron Hamiltonians: Huckel theory for conjugated systems (linear and cyclic). Resonance energy and bond order.

Unit-3: Quantum Chemistry 2

Many-electron systems: Closed and open shells. Antisymmetry principle and antisymmetrization operator. Independent particle model (IPM). The He-atom problem. Hartree and Hartree-Fock methods for closed shells. Koopman's theorem; Brillouin's theorem. Roothan equation. Problems with open-shell systems. Limitation of IPM: electron correlation. Multideterminantal wave function and CI.

Unit-4: Kinetics 3

Linear free energy relationship: effect of substituents; Hammett and Taft constants. Hammett acidity function. Rate processes and some physical phenomena. Statistical approach to rate theory: Hinshelwood, RRK and RRKM theories.

Unit-5: Chemistry of Excited States

Rotational, vibrational and electronic excited states. Excited state isomerisation reaction. Predissociation. State-specific predissociation and photofragmentation, excited state dynamics. Spectroscopy of cold molecules; single molecule spectroscopy.

Course ID: Chem/ThSI/402

Unit-1: Magnetochemistry 2

Introduction: Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility, determination of magnetic susceptibility (methods like

Gouy, Faraday, SQUID). Curie and Curie-Weiss Law and their derivations, Quantum theory of paramagnetic susceptibility – Van Vleck equation, its derivation and applications under different conditions of energy level gaps in comparison to room temperature, Temperature Independent paramagnetism (TIP). Magnetic properties of free ions (first order and second order Zeeman effects), spin-orbit coupling with special reference to Sm^{3+} and Eu^{3+} . Antiferromagnetic interactions in inorganic compounds; direct and superexchange interactions with reference to polynuclear metal complexes and oxide/halide salts of transition metals, magnetic materials and molecular magnets.

Unit-2: Bioinorganic Chemistry 3

Metal storage and transport proteins: transferring, ferritin, ceruloplasmin, calmodulin. Electron transport proteins: cytochromes, ferredoxins and rubredoxins, blue copper proteins. Redox metalloenzymes: catalase (both Fe and Mn), Ascorbate oxidase, peroxidase, superoxide dismutase, cytochrome c oxidases.

Nitrogen fixation. Cobalamins including vitamin and coenzyme B12.

Structural/functional models of some of the above-mentioned systems.

DNA – Metal complexes interactions. Antitumor activities of metal complexes and structure-activity relationship.

Unit-3: Thermal Methods of Analysis

TGA, DTG and DTA: Principles and methods, presentation of data. DSC: A brief outline and a comparative discussion with DTA. Instrumentation: TG, DTA and DSC; basic principles, outline, schematic diagrams of the instruments.

Factors affecting results of thermal analysis: Applications of thermal methods of analysis in solid state reactions, decompositions of materials; desolvation/deaquation in inorganic complex compounds, phase transition, reaction kinetics.

Unit-4: Spectroscopy 1

Survey of metal centered transitions of 3d, 4d, and 5d metal ion complexes. f-f spectra of lanthanides and actinides. Bonding parameters and structural evidences from electronic spectra. Charge transfer spectra, CD, ORD, and MCD spectra and absolute configuration of coordination compounds. Cotton effect and Faraday effect, stereoselective and stereospecific effects.

Unit-5: Nuclear Chemistry

Nuclear models – Nuclear forces, liquid drop model, Fermi gas model, Magic numbers. Nuclear spin and nuclear isomerism. Nuclear reactions – energetics, mechanism and models, nuclear fission and nuclear fusion. Nuclear reactors and particle accelerators. Interaction of radiation with matter.

Course ID: Chem/ThSO/402

Unit-1: NMR Spectroscopy II

Application of DEPT, ^1H - ^1H COSY, ^1H - ^{13}C HETCOR, HMBC, HMQC, HSQC, TOCSY, NOESY in structure elucidation of organic compounds, reaction monitoring etc., Solid state NMR (^{13}C -CP-MAS), Chemical Shift Anisotropy and Cross Polarization.

Unit-2: Bio-organic Chemistry

Molecular models of biological receptors, design, synthesis and binding studies of synthetic receptors. Enzyme models, micelles, biopolymers, remote functionalization reactions, catalytic antibodies, principle of gene synthesis. Proteins, peptides and amino acids.

Unit-3: Medicinal Chemistry 2

Mechanism of action and synthesis of some non-steroidal anti-inflammatory drugs (NSAIDs).

Classification and mechanism of action of antibiotics. Gram positive and gram negative microorganisms. Synthesis of penicillin-G, penicillin-V, amoxicillin, chloramphenicol, norfloxacin, cephalosporins and other new generation antibiotics.

Introduction to cardiovascular drugs, cardiovascular diseases, lipoproteins (LDL, HDL etc.) and their role in atherosclerosis. Mechanism of action of some cardiovascular and antianginal drugs (Statins and other nitrate drugs). Chemistry and mode of action of some important antihistamines and anti-ulcer agents (ranitidine, famotidine, omeprazole, lansoprazole, etc.). Local anti-infective drugs. Antineoplastic agents. Antimalarial, anticholinergic and psychotic drugs (diazepam, oxazepam, chlorpromazine, lithium, alprazolam, barbiturates etc.).

Unit-4: Carbohydrate Chemistry

Basic structure and type of sugars. Chemistry of sucrose, maltose and gentiobiose. Glycosides, protection and deprotection. O-glycosylation and C-glycosylation. Deoxy-sugars, amino sugars, glycolic sugars and their synthetic and biological aspects. Carbohydrates as chiral pools in organic synthesis.

Chemistry of naturally occurring oxygen heterocyclic compounds, polyphenolics and other antioxidants.

Unit-5: Bond activation and functionalization

Mechanisms of C-H bond activation with transition metals: Oxidative addition, sigma bond metathesis, electrophilic and metalloradical activation. Organic synthesis involving chelation-assisted C-H activation, ortho-C-H activation, C-H activation in heterocycles and base-assisted C-H activation. C-H, C=C and C≡C activated annulation reactions. Important synthetic approaches via C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis.

Course ID: Chem/ThSP/402

Unit-1: Quantum mechanics 3

Coordinate, momentum and matrix representations. Schrodinger and Heisenberg Pictures. Virial and Hellmann-Feynman theorems; applications. Generalized uncertainty relation. Momentum eigenfunctions, delta function (properties and representations) and Fourier transformation. Projection operators. Time reversal.

Unit-2: Perturbation theory

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications. Matrix perturbations. Degenerate perturbation theory. First order lifting of degeneracy and hybridization. The Stark effect.

Unit-3: Statistical Mechanics 1

Phase space; ergodic hypothesis; Liouville's theorem. Concepts of different ensembles with applications to selected systems. Fluctuations. Ideal Fermi and Bose gases. Planck's radiation formula. System of interacting molecules; treatment of imperfect gases.

Unit 4: Statistical Mechanics 2

Einstein's theory of Brownian motion; Langevin equation; fluctuation-dissipation relation; effect of friction. Discussion on the Fokker-Planck equation.

Unit-5: Theoretical Spectroscopy 1

Perturbative dynamics. Semiclassical treatment of radiation-matter interaction – first order and second order effects. Golden rule. Einstein's A, B coefficients. Connection of results with experimental quantities. Two-level system and Rabi oscillations

Course ID: Chem/ThSI/403

Unit-1: Chemical Bonding

MO theories in inorganic molecules: Empirical MO – Huckel theory, examples; symmetry adapted MO; symmetry and group theoretical methods for qualitative MO energy level diagram of AB_n types of molecules (n = 1 – 6); analogous MO treatment for transition metal complexes. Walsh diagram, Construction of Walsh correlation diagram for AB_n (n = 2 – 4) types of molecules. Study of variation of energies of MO with change in bond angle. Shapes of small molecules: VSEPR model, symmetry and group theoretical methods for construction of hybrid orbitals. Relativistic effects and its consequences: Concept and applications.

Unit-2: Molecular Excited States

Basic theories: different photonic and deactivation processes, energy level diagram. Morse curve, fluorimetric reagents, effect of substitution (on aromatic system), structural and environmental factors on photoluminescence; quenching and non-quenching extinction of fluorescence, pi-pi states, cation and anion sensing fluorescent molecules, low temperature and room temperature phosphorescence.

Chemiluminescence: Theory, mechanism and applications.

XRF: Basic principles and applications.

Unit-3: Spectroscopy 2

Application of IR, Raman, ESR, Mössbauer and PES in inorganic chemistry (examples with simple and complex inorganic compounds including organometallic and cluster compounds and bioinorganic systems).

NMR Spectroscopy: ¹H NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, magnetic susceptibility and resonance shifts. ¹¹B, ¹³C, ¹⁹F, ²⁷Al, ³¹P-NMR Spectroscopy with typical examples.

NQR Spectroscopy: Principle, nuclear quadrupole coupling constant, structural information from NQR spectra.

Unit-4: Electrochemical methods

Voltammetry: cyclic voltammetry, polarography, anodic stripping voltammetry; amperometry, coulometry, electrogravimetry: Basic principles and applications; high frequency titrations - basic concept and applications, ion-selective electrodes – concept and applications. Electrogravimetry, Cyclic Voltammetry, Spectroelectrochemistry: General concept and applications.

Unit-5: Chemistry of the Pt group metals

Pt group metals: Oxidation states, valence preferences toward pi-donor and pi-acceptor ligands. The Pt-metal chemistry in particular with C, N, O, P and S donor ligands: synthesis, structure and characterization. Structure and bonding in acetate complexes, radical complexes. Dinitrogen complexes of Ru and nitrogen fixation: structure and bonding in dinitrogen complexes of Ru, trans effect, use of Pt metals in catalysis and in medicines. Preparation and properties of historically important compounds like Creutz-Taube compound, Vaska's complex, Magnus' green salt, Vauquelin's pink salt, Krogmann's salt, etc.

Course ID: Chem/ThSO/403

Unit-1: Nanoscience and Biomimetic Chemistry

Basic concept on nanoparticles, quantum dot and nanocluster, surface atom effect, quantum size effect, nonmetal to metal transition, special properties of nanoparticles, important routes for fabrication of nanoparticles and porous nanomaterial, method of characterization, their application as smart catalyst in organic synthesis (e.g. C-C, C-N, C-O coupling reactions under reductive and oxidative conditions). Basic definitions of Biomimetics, application of supramolecular chemistry to Biomimetic design, relation to the designing of drugs and synthetic materials, involvement of organic chemistry in Biomimetics, classification of different Biomimetic fields – Peptidomimetics, Membranemimetic, Nucleic acid mimics.

Unit-2: Green Chemistry and PTC

Green chemistry- overview, Twelve Principles, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave. Solvent free organic reactions. Phase Transfer Catalyst – Theory of Phase transfer equilibrium, macrocyclic and macrobicyclic effect, application of quaternary ammonium salt, crown ether and cryptand in organic transformations.

Unit-3: Nucleoside and Nucleotide

Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Amino-acids-protein biosynthesis. Interactions of nucleic acids with small molecules. Structural features of DNA and RNA.

Unit-4: Natural Products as Lead Drug

Synthesis and mechanism of, anti-tumor, antiviral (AIDS, HIV, Herpes and Pox), anti-sense agent.

Unit-5: Synthetic Methodology 4

Alkylation of enolates and enamines, Reductive alkylations with special reference to asymmetric alkylations. Use of blocking groups, use of activating groups, alkylation of anions from 1,3-dithiane, alkylation of dihydro-1,3-oxazines. Umpolung reactions.

Course ID: Chem/ThSP/403

Unit-1: Solids

Reciprocal lattice. Structure factor. Fourier synthesis. Band theory, band gap. Metals and semiconductors – intrinsic and extrinsic semiconductors. Superconductivity. Special properties of nanomaterials and nanoparticles.

Unit-2: FT Spectroscopy: FT NMR and FTIR

Advantages of time-domain vs. frequency-domain studies. Principles of FT-IR and pulse-FTNMR with instrumentation. 1D vs. 2D NMR. Coherence and polarization transfer experiments. Determination of three dimensional structure of molecules using NMR spectroscopy.

Unit-3: Group Theory 2

MO theory with applications to σ and π bonding and construction of hybrid orbitals. LFT with applications to splitting of terms and levels in different coordination environments and construction of energy level diagrams. Applications of symmetry principles in Woodward-Hoffman type reactions.

Unit-4: Lasers and Masers

Principles of Maser and Laser action. Population inversion (two/three/four level systems). Basic elements in laser (resonator, Gain medium, Pumping technique). Characteristics of laser radiation (coherence:

temporal/spatial; polarization, monochromaticity, intensity). Single mode and tunable laser. Harmonic generation. Applications.

Unit-5: Electronic Spectroscopy

Molecular orbitals, classification of electronic states, electronic and vibronic selection rules for diatomic and polyatomic molecules, vibrational coarse structure (progressions and sequences), repulsive states

Course ID: Chem/LS/404

1. Write-up of review/literature survey
2. Continuous assessment and grand viva-voce

Course ID: Chem/LS/405

1. Write-up of project report
2. Oral presentation and discussion around the project work

Appendix

Detailed Chemistry Practical Worksheet

Chem/LG/105: Practical Inorganic Chemistry

- A. Semi-micro inorganic qualitative analysis: Special elements (uncommon): Be, Th, U, Ce, Mo, W, Zr, Ti (in their stable oxidation state/states) with commonly available anions (single element and binary mixtures).
- B. Determination of stability constants by pH-metric methods.
- C. Analysis of drugs like Ascorbic acid, Paracetamol, Isoniazide.

Chem/LG/204: Practical Organic Chemistry

- A. Identification of single organic compound (solid/liquid) with one or more functional group(s) through preparation of derivatives.
- B. Organic preparations (name reaction based/else) including methods of purification (e.g., crystallization, steam distillation, vacuum distillation, sublimation, etc.).

Chem/LG/205: Practical Physical Chemistry

- A. Analytical experiments: Iodination of acetone, Decomposition of H_2O_2 [by FeCl_3], Order of a reaction [e.g., $\text{BrO}_3^- - \text{I}^-$], Co-ordination number of Cu in $[\text{Cu}+(\text{NH}_3)_4]^{2+}$, Solubility product by precipitation method [e.g., of PbI_2], Isoelectric point of gelatine sol (viscometer)
- B. Instrumental experiments
Conductometry: Ostwald's dilution law, mixed halide composition, CMC, verification of Onsager equation.
Polarimetry: Inversion of Cane sugar.
Potentiometry: E_0 of Ag/Ag^+ and $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$, pK_a of AcOH .
Colorimetry: Job's method, iodination of acetone.

Chem/LSI/304: Practical Special Inorganic Chemistry

- A. Composition of a coordination compound by Job's/Mole-ratio/Slope-ratio method.
- B. DNA-Metal complex interactions (Spectrophotometrically).
- C. Synthesis and characterization of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands
- E. Preparation of optically active inorganic coordination compound and measurement of its optical activity with a polarimeter.

Chem/LSI/305: Practical Special Inorganic Chemistry

- A. Magnetic susceptibility/moment measurement of coordination compounds by Gouy balance.
- B. Kinetic studies of at least two reactions.
- C. Ion-exchange experiments (to determine strength/concentration of Metal ion or anion)
- D. CD Experiments
- E. Electrochemical Experiments

Chem/LSO/304: Practical Special Organic Chemistry

- A. Multistep organic preparations: Reactions may include (i) Benzaldehyde to Diphenyl acetic acid, (ii) Acetanilide to Sulphanilamide, (iii) Phthalic acid to 2-Iodobenzoic acid, etc.
- B. Extraction and purification of selected natural products (any two: Caffeine, Nicotine, Protein, beta-Carotene, Eucalyptus, etc.).

Chem/LSO/305: Practical Special Organic Chemistry

Chromatographic separation with TLC monitoring, and identification of the components of a binary mixture of organic solids by (A) chemical and (B) spectroscopic methods. Examples are (i) Anthracene + Benzoin, (ii) Benzil + Benzoin, (iii) Phenanthrene + Benzoic acid, etc.

Chem/LSP/304: Computer applications in Chemistry 2

- A. Formatting statements, uses of data files (r/w), subroutines and function subprograms.
- B. Use of 'RAND()': diffusion and the random walk problem, variants of the problem.
- C. Numerical integration and differentiation; position-momentum uncertainty products for the box and oscillator problems with given wave functions, etc.
- D. Solutions of differential equations by Euler and Runge-Kutta methods; finding out Schrodinger stationary states for the particle-in-a-box, harmonic oscillator and related problems; applications to radioactive equilibrium, etc.
- E. Interpolations (Newton, cubic spline, etc); extrapolations (Richardson, Pade, etc); applications.
- F. Matrix multiplication; diagonalization of matrices; applications to Huckel pi systems.

Chem/LSP/305: Practical Special Physical Chemistry

Autocatalysis by Mn^{2+} in permanganate-oxalic acid reaction (analytical/colorimetric)
Persulfate-iodide reaction: ionic strength effect (analytical)
Activation energy (H_2O_2 decomposition, analytical)
Ternary phase diagram (analytical)
Iodination of aniline (analytical/colorimetric)
 ΔpK_a of beta naphthol (spectrophotometric)
Mimicking antibiotic kinetics (spectrophotometric)
Quenching of fluorescence (fluorimetric)

Basic Concepts of Chemistry

Chem/TH/EP/305

(To be offered to students of other departments)

CBCS PAPER

Unit-1: Green Chemistry

Environmental Hazards and Pollution.

Green Chemistry-definition, need for Green Chemistry, limitations in the pursuit of Green Chemistry, basic principles, Applications of Green Chemistry to Chemical Synthesis.

Unit 2: Basic idea of crystal field theory

Valence Band theory, Basic idea of crystal field theory, Splitting of d-orbitals octahedral and tetrahedral, square planar, fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environment, Octahedral site preference energy, spinel and inverse spinel, hole formalism, inversion and equivalence reactions, splitting of dn terms in octahedral and tetrahedral fields, Tetrahedral distortion and Jahn Teller effect. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy.

Unit 3: Essential of Inorganic chemistry

Classification of metal ions and their roles in various basic chemical reactions in biological systems. Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs (examples only), metal dependent diseases.

Unit 4: Thermodynamics

Introduction to thermodynamics- 1st and 2nd law of thermodynamics, Thermochemistry and its applications, Physical concept of Entropy and auxiliary state functions (G and A), criteria for spontaneity and equilibrium, application to biological systems.

Unit 5: Classification of organic reactions and study of their mechanism

1. Substitution Reactions
2. Addition Reactions
3. Elimination Reactions
4. Rearrangement Reactions
5. Oxidation Reactions
6. Reduction Reactions
7. Oxidative Coupling
8. Reductive Coupling

Modern Concepts of Chemistry
Chem/TH/EP/306
(To be offered to students of other departments)
CBCS PAPER

Unit-1: Nanoscience

Introduction to nanoworld, Fundamental theories of nanoparticles (NPs), 0D, 1D and 2D nanoparticles and their physical, optical, electronic, magnetic properties, Methods of fabrication of metal organic and composite NPs, Application of NPs, nanoelectronics and devices.

Unit 2: Drugs & Pharmaceuticals:

Drug discovery, design and development. Preparation of Aspirin and magnesium bisilicate (Antacid). Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT-Zidovudine)

Unit 3: Biomolecules:

Structure and function of Biomolecules: Protein, nucleic acid, carbohydrates and lipids. Membrane structure. Biomolecular complexes: Protein–ligand, Enzyme–substrate and Drug–DNA. Examples

Unit 4: Rotational and Vibrational Spectroscopy:

Rigid rotors, selection rule for rotational spectra, harmonic oscillator, selection rule for vibrational spectra, anharmonicity, appearance of overtones; Raman scattering.

Unit 5: Atomic Structure and Spectra

Atomic spectra: Hydrogen atom spectra, orbital and spin angular momentum; Stern-Gerlach experiment, spin-orbit interaction, spectral term symbols.