CHEMISTRY SYLLABUS

Two-Year Four-Semester PG Course in Chemistry

DHWU
2017

Syllabus for Two-Year Four-Semester PG Course in Chemistry

DHWU
COURSE STRUCTURE

Two – Year, 4 – Semester PG Course in Chemistry: Grand Total Marks - 1000

(First Year) First Semester:

Paper	Subject	Marks in Semester Exam.	Marks in Midterm Evaluatiion /Sessional	Total	Periods/ Week	
Chem/ThG/101	Chemistry Theory General	40	10	50	4+1	
Chem/ThG/102	Chemistry Theory General	40	10	50	4+1	
Chem/ThG/103	Chemistry Theory General	40	10	50	4+1	
Chem/LG/104	Chemistry Laboratory General	30	20	50	3 x 3pds = 09	↑
Chem/LG/105	Chemistry Laboratory General	30	20	50	2 x 3pds = 06	↓
Total				250	30 (15 Th +15 Lab)	

(First Year) Second Semester:

Paper	Subject	Marks in Semester Exam.	Marks in Midterm Evaluation /Sessional	Total	Periods/ Week	
Chem/ThG/201	Chemistry Theory General	40	10	50	4+1	
Chem/ThG/202	Chemistry Theory General	40	10	50	4+1	
Chem/ThG/203	Chemistry Theory General	40	10	50	4+1	
Chem/LG/204	Chemistry Laboratory General	30	20	50	3 x 3pds = 09	↑
Chem/LG/205	Chemistry Laboratory General	30	20	50	2 x 3pds = 06	↓
Total				250	30 (15 Th +15 Lab)	

ThG: Theory General
LG: Laboratory General

(Second Year) Third Semester:

Paper	Subject	Marks in Semester Exam.	Marks in Midterm Evaluation /Sessional	Total	Periods/ Week	
Chem/ThG/301	Chemistry Theory General	40	10	50	4+1	
Chem/ThS/302	Chemistry Theory Special	40	10	50	4+1	
Chem/ThS/303	Chemistry Theory Special	40	10	50	4+1	
Chem/LS/304	Chemistry Laboratory Special	30	20	50	2 x 3pds = 06	↑
Chem/LS/305	Chemistry Laboratory Special	30	20	50	3 x 3pds = 09	↓
Total				250	30 (15 Th +15 Lab)	

(Second Year) Fourth Semester:

Paper	Subject	Marks in Semester Exam.	Marks in Midterm Evaluation /Sessional	Total	Periods/ Week	
Chem/ThS/401	Chemistry Theory Special	40	10	50	4+1	
Chem/ThS/402	Chemistry Theory Special	40	10	50	4+1	
Chem/ThS/403	Chemistry Theory Special	40	10	50	4+1	
Chem/LS/404	Chemistry Laboratory Special	30	20	50	2 x 3pds = 06	↑
Chem/LS/405	Chemistry Laboratory Special	30	20	50	3 x 3pds = 09	↓
Total				250	30 (15 Th +15 Lab)	

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

$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/ThS : Chemistry Theory Special
Chem/ThSI: Chemistry Theory Special Inorganic
Chem/ThSO: Chemistry Theory Special Organic
Chem/ThSP: Chemistry Theory Special Physical

Chem/LG : Chemistry Laboratory General
Chem/LS : Chemistry Laboratory Special
Chem/LSI : Chemistry Laboratory Special Inorganic
Chem/LSO : Chemistry Laboratory Special Organic
Chem/LSP : Chemistry Laboratory Special Physical

Semester – I

Course ID: Chem/ThG/101

Unit-1: Symmetry
Symmetry elements and symmetry operations. Group theory. Group multiplication tables and molecular point groups. Platonic solids. Stereographic projections of point groups. Introduction of periodic symmetry.

Unit-2: Coordination Chemistry 1
Crystal field theory: Splitting of d-orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral 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. 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. Limits of applicability of crystal field theory.

Unit-3: Bioinorganic Chemistry 1
Elements of life: basic reactions in biological systems and roles of metal ions. Bioenergetic principle and role of ATP. Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Transport across biological membrane: Na^+-K^+-ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, 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 Bailer 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 aromaticty, annulenes, heteroannulenes, fullerenes (C_{60}), alternant and non-alternant hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods-Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene,Walsh orbitals of cyclopropane and cyclobutane, Hammett equation and its modifications, HSAB principles.

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, alkyl ketone effect, 2- halo ketone effect, allylic strains ($A^{1,2}$ and $A^{1,3}$), decalin and their derivatives; perhydroanthracene, perhydrophenanthrene etc., Felkin-Anh, Cieplak and Zimmerman-Traxler Models; Addition Reactions to Carbonyl Compounds.

Unit-3: **Pericyclic Reactions 1**

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, Dewer-Zimmermann approach, Mobius and Huckel systems. 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.

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, A_2B_2 in proton NMR. Introduction to ^{13}C-NMR spectroscopy. Application of NMR spectroscopy and other spectroscopical techniques to simple structural and mechanistic problems.

Unit-5: Natural Products 1

Isoprene rule, Structure elucidation (by chemical and spectroscopic methods), Synthesis, Biogenesis and Biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. Structural types: general introduction, general study and structural features of sesqui-, di- and tri-terpenes, carotenoids and chemistry of their representative members.

Course ID: Chem/ThG/103

Unit-1: Thermodynamics 1
Chemical potential. Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures.
Thermodynamics of ideal and non-ideal binary solutions: excess functions; partial molar properties. Gibbs Duhem equation: uses. Different scales of activity coefficients for solutes and solvents.

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: 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.

Course ID: Chem/LG/104

1. Use of standard commands to write elementary programs.
2. 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: 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-2: Coordination Chemistry 2
Ligand field theory: Experimental evidences of metal ligand overlap, spin-orbit coupling and interelectronic repulsion parameters in complex ions/free ions. Metal-centered electronic spectra of transition metal complexes: microstates, determination of ground and all excited state terms of d^n ions, splitting of d^n terms in octahedral and tetrahedral fields; electronic structure and bonding in ML_4 and ML_6 complexes on the basis of symmetry and overlap principles and their MO energy level diagrams, Orgel diagrams (qualitative approach), hole formalism – inversion and equivalence relations; selection rule for spectral transitions, d-d spectra and crystal field parameters; Nephelauxetic effects. Qualitative idea of Tanabe-Sugano diagrams; charge transfer spectra. Magnetic properties of coordination compounds: spin and orbital moment, spin-orbit coupling, quenching of orbital moment, spin only formula.

Unit-3: 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 $K[Pt(C_4H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$ and $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination; electrophilic and nucleophilic reactions of coordinated ligands.

Unit-4: Solid-state Chemistry 1
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.

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 metal-atom 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 f-block elements with comparison, lanthanide shift reagents and uses of lanthanides.

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-pi-methane, oxo di-pi methane and aza di-pi methane rearrangements,Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, $S_{RN}1$ 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- Wordsworth-Emmons 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 2

Familiarity with methods of structure elucidation (chemical & spectroscopic methods). Biosynthesis, synthesis and biological activity of alkaloids (nicotine, atropine, coniine and papaverine).

Course ID: Chem/ThG/203

Unit-1: Quantum Mechanics 2
Bound-states and their properties. Box with finite walls; the Kronig-Penney model and formation of bands. 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: 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.

Unit-4: Statistical Thermodynamics
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-5: Interfacial Chemistry
Curved surfaces: Young-Laplace and Kelvin equations. Adsorption on solids: BET equation. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; emulsions.

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. N_2, O_2, 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: Emission Spectroscopy
FC principle. Mirror-image symmetry and its violation. Radiative and radiationless deactivation. Polarization characteristics of emission. Quenchers and lifetime variations.

Unit-5: FT Spectroscopy
Advantages of time-domain vs. frequency-domain studies. Principles of FT-IR and pulse-FT-NMR with instrumentation.

Course ID: Chem/ThSI/302

Unit-1: 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-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: Group Theory

Group theory and quantum mechanics (elementary ideas); representation of point groups, reducible and irreducible representations, definitions of classes and character; statement of grand orthogonality theorem, construction of character table, reduction formula; direct product representation and its uses; symmetry of normal modes, normal mode analysis, selection rules for IR and Raman transitions. Hybridization.

Unit-4: Solid-state Chemistry 2

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, X-ray diffraction analysis (spectral analysis, particle-size determination, etc.).

Unit-5: 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 metatheses reaction of alkenes and alkynes; Ziegler-Natta catalysis, photodehydrogenation catalyst (platinum POP).

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: ^{1}H and ^{13}C NMR principles, rules for carbon 13 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: Asymmetric Synthesis 1

Principles and newer method of asymmetric synthesis (including enzymatic and catalytic nexus), enantio- and diastereoselective synthesis. Reactions of enolates (α–substitution), Addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, Asymmetric hydroboration, Conjugate additions.

Unit-4: Bio-active Molecules

Chemistry of porphyrins, lipids, polyunsaturated fatty acids, arachidonic acid cascade, prostaglandins – structure and synthesis. Steroids : General methods of study and structural type. Chemistry of cholesterol, hormones, bile acids, vitamins of D – group, diosgenin.

Unit-5: Medicinal Chemistry 1

Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics.

Vitamins - Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B_1, B_6 and folic acid, etc.

Drugs - Introduction and classification of drugs, brief discussion on drug targets. Sulphur drugs, anti tubercular drugs, anti diabetic drugs and newer generation of antacids.

Course ID: Chem/ThSP/302

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: 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-3: Valency
Born-Oppenheimer approximation and beyond. Avoided crossings. Virial theorem and chemical bonding. Theories of valence: VB and MO. Discussion on H_2^+ and H_2; dissociation limits.

Unit-4: Thermodynamics 2
State functions. Legendre transformation; Energy and entropy representations; Massieu functions; minimum and maximum principles. Stability conditions; the Le Chatelier principle. Thermodynamics of phase transitions.

Unit-5: 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.

Course ID: Chem/ThSI/303

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. Nitrogen fixation. Cobalamins including vitamin and coenzyme B12.
Structural/functional models of some of the above-mentioned systems.

Unit-2: X-ray crystallography 1
Fundamentals of X-ray, crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their proper ties. Diffraction of X-ray, lattice planes, indices, Brag's condition, reciprocal lattice and its relation to direct lattice; Bragg's law in reciprocal space.

Unit-3: 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-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: 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/303

Unit-1: 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, Heathcock modification, Wickterle annelation, Halo ketal annelation – cation effect on this reaction, Woodward annelation and Danishefsky's modification with phosphoranes), Ring closure reactions (Dieckmann, Ruzicka, Thorpe cyclisation, Acyloin condensation, etc.) and other miscellaneous cyclisations. Ring formation via polyene cyclisation.

Unit-2: 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.

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 Baeyer-Villiger rearrangement. Ionic hydrogenation, synthetic use of TMSCN, TMSNCO, TMSI, TMSNHCOMe, $TMSN_3$ etc.

Organotin reagents for selective reactions.

Unit-4: Medicinal Chemistry 2

Pharmacodynamics: different types of drugs and drug targets, drug binding forces, role of enzymes. Drug – receptor interactions, mechanism of drug action, agonists, antagonists. Affinity, efficacy and potency of a drug, dose-response curves.

Pharmacokinetics**:** drug absorption, distribution, metabolism (Phase-I and Phase-II transformations), excretion, drug formulation and others.

Unit-5: Pericyclic Reactions 2

Diels – Alder reactions : Regiochemistry and stereochemistry of Diels – Alder reaction, intramolecular Diels – Alder reactions, retro Diels – Alder reactions, asymmetric Diels – Alder reactions, Diels – Alder reactions of inverse electron demand, hetero Diels – Alder reactions and Lewis acid catalysed Diels – Alder reactions.

Cycloaddition reactions with ally cations and allylanions, 1,3–dipolar cycloaddition reactions, sigmatropic rearrangements of charged systems.

Course ID: Chem/ThSP/303

Unit-1: 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-2: Electrochemistry 1

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.

Unit-3: 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.

Unit-4: Vibration-rotation Spectra

Principles. Rotational coherence spectroscopy; rotational and vibrational spectra (electronic excitation: pump-probe technique) of excited and transient states. Time-resolved IR, 2-d IR, rotovibrational spectra.

Unit-5: NMR Spectroscopy

1D vs. 2D NMR. Coherence and polarization transfer experiments. Determination of three-dimensional structure of molecules using NMR spectroscopy.

Course ID: Chem/LSI/304

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

Course ID: Chem/LSI/305

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

Course ID: Chem/LSO/304

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

Course ID: Chem/LSO/305

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/304

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

Course ID: Chem/LSP/305

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

Semester - IV

Course ID: Chem/ThSI/401

Unit-1: X-ray Crystallography 2

Methods of growing single crystals, crystal mounting, experimental diffraction methods (Laue method, rotating crystal method), Geometric data collection (simple examples), structure factor, structure solution, structure refinement, R value, systematic absence, heavy-atom method. Fourier synthesis, Patterson function.

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, photo-splitting 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, Zintle 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 3

Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules, helicity rules, exceptions and excitation chirality; atomic and conformational asymmetry. Chiral analysis by polarimeter, NMR, GC, HPLC and Capillary Electrophoresis (CE) methods. Baldwin's Rules - applications, hydrolytic kinetic resolution.

Unit-2: Asymmetric Synthesis 2

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 2

Pyrimidines, pyridazines, pyrazines, purines, pteridines, compounds with oxygen and sulfur hetero atoms. Role of heterocyclic compounds in biological systems.

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 Ziegler-Natta 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: 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: 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.

Unit-4: 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-5: 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.

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
Transport of ions across membranes, Na/K ion pump. Metal storage and transport proteins: transferring, ferritin, ceruloplasmin, calmodulin. Oxygen binding and transport proteins: hemoglobin, myoglobin, hemerythrine, hemocyanin. 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.
Hydrolytic enzymes: Carboxy peptidase, Carbonic anhydrase. 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: 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.

Course ID: Chem/ThSO/402

Unit-1: NMR Spectroscopy 3

Application of DEPT, ^{1}H-^{1}H COSY, ^{1}H-^{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, biomimetic chemistry, 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 3

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, *De novo* design, Molecular Recognition, Receptor Based Molecular Modeling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective dugs, Antimalarial, Anticholenergic and CNS-active drugs.

Unit-4: Carbohydrate Chemistry

Basic structure and type of sugars. Protection and deprotection. Deoxy-sugars, amino sugars, glycal sugars and their synthetic aspects. Synthetic approach (Combinatorial) towards polysaccharides of biological and industrial importance. Carbohydrates as chiral

pools in organic synthesis.

Unit-5: Natural Products 3

Structure, transformation and biosynthesis of alkaloids from terrestrial and marine sources; Chemistry of quinoline alkaloids with special reference to cinchona group; Chemistry of isoquinoline alkaloids – morphine group; structure, transformations, synthesis of simple and monoterpenoid derived indole alkaloids – yohimbine, reserpine, strychnine, ellipticine, lysergic acid.

Course ID: Chem/ThSP/402

Unit-1: 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-2: Non-equilibrium thermodynamics
Characterization of Non-equilibrium states: Entropy production rate; energy dissipation. Flux-force relations (phenomenological equations) with suitable examples. Microscopic reversibility and detailed balance. Coupling of irreversible processes. Onsager reciprocal relations. Non-equilibrium stationary states.

Unit-3: Electrochemistry 2
Ion Solvent interaction: concept and applications. Solvation number and its determination. Ion-solvent-non-electrolyte interactions: Salting-in and salting-out phenomena.
Ion-Association: Bjerrum and Fuoss treatments for ion-pair formation and conductance minima; Walden's empirical rule.

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: 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.

Course ID: Chem/ThSI/403

Unit-1: Crystal Field and Ligand Field Theories
Crystal field splitting of orbital degeneracy of free ions – group theoretical treatment, calculation of crystal field splitting of d energy level: (i) electrostatic potential due to octahedral distribution of point charges – expansion in terms of spherical harmonics (with derivation), similar potentials due to tetrahedral, tetragonal and square planar distribution (derivation not required) (ii) effect of octahedral/tetrahedral potential on d orbital – perturbation calculation on energy splitting.
Effect of spin-orbit coupling, Tanabe-Sugano diagram, normal modes and normal coordinates of vibration, symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.
Vibronic coupling and its group theoretical consideration and implications; Jahn-Teller effect – origin, first-order and second-order Jahn-Teller effect with examples.

Unit-2: 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-3: 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 florescent molecules, low temperature and room temperature phosphorescence.

Chemiluminescence: Theory, mechanism and applications.

XRF: Basic principles and applications.

Unit-4: 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: $_1$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-NMR Spectroscopy with typical examples.

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

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, Membranemimeticl, 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. Covalent 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 and DNA cleaving agents.

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: 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-3: 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.

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: Theoretical Spectroscopy 2

Selection rule for vibrational spectra, anharmonic correction by perturbation – appearance of overtones; selection rule for rotational spectra; nuclear spin and rotational energy levels. Stark effect. Raman scattering, selection rule for rotational-vibrational Raman effect. Non-linear scattering phenomena.

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/104: Computer Applications in Chemistry 1

A. Computer: components; storage devices; WINDOWS and LINUX environments.
B. Elements of programming: variables; library functions; ‘do’ loop; control and ‘if’ statement.
C. Use of standard commands to write elementary programs, especially (i) sorting and ordering, (ii) linear regression, (iii) covariance and correlation coefficient (data from standard books), (iv) iterative solution (Newton-Raphson) of equations, etc.
D. Uses of standard free softwares (any two/three: Avogadro, Schrodinger, PCMODEL, RASMOL, REAXIS, ChemOffice, DTMM, etc.) for structure optimization/molecular graphics/ orbital shapes/rotational barriers/ structure-activity relationships/stabilities of conformational isomers/bond energy/formation energy, etc. and some others for studying reactions/spectral predictions of various organic/inorganic molecules.

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., BrO_3^- - $I^{-]}$
Co-ordination number of Cu in $[Cu^+(NH_3)_4]^{2+}$
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 $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$, 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. Flame photometric experiments (Na, K).
D. Preparation of at least two inorganic coordination compounds and their physicochemical characterization. (e.g., coordination compounds like $[Mn(acac)_3]$ or $[Fe(acac)_3]$, $[Co(NH_3)_6]Cl_3$, $[Ni(en)_3]Cl_2$, $[Et_4N][MnX_4]$, X = Cl, Br, NCS, etc.).
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: Caffine, 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 napthol (spectrophotometric)
Mimicking antibiotic kinetics (spectrophotometric)
Quenching of fluorescence (fluorimetric)