SYLLABUS

FOR

TWO-YEAR FOUR-SEMESTER
M. Sc. COURSE IN **CHEMISTRY**

2020

RANI RASHMONI GREEN UNIVERSITY

DEPARTMENT OF CHEMISTRY
RANI RASHMONI GREEN UNIVERSITY

TWO-YEAR FOUR-SEMESTER M. Sc. COURSE IN CHEMISTRY

COURSE STRUCTURE

DURATION	SEMESTER				TOTAL MARKS
	I JULY-DEC	II JAN-JULY	III JULY-DEC	IV JAN-JUNE	
MARKS	**300**	**300**	**250**	**250**	**1100**
COURSE TYPE	THEO PRAC	THEO PRAC	THEO PRAC	THEO PRAC	
COMPULSARY (CHEM)	**150 100**	**150 100**	**100 100**		**700**
CREDIT POINTS	**(12) (8)**	**(12) (8)**	**(8) (8)**		**(56)**
CHOICE BASED (CHEM OR OTHER)	**50**	**50**	**50**	**150 100**	**400**
CREDIT POINTS	**(4)**	**(4)**	**(4)**	**(12) (8)**	**(32)**
Total Marks	**200 100**	**200 100**	**150 100**	**150 100**	**1100 (88)**

Total Credit Points: **88**

SEMESTER-I (Marks: 300)

Course ID	Marks/Credit			
	Theo	Credit	Prac	Credit
CHEM-C11	50	4	-	-
CHEM-C12	50	4	-	-
CHEM-C13	50	4	-	-
NON-CHEM-CB11/CB12	50	4	-	-
CHEM-C14	-	-	100	8
Total	200	16	100	8

SEMESTER-II (Marks: 300)

Course ID	Marks/Credit			
	Theo	Credit	Prac	Credit
CHEM-C21	50	4	-	-
CHEM-C22	50	4	-	-
CHEM-C23	50	4	-	-
NON-CHEM-CB21/CB22	50	4		
CHEM-C24	-	-	100	8
Total	200	16	100	8

SEMESTER-III (Marks: 250)

Course ID	Marks/Credit			
	Theo	Credit	Prac	Credit
CHEM-C31	50	4	-	-
CHEM-C32	50	4	-	-
CHEM-CB33I/ -CB33O/ -CB33P	50	4	-	-
CHEM-C34	-	-	100	8
Total	150	12	100	8

SEMESTER-IV (Marks: 250)

Course ID	Marks/Credit			
	Theo	Credit	*Project	Credit
CHEM-CB41I/ -CB41O/ -CB41P	50	4	-	-
CHEM-CB42I/ -CB42O/ -CB42P	50	4	-	-
CHEM-CB43I/ -CB43O/ - CB43P	50	4	-	-
CHEM-CB44	-	-	100	8
Total	150	12	100	8

*Consisting of Review (30 marks), Project Work (50 marks) and Grand Viva (20 marks)

Syllabus

Semester-I

Course ID: CHEM-C11

Unit-1: Symmetry and Group Theory

Symmetry elements and symmetry operations, introduction to group theory, matrix representation of symmetry operations, multiplication tables and molecular point groups, reducible and irredicible representations, classes of symmetry operations, statement of Great Orthogonality Principle (without derivation) and construction of character tables, (viz C_{2v}, C_{3v}, D_2 and C_{2h})

Unit-2: Coordination Chemistry-1

CFT, splitting of d-orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal, octahedral and cubic fields of similar and dissimilar ligands; CFSEs in weak/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, CFAE, labile and inert complexes

Unit-3: Bioinorganic Chemistry-1

Elements of life, basic reactions in the 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 disease: Wilson's disease, Alzheimer disease; metal complexes as drugs: Pt, Rh, Ru and Au drugs; toxic effects of metal ions and detoxification by chelation therapy

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 centers in ionic crystals; band theory and band gap: metals, insulators, semiconductors (intrinsic and extrinsic)

Unit-5: Electrochemical Analyses

Principles and applications of electrogravimetry, coulometry, voltammetry, polarography, differential pulse polarography, anodic stripping voltammetry, amperometry and cyclic voltammetry

Course ID: CHEM-C12

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}), alternate and non-alternate 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

Winstein-Holness equation, Curtin-Hammett principle; conformational analysis of cyclohexane, cyclohexene, 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, carbene addition; rationalization based on Frontier MO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Sommelet, Hauser, Cope and Claisen rearrangements, Ene reaction, Wittig rearrangement

Unit-4: NMR Spectroscopy-1

Principle, instrumentation and different techniques (CW and FT) of NMR spectroscopy; factor 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 structure and mechanistic problems

Unit-5: Natural Products-1

Terpenoids: Isoprene rule, structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis and biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes; structural types: general introduction to sesqui-, di- and tri-terpenoids

Course ID: CHEM-C13

Unit-1: Atomic Structure

Zeeman Effect (normal and anomalous), fine structure, spin-orbit interaction; effect of high magnetic field, Lande g factor, atomic (and molecular) terms, fine structure

Unit-2: Quantum Mechanics-1

Postulates and their analyses; properties of operators and commutators; equation of motion, stationary states, Ehrenfest's theorem and uses, Barrier problems

Unit-3: An Overview on Elementary Nanochemistry

Quantum mechanical approach for the elucidation of density of states; carbon based nanostructured material(s) - synthesis, structural characterization and spectroscopic properties; preparation of metal nanoparticles (Zn, Ag, Au) using simple chemical technique and study of their optical properties; green synthesis of nanoparticles

Unit-4: Kinetics-1

Fast reactions, oscillatory reactions, autocatalysis, electrode kinetics; Nernst, Butler-Volmer and Tafel equations

Unit-5: Absorption Spectroscopy

Principles, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and $d \rightarrow d$ transitions; solvent effects, weak- and CT-interactions; vibronic and spin-orbit couplings

Course ID: EVS-CB11

Unit-1: Basic Concept of Environment

Basic concepts of environment and environmentalism, environmental education and awareness, environmental ethics and global imperatives, basic concept of sustainable development

Unit-2: Ecosystems and Ecology

Ecosystems: types, structures and function; energy flow in ecosystem, biogeochemical cycle, population and community ecology, niche and habitat concept, succession, biodiversity and conservation biology

Unit-3: Energy and Environment

Energy, environment and society; renewable and nonrenewable energy resources, types of alternative energy, energy security and energy audit

Unit-4: Green Technology

Applications of green technology, green infrastructure, green Chemistry, green planning and economy

Unit-5: Current Environmental Issues in India

Environmental movements and related issues; water, energy and waste management issues, joint forest management, man-animal conflict, ecological restorations, environmental pollution, extreme weather events, land use related issues

Course ID: CHEM-C14

Qualitative analysis of mixture of inorganic compounds; separation of inorganic compounds (cations and anions) by ion exchange column and their estimation; analysis of alloys - brass, steel, bronze etc by spectrophotometry, complexometry, redox titration and garvimetry; analysis of ores/minerals - dolomite, bauxite etc; syntheses and characterization of some coordination compounds of 3d metal ions, for examples, $[VO(acac)_2]$, $[Cr(acac)_3]$ (acacH = acetylacetone), $K_3[Fe(ox)_3]$ (ox = oxalate), $[Co(NH_3)_6]Cl_3$, $[Ni(en)_3]Cl_2$ (en = ethylenediamine), $[Cu(oxin)_2]$ (oxinH = 8-hydroxyquinoline), etc

Semester-II

Course ID: CHEM-C21

Unit-1: Chemical Bonding

Variation method, LCAO method; molecular orbital theory of H_2^+, H_2, homo- and hetero diatomic, triatomic and polyatomic (including T_d, O_h, and D_{4h} coordination complexes) molecules/ions; electron pair wave function, VB theory and its application to H_2 molecule, comparison of VB and MO theories

Unit-2: Coordination Chemistry-2

Metal-centered electronic spectra of transition metal complexes; microstates, determination of ground and excited state terms of d^n ions, splitting of d^n terms in O_h and T_d fields, Orgel diagrams (qualitative approach), hole formalism – inversion and equivalence relations, selection rule for spectral transitions, d-d spectra and CF-parameters, nephelauxetic series; magnetic properties of coordination compounds: spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, room- and variable-temperature magnetic moments

Unit-3: Organometallics-1

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, isolobal and isoelectronic relationships; 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 $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$, etc; reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination

Unit-4: Selected Topics on the Chemistry of s- and p-Block Elements

Structure and bonding in higher boranes based on Lipscomb's topological concept, Wade's rules, borohydride $B_nH_n^{2-}$ anions, carboranes, metalloboranes, hydroboration reactions; alkali metal complexes with macrocyclic ligands (crown ethers, cryptates and spherand); aqueous and complex chemistry of beryllium and

aluminium, basic beryllium compounds; main group organometallics: classification, syntheses, reactions, structure and bonding and applications of typical ones

Unit-5: Errors in Chemical Analysis

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; standardization and calibration; least squares method for calibration plots; minimizing error, sensitivity and detection limit

Course ID: CHEM-C22

Unit-1: Photochemistry-1

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *Cis-trans* isomerization, Paterno-Buchi reaction, Norrish type-I and -II reactions, photoreduction of ketones, di-pi-methane rearrangement, photochemistry of arenes, photoreaction in solid state, method of generation and detection (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications; cyclisation of radicals

Unit-2: Synthetic Strategy

Retrosynthetic analysis, disconnection approach, typical examples to ilustrate the disconnection approach, functional group interconversion, umpolung (1,3-dithiane), convergent synthesis

Unit-3: Heterocyclic Chemistry-1

Synthesis and reactivity of pyridine, quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole, isooxazole and their applications in organic synthesis

Unit-4: Synthetic Methodology

Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates; chemistry of organophosphorus compounds, phosphorus ylides and chiral phosphines; chemistry of organosulphur compounds, sulphur-stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylides, chiral sulphoxides

Unit-5: Natural Products-2

Alkaloids: Classifications, familiarity with methods (chemical and spectroscopic) for structure elucidation, biosynthesis, synthesis and biological activity of alkaloids like nicotine, atropine, coniine and papaverine

Course ID: CHEM-C23

Unit-1: Quantum Mechanics-2

Bound-states, box with finite walls; Kronig-Penney model, energy-spectrum of electrons and band formation; harmonic oscillator (wavefunction and operator methods); elements of variational method

Unit-2: The H-Atom Problem

Cartesian and polar coordinates, center of mass and relative coordinates, general forms of solutions and orbital specifications, spherical harmonics, real and complex orbitals, role of constants of motion; concept of antihydrogen

Unit-3: Kinetics-2

Potential energy surface – analysis of molecular geometry and chemical reaction dynamics, reaction coordinates and reaction paths, saddle point; BEBO method; absolute rate theory, sample case studies; 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, applications to chemical/ionization equilibrium; equipartition principle, Gibbs paradox and quantum statistics, blackbody radiation

Unit-5: Interfacial Chemistry

Analysis of surfaces, curved surfaces: Young-Laplace and Kelvin equations, adsorption on solids: BET equation, micelles, reverse micelles, micellization equilibrium, thermodynamics of micellization; micro- and macro-emulsions

Course ID: EVS-CB-21

Unit-1: Natural Resource Management and Sustainability

Concept of natural resources, water resources, mineral resources, energy resources, land resources, forest resources; bio-resources and management; sustainable use of resources

Unit-2: Waste Management

Solid, liquid and gaseous wastes; pollution from untreated waste disposal/discharge, toxic effects of waste, waste segregation, handling and management; analysis and treatment of wastes, domestic and industrial waste management, resource recovery and reuse, waste to energy; zero liquid discharge: concept, laws and policies for pollution prevention and waste management

Unit-3: Urban Ecosystem and Management

Urbanization, development induced population displacement, environment in an urban setting, urban dwelling, heat islands, urban interface with the environment,

natural spaces in a city; pollution due to population explosion and habitat degradation, planning and environmental management

Unit-4: Hazards and Disaster Management

Hazards, disasters, risks and vulnerability; earthquake, flood, cyclone and tsunami; mitigation and preparedness; disaster management, national policies and programs, role of local bodies, case studies on major natural disasters

Unit-5: Regulations for Environmental Management

Environmental impact assessment-regulations, notifications and amendments, environmental monitoring and role of regulatory agencies, coastal regulatory zones, special economic zones, environmental audit, corporate environmental responsibility

Course ID: CHEM-C24

Identification of single organic solid and liquid compounds; chromatographic separation and identification of the components in binary mixtures of organic solids and liquids; single-step/multi-step synthesis of selected organic compounds, drugs and drug-analogues using classical/greener benign method and their purification

Semester-III

Course ID: CHEM-C31

Unit-1: IR and UV-Vis-NIR Spectral Study

IR: Basic elements, elucidation of geometric and electronic structures, stereochemistry, bonding and reaction pathways in organic, inorganic, coordination and organometallic compounds; characteristic group frequencies: stretching and bending vibrations and their secondary shifts due to coordination, new bands upon coordination; characterization of varied geometrical and linkage isomers in different polyhedra; FTIR and interpretation of spectra

UV-Vis-NIR: Principle, spectral analysis of organic, inorganic, coordination and organometallic compounds, determination of analyte concentration; electronic transition time, designation of bands, effect of solvents, characteristic absorptions of varied chromophoric systems, kinetics and mechanistic study; vibrational structures, selection rules and their violations, elementary idea on spectra of d^n and f^n ions

Unit-2: NMR Spectral Study

Overview, spin-spin coupling: through space and through bond, ^{1}H NMR spectra of dia- and paramagnetic organic, inorganic, coordination and organometallic species; study on electronic and structural properties; dipolar/contact shift, magnetic susceptibility and resonance shifts; techniques for simplification of complex spectra, decoupling: gated/inverse gated, principles of NOE; fluxionality, dynamic equilibrium, matalloligand behaviour, hapticity, probing chemical reactivity and reaction pathways (intra-/intermolecular, stereo-retentive/-dynamic); techniques for simplification of complex spectra; ^{11}B, ^{13}C, ^{19}F, ^{31}P, ^{195}Pt-NMR study with typical examples

Unit-3: Mössbauer, Photoelectron and X-ray Fluorescence Spectral Study

Mössbauer: Fundamentals, recoilless transition, Mössbauer effect, Doppler effect; isomer shift - unit and factors affecting; quadruple interaction, magnetic interaction; information on spin/oxidation state, electronic structure, bonding and electron exchange reaction; typical spectra of Fe, Sn, I, etc compounds and biological systems

Photoelectron: photoionization, core level (XPS, ESCA) and valence level (UPS) experiments, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about nature of molecular orbital from UPS, UPS of simple diatomic molecules like N_2, O_2, CO, HCl etc

X-ray Fluorescence: Principle, instrumentation and application in quantitative analysis

Unit-4: EPR and Auger Electron Spectral Study

Principle, internal standard, line-width, derivative spectrum, relaxation time, frozen glass and low-temperature study, doping, factors affecting g values, hyperfine/ superhyperfine interaction, ZFS, anisotropy in magnetically equivalent and nonequivalent set of nuclei, intensity, Kramer's transition, spin densities and McConnell relationship; structural information of organic radicals, inorganic molecules/molecular ions and coordination compounds; conjunctive study with electrochemistry in probing electron-transfer site, covalence in M-L bond

Auger Electron: Principle, transition of Auger electron, Auger effect, quantitative analysis, probing chemical and compositional surface structure, applications

Unit-5: Mass and CD-ORD-MCD Spectral Study

Mass: Working principle; ion generation: EI, CI, ESI, FAB, MALDI-TOF; ion-detection/-analysis/-abundance; molecular ion-/metastable/isotope- peak; ion-molecule interaction, fragmentation patterns analysis, McLafferty rearrangement; nitrogen rule; mass analysis and mass accuracy; structure determination by major hyphenated mass spectral methods like GC-MS, LC-MS, MS-MS, etc

CD, ORD and MCD: Background, molecular dissymmetry, electronic/vibrational chiro-optical properties; spectral study and absolute configuration/conformation of organic, inorganic, coordination and organometallic compounds; biological samples; Cotton effect and Faraday effect, octant rule, axial halo ketone rule, lactone sector rule; symmetry of electronic levels

Course ID: CHEM-C32

Unit-1: Nuclear Chemistry

Fundamentals, nuclear composition, nuclear models - liquid drop model, Fermi gas model, nuclear forces, strong/weak interaction; nuclear angular momentum, magnetic dipole/electric quadruple moments in terms of shell model, parity of nuclear energy states; semi-empirical binding energy (BE) equation, mass parabola and application of BE equation; magic number and its derivation from nuclear potential well; calculation of nuclear spin, nuclear isomerism and non-optical transitions; nuclear reaction dynamics and its cross-section, energetic, mechanism and models, compound nucleus theory; nuclear reactors and particle accelerators; nuclear excitation, idea of nuclear temperature and entropy, interaction of radiation with matter

Unit-2: Photochemistry-2

Photoactive compounds, photonic molecules, modes of photo-excitation in free and coordinated molecules: d-d/LF, CT, intervalence, $\delta \rightarrow \delta^*$ excitations; excimers/exciplexes, life-time, cage effect, prompt/delayed reaction, triplet-triplet annihilation; mirror image rule, Stokes shift in photoluminescence; Kasha's/ Vavilov's/Adamson's rules; chemical actinometer, photosensitization reaction and photosensitizer, quenching and quenchers; tribo-/lyo-/bio-luminescence; photo-nonredox/-redox reactions; tuning of quantum yield, photocatalysis, flash/laser flash photolysis; photochemistry of $[Ru(bpy)_3]^{2+}$ in water splitting, photosynthesis and role of porphyrin π-cation radical, solar energy conversion and storage; sensing of biologically relevant cations/anions: chemo-sensors and chemodosimeters; use of TiO_2 as green photocatalyst

Unit-3: Bioinorganic Chemistry-2

Reversible oxygenation in life process, O_2-uptake proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin, model systems; electron transport proteins: cytochromes, Fe-S proteins –f erridoxins; respiratory electron transport chain, cytochrome c oxidase, photosynthetic electron transport chain-chlorophyll, PS-I and PS-II, biological (nitrogenase) and abiological nitrogen fixation

Unit-4: Environmental Chemistry

Overview, characteristics of litho-/hydro/atmo/bio-sphere; emission of gases, volatile organic compounds, viable-/nonviable particulates in atmosphere; classical/photochemical smog and mechanism of formation; chemistry of stratospheric ozone depletion, Antarctic ozone hole formation, acid rain and their consequences; threshold limit value (TLV), monitoring and determination of atmospheric gases and particulates; major water pollutants - chemical discharge, biodegradation of organic matters, nutrients in aquatic ecosystem, eutrophication, sewage and their control; BOD and COD and their determinations; soil pollution - pesticides, herbicides, fertilizers, polymers, plastics, radioactive waste, E-waste; bio-/nonbio-degradable pollutants; waste management, C, N, K, P determinations

in soil; diseases due to pollution; control of indoor and outdoor environments; smart chemistry, smart environment and sustainable development

Unit-5: Green Chemistry

Basic principles and green ChemisTREE diagram, cost-effective safer synthetic techniques and methods, catalytic-/biocatalytic method, atom economy, conservation of raw materials, design of energy efficient processes; reduction in consumption of non-renewable resources, greener and benign organic/inorganic one-pot syntheses using aq. solvent, ionic liquid, supercritical fluid and microwave; comparison with traditional methods; solvent free inorganic and organic reactions; impact on environment, green economy in blue world, cultural drive conductive to sustainable civilization; chemistry of past, present and future

Course ID: CHEM-CB33I

Unit-1: Chemical Application of Group Theory-1

Group theory and quantum chemistry; cyclic point groups, construction of their character tables (C_3, C_4 etc) and uses; reduction formula, direct product representation and its uses, symmetry of normal modes of vibrations, selection rules for IR and Raman transitions; stereographic projection of thirty-two crystallographic point groups

Unit-2: Spectral Study and Thermal Analysis

Spectral study: exposition of ligational motifs and chelate loop size, structural distortion, M-L bonding and effective π-acceptance center, redox site of non-innocent ligands, μ-bonding and hapticity, electrophilicity/nucleophilicity from IR and NMR results; ascertaining d-d and f-f transitions and CT transitions - MLCT, LMCT, IVCT, MMCT and LLCT in different types of compounds; spin-allowed and spin-forbidden transitions and their intensity stealing

Thermal Analysis: Fundamentals, instrumentations, working principles of different methods of analysis - TGA, DTA and DSC; reference materials, thermogram, thermal degradation and different thermal events, enthalpy change; phase transition, thermal stability of covalent and non-covalent bonds, ascertaining poymer crystallinity, single crystal phase transformation; thermochromism, thermochemiluminescence; application of DSC and modulated differential scanning calorimetry (MDSC) in food and drug industries

Unit-3: Magnetochemistry-1

Background, different magnetic materials; magnetic susceptibility measurements: Gouy method, Faraday method, vibrating sample magnetometer (VSM), SQUID and Evans (NMR) method; Curie's law, Curie-Weiss law, Curie-Langevin-Debye equation and significance; magnetically dilute and concentrated systems, Curie and Neel temperatures, cooperative magnetism, anomalous and subnormal magnetic moments, Bose-Stoner equation and different magnetic equations; diamagnetic susceptibility, Pascal's constants and its uses; Lande interval rule,

microstates, multiplet, multiplet width, hole formalism, energies of J levels, anisotropy in magnetic susceptibility

Unit-4: Complex Equilibria

Overview, stability of mononuclear, polynuclear and mixed ligand complexes; thermodynamic, kinetic and conditional stability constants; stepwise and overall formation constants and their relations, trends in stepwise formation constants, anomalous stability order; factors affecting stability order: internal/external, statistical/non-statistical; synergistic action to stabilize ternary complexes; stability and reactivity of mixed ligand complexes with reference to chelate effect, thermodynamic and kinetic aspects; macrocyclic effect, preorganization energy, entropic favour and enthalpic favour; pH-metric, spectrophotometric and polarographic determinations of binary formation constants, formation function and formation curve

Unit-5: Electrochemical study

Fundamentals, experimental findings of CV, DPV and coulometry; delving reversible/quasi-reversible/irreversible electrochemical/chemical processes in model compounds; electroinduced reactions: protic and electroprotic equilibria, electrocatalysis, electropolymerisation, electrochemiluminiscence, electro-synthesis, electrocrystallization; evaluating comproportionation constant; OTTLE, membrane electrode, electrode-solution interface layer, gas-sensing probe, surface-modified electrode; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA systems; photo-/spectro-electrochemistry, excited state potential and excimer structure simulation; redox orbital, redox series, redox isomer, electron hopping, spatially isolated orbital; single-/multi-chelate ring model; synergistic experiments and exposing electron transfer site, model cases correlating biological processes

Course ID: CHEM-CB33O

Unit-1: NMR Spectrscopy-2

^{1}H and ^{13}C NMR: principles, instrumentations; rules for carbon-13 calculations; enumeration of antiaromatic/aromatic/quasiaromaic/superaromatic systems; nuclei with negative NOE. problems on NOE, relaxation process, population transfer; NMR shift reagents and their applications, 2D-NMR and its applications; off-resonance decoupling, heteronuclear coupling: C-F and C-P; DEPTexperiment, application of NMR and other spectroscopic techniques to structural and mechanistic problems

Unit-2: Stereochemistry-2

Static and dynamic, Curtin-Hammett principle; 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-3: Heterocyclic Chemistry-2

Synthesis and reactions of aziridines, azetidines, oxazoles, thiazoles, imidazoles, isoxazoles, isothiazoles, pyrazoles and higher azoles and corresponding fused systems; nomenclature of bicyclic and tricyclic fused systems; introduction to the chemistry of azepins, oxepins, thiepins and their aza-analogues; phosphorus and selenium containing heterocycles; cyclazines

Unit-4: Asymmetric Synthesis-1

Principles and newer method of asymmetric synthesis (including enzymatic and catalytic nexus), enantio- and diastereoselective synthesis, addition to carbonyl compounds, reactions of enolates (α–substitution), addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, hydroboration, conjugate additions, Diels-Alder cycloaddition, cyclopropanation

Unit-5: Medicinal Chemistry-1

Pharmacodynamics: drugs and drug targets, drug binding forces, role of enzymes; drug-receptor interactions, mechanism of drug action, agonists, antagonists

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

Antibiotics: Penicillins, cephalosporins, macrolides, tetracyclins, etc; new to newer generation of antibiotics

Natural Products as Lead Drug: Synthesis and mechanism of anti-tumor, antiviral, anti-sense and DNA cleaving agents

Course ID: CHEM-CB33P

Unit-1: Biophysical Chemistry

Structure and function of biomolecules: protein, nucleic acid, carbohydrates and lipids; membrane structure and ion channel; biomolecular complexes: protein-ligand, enzyme-substrate and drug-DNA; examples; techniques for study of biomolecular structure and function: fluorescence and CD

Unit-2: Solution Thermodynamics and Electrochemistry

Partial molar quantities, thermodynamics of ideal and non-ideal binary solutions, activity coefficients and determinations for electrolytes and non-electrolytes; ion-ion interactions, 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

Fundamentals, classification, different synthetic methods, kinetics of polymerization; molecular weight and its determination, polydispersity index, some specific methods for molecular weight determination of biopolymers – gel filtration; SDS – PAGE for proteins, Agarose gel method for nucleic acids; thermodynamics of polymer solution, polymer conformation; polymer engineering

Unit-4: Vibration-Rotation Spectra

Principles, rotational coherence spectroscopy, rotational and vibrational spectra (electronic excitation: pump-probe technique) of excited and transient states; quantum coupling, hybrid bands, parallel and perpendicular bands; time-resolved IR, rotovibrational spectra of homo-/hetero di-/poly- atomic linear molecules

Unit-5: Mathematical Concepts

Elements of calculus, extremum principles, constrained extremization; power series: convergence and divergence; Taylor series and Fourier series; vectors and linear vector space: matrices

Course ID: CHEM-C34

Experiments in kinetics and equilibrium; instrumental methods (variable-temperature, if does arise): conductometry, potentiometry, polarimetry, colorimetry, pH-metry, spectrophotometry, fluorimetry, etc for standard systems and beyond; experiments on surface chemistry: determination of CMC by conductometric, tensiometric, viscometric and spectrophotometric methods; study on charge transfer/EDA complexes

Data processing and elementary numerical techniques; computer programming in FORTRAN for problems of chemical interest; learning chemistry with computers: molecular structures, MO theory with small molecules

Semester-IV

Course ID: CHEM-CB41I

Unit-1: Chemical Application of Group Theory-2

Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, correlation diagram, Tanabe-Sugano diagram; effect of lowering of symmetry on the orbitals and energy levels, correlation table; justification of Laporte selection rule and spin selection rule, vibronic coupling and vibronic polarization, polarization of electronically allowed

transitions; symmetry adapted linear combinations (SALCs); MO of homo-/hetero-nuclear diatomic molecules, MO of polynuclear AB_n type molecules, Walsh diagram, molecular term symbols

Unit-2: Solid State Chemistry-2

Fundamentals, crystallization processes and crystal synthesis, crystal orbital; ionic, covalent, H-bonded, metallic and molecular solids; Laves principles, Zachariasen rules, Ruddlesden-Popper phases, Chevrel phases; silicates - single-/double chain, 3D network, pyroxene, amphibole, talc, mica, clay, zeolite, zeotypes and hyper-/super-tetrahedral frameworks, ZSM-5 and its uses; ferro-/antiferro-/pyro-/piezo-electric materials, solid electrolytes; foreign materials doping, kernel, high entropy alloys and uses; antisite defect, crystallographic shear and Wadsley defect; Krogmann's salt – metallic rod, Bechgaard salt - organic molecular superconductor, Josephson junction, tokamak, maglev

Unit-3: Inorganic Chains, Rings, Cages and Clusters

Inorganic catenation - 1D chain, 2D sheets and 3D networks; homo-/hetero-cyclic systems; briging units, capping principle, inorganic and coordination polymers, iso- and hetero chains, linear chains and ladder-/parquet-/lattice-polymers; homo-/heterocyclic Si-O rings and cages; low nuclearity and high nuclearity carbonyl clusters, carbide, nitride, chalcogenide and halide containing clusters; Nb, Ta, Mo and W clusters; M-M bonding in single and multiple bonded compounds, multidecker molecules, fullerenes, torus/Zintl/water clusters; cluster-surface analogy, structures and bonding, skeletal electron (Elm) counting, Wade-Mingos-Lauher rule; Jemmis unified mno rules covering PSEPT, Wade-Mingos-Lauher rules and Huckel's rule

Unit-4: Bioinorganic Chemistry-3

Compartmentalization (homeostasis) and specific activity of metal (M) ions, selectivity filter, M-ion activated proteins; transport, storage, transfer and transcription; O-atom transport and storage, electron transfer, selective transport and storage of Fe, potential-gated K^+-ion channel, Zn-transcription, Ca-signaling; catalytic processes – acid-base catalysis, enzymes dealing with H_2O_2 and O_2, O-atom transfer by Mo-/W-enzymes; light-harvesting antenna; some specific functions of proteins – (i) oxidation and reduction by Fe, Mn, Cu and Mo, (ii) radical-based rearrangements by Fe and Co, (iii) Me-group transfer by Co; hydrolysis by Zn, Fe, Mg, Mn and Ni, (iv) DNA processing by Zn, (v) conformation setting by Ca; siderophore, ionophoric activity, chemiosmotic theory, electrogenic proton pump, respiratory chain, M-ions in genetic information transfer, basket porphyrin, model compounds as structure-function analogue, opportunity existing and future potential

Unit-5: Highlighting Chemistry of d-Block Elements

General electronic configuration, wider aspects of periodicity/aperoiodicity and diffusion cartograms; common/uncommon oxidation states; aqueous, redox and coordination chemistry; group characteristics and periodic trends; ligand

design/synthesis using molecular mechanics/engineering, tailoring of pendant arm; coordination compound design/synthesis and different synthetic protocols: thermal, cryo-/mechano-/electro-/photo-/sono-chemical, solvothermal, sol-gel methods, etc; reaction conditions from thermodynamic and kinetic aspects; synthesis of mixed-valence, homoleptic/heteroletic and homonuclear/heteronuclear mono/di-/poly-meric stoicio-/nonstoichio-metric compounds stressing on electric, electronic and magnetic properties and commercial uses; homo-/hetero-geneous catalysts with precise steric and electronic factors controlling pliancy of substrates; modeling biphasic transport and ionophoric activity, aggregation, extrusion and reaggregation reactions; specific compounds like molybdenum blue, Creutz-Taube ion, ruthenium red, Vaska complex, Wolffram's red, Magnus' green, etc; important breakthrough in chemistry and related disciplines

Course ID: CHEM-CB41O

Unit-1: Stereochemistry-3

Static and dynamic; chiroptical properties of organic molecules: origin, theory; 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; Curtin-Hammett principle and Wenstein-Eliel equations; conformation, reactivity and mechanism

Unit-2: Asymmetric Synthesis-2

Reduction of C=C double bonds, carbonyl and imine groups; oxidation: epoxidation, dihydroxylation and aminohydroxylation; rearrangement: [3,3]-Sigmatropic, (2,3)-Wittig, alkene isomerisation; hydrolysis and esterification

Unit-3: Heterocyclic Chemistry-3

Advanced: Indoles, pyrimidines, pyridazines, pyrazines, purines, pteridines, compounds with oxygen and sulfur hetero atoms; role of heterocyclic compounds in biological systems

Unit-4: Organometallic Chemistry-2

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 coupling; Ziegler Naata reaction, olefin metathesis, Tebbe's reagent, Pauson-Khand reactions; Volhsrdt co-trimerisation, functional organometallic compounds; use of nontransition metal Zn, Cd, Hg, In and Sn

Unit-5: Supramolecular Chemistry-1

From molecular to supramolecular chemistry: factors leading to strong binding (non-covalent cooperative interactions); new molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific

recognition processes; supramolecular reactivity and catalysis, switching devices; self-assembly of supramolecular aggregates, crystal engineering

Course ID: CHEM-CB41P

Unit-1: Angular Momentum

Constants of motion, representations, commutation relations, Step-up/step-down operators, quantization, spin and Pauli matrices, matrix representations of total angular momentum operators, many-electron systems

Unit-2: Valency

Born-Oppenheimer approximation and beyond, avoided crossings, Virial theorem and chemical bonding, theories of valence: VB and MO, model Hamiltonians: basic idea

Unit-3: Quantum Mechanics-3

Linear vector space: coordinate, momentum and matrix representations; pictures, constant of motions; Virial, hypervirial and Hellmann-Feynman theorems; sum rules, generalized uncertainty relation, Delta function and Fourier transformation, time reversal

Unit-4: Perturbation Theory

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications, Brillouin-Wigner theory, degenerate perturbation theory – Stark effect, first- and second order lifting of degeneracy

Unit-5: Time-dependent Quantum Processes

Perturbative dynamics, semiclassical treatment of radiation-matter interaction – first order and second order effect,. Golden rule, Einstein's A, B coefficients, connection of results with experimental quantities, two-level system

Course ID: CHEM-CB42I

Unit-1: Magnetochemistry-2

Design, synthesis and isolation of different magnetic materials; cryogenic magnetic study, first-/second-order Zeeman effect, van Vleck equation and its application, TIP, magnetic interactions in di-/polynuclear compounds and clusters; mechanism of exchange interactions, Bleaney-Bowers equation, Kahn's spin polarization, Goodenough-Kanamori-Anderson rules, antiferro-magnetism (AF), ferromagnetism (F), spin crossover, spin state isomerism and bistability; single chain magnet, single molecule magnet and storing and processing of data; accidental orthogonality, spin canting, canted-F, canted-AF, spin frustration, admixed-spin, metamagnetism, superdia-/superpara-magnetism, long-range ordering; magnetization vs field studies, Fermi contact/pseudo-contact shift; magnetotherapy – alternative medicine and future prospect

Unit-2: Separation Techniques

Overview, successive extraction and separation; techniques of solvent extraction: Craig extraction and counter current distribution; ionic liquid assisted and supercritical solvent extractions; chromatography: mathematical relationship of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography, band broadening and column efficiency, van Deemter equation, column resolution; gas chromatography, high performance chromatography, supercritical fluid chromatography ion-chromatography, size-exclusion chromatography and capillary electrophoresis: principles, methods, comparison and applications

Unit-3: Inorganic Reaction Mechanism

Introduction; stoichiometric/intimate mechanism; D, A, I_a, I_d and IP mechanisms, reaction profiles, rate determination techniques, rate laws and factors affecting; reaction parameters ($\Delta H^{\#}$, $\Delta S^{\#}$, $\Delta V^{\#}$) and diagnosis of mechanism, mechanisms of substitution reactions in O_h and sq planar d^n ion complexes: solvent exchange, aquation, anation, base hydrolysis, acid-catalyzed aquation, pseudo-substitution; Eigen-Wilkins mechanism, Hammett and Taft plots; nucleophilicity and rate scales, Edward scale, ^{n}Pt scale, Gutmann donor number, Drago E & C scale; mechanisms of isomerization (geometrical/linkage) and racemization, Ray-Dutta/Bailar twist mechanism; stereospecificity, *cis*-/*trans*-effect, different theories and synthetic uses, *trans*-influence, stereoretentive/stereodynamic path; inorganic functional group and reactions on coordinated ligands

Redox reactions: complementary and non-complementary, self-exchange; OSET/ISET mechanism: steps involved, factors favouring, frontier orbitals involved; Franck-Condon barrier, potential energy diagram, redox catalyzed substitution reactions, Marcus theory, fast redox reactions in biological systems

Unit-4: Supramolecular Chemistry-2

Concept and language, new horizon and scientific/technological landscape, building blocks: geometry setter, blocker, spacer and counter ions; atomic/ molecular valence, bifunctional ligand, supramolecular orbital, pallet of non-covalent forces like H-bonding, π…π, C-H…π, halogen…π, S…π, etc interactions and harnessing them; synthesis using secondary building units, modular chemistry and reticular chemistry; supramolecular arrays/-isomerism; isolation of different advanced functional materials; allosterism, principle of three C's, lock and key principle, host-guest interaction, superstructures in inorganic/metallo-organic/ organometallic compounds; innocent 0D-/smart 1D-/flat 2D-/intriguing 3D-architectures/hierarchies, supramolecular devices

Unit-5: Chemistry of f-Block Elements

Abundance, extraction, separation and recovery of lanthanoids; atomic parameters, nuclear properties and syntheses of elements; general electronic configuration, valence orbitals and anomalous nature; lanthanoid (Ln) and actinoid (An) contractions and consequences; relativistic effect, group characteristics and

periodic trends, alloys and their uses; oxidation states, yl-ions and linear structures; aqueous, redox, coordination and organometallic chemistry and comparison with d-block elements; absorption spectroscopy, luminescence behaviour, antenna effect, quantum cutting and solar photovoltaic cell; magnetic properties, LSR; neo-coordination chemistry; electronic, optical and magnetic properties exploited in technology, Ln-compounds as high temperature superconductors; lessons from chemistry of f-block elements

Course ID: CHEM-CB42O

Unit-1: NMR Spectroscopy-3

Application of ^{1}H-^{1}H COSY, ^{1}H-^{13}C HETCOR, HMBC, HMQC, HSQC, NOESY in structure elucidation of organic compounds, solid state ^{13}C-NMR (CP-MAS) and chemical shift anisotropy

Unit-2 Bio-Organic Chemistry

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

Unit-3: Medicinal Chemistry-2

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 drugs, antimalarial, anticholenergic and CNS-active drugs

Unit-4: Carbohydrate Chemistry

Basic structure and type of sugars; protection and deprotectio;. 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

Derivatized Alkaloids: Structure, transformation and biosynthesis of alkaloids from terrestrial and marine sources; chemistry of quinoline alkaloids with cinchona group, isoquinoline alkaloids with morphine group; alkaloids derived from pyrrolidine, piperidine ring systems and from ring systems containing two N-atoms; peptide alkaloids, macrocyclic alkaloids; chemistry of simple and monoterpenoid derived indole alkaloids – yohimbine, reserpine, strychnine, ellipticine, lysergic acid, representative examples of Iboga and Aspidosperma type indole alkaloids

Course ID: CHEM-CB42P

Unit-1: Statistical Mechanics-1

Phase space; ergodic hypothesis; Liouville's theorem, concepts of different ensembles with applications to selected systems, fluctuations, perfect gas and the Sackur-Tetrode equation, system of interacting molecules; treatment of imperfect gases

Unit-2: Statistical Mechanics-2

Formulation of quantum statistical mechanics: pure and mixed states, density matrix, quantum Liouville theorem and its consequences, quantum statistics and ensembles, specific heat of electron gas, Debye theory, Bose condensation

Unit-3: Kinetics-3

Rate processes and some physical phenomena, statistical approach to rate theory: Hinshelwood, RRK and RRKM theories

Unit-4: Quantum Chemistry-1

Variation method as an approximate method – basis and applicability, linear variation method – secular determinant, nonvariational-nonperturbative approximate methods – elementary exposure, many–electron systems, closed and open shells, antisymmetry principle and antisymmetrization operator, independent particle model (IPM), HK theorem and elements of DFT, Applications of DFT – KS and related functions

Unit-5: Quantum Chemistry-2

Hartree and Hartree Fock methods for closed shells, Koopman's theorem, limitation of IPM; electron correlation, restricted and unrestricted Hartree-Fock methods (elementary idea), multideterminantal wave function and CI, Brillouin's theorem, Roothan equation

Course ID: CHEM-CB43I

Unit-1: Crystallography

Diffraction of X-ray, Brag's condition, Brag's law in reciprocal lattice, Ewald sphere; X-ray crystallography instrumentation, goniometer, geometric data collection, crystal mosaicity and beam divergence, completeness of data collection, crystal to detector distance vs resolution, atomic scattering factor, structure factor, intensity of diffracted beam, Friedels Law, systematic absences, temperature factor on the intensity of diffracted beam; principles of electron and neutron diffraction methods

Unit-2: Chemistry of Elements in Biology and Medicine

Fundamentals, metallome and metallomics, inorganic composition of living organism, ligand binding, support structure specificities, transport, transcription,

biochemical signaling, biosensors, biological cycles, dynamic properties, regulation, biominerals, bioinspired reactions/catalyses, bioinformatics, future directions

Metallodrug discovery – a background; biocojugation, diagnosis, prognosis, treatment and prevention of diseases; efficacy of recent inorganic and related complexes in cancer treatment, phototherapy, anti-arthritis drugs, Bi in treatment of gastric ulcers, Li in treatment of bipolar disorders, Zn-cyclams as anti-HIV agents, Gd in magnetic resonance imaging (MRI), inorganic drugs against post-operative stress; tomography, ^{18}FDG, PET, SPECT, RIA; drug-delivery vehicles – a paradigm shift

Unit-3: Organometallics-2

Overview, Jesiphos and related ligands; stereochemical non-rigidity and pliancy, haptotropic shift, variable-temperature spectral analysis and structural characterization; Dewar-Chatt-Duncanson bonding model, Agostic interaction; language of catalysis and catalysis by organometallic compounds; Wilkinson's catalyst, Tethered catalyst, Ziegler-Natta catalyst and Cossee-Arlman mechanism, Kaminsky catalyst; Tolman catalytic loop, syntheses gas - WGSR, hydroformylation, Monsanto acetic acid process, Wacker-Smidt process, C-H activation, CO_2 fixation, water oxidation, Cativa process, hydro-silation/-phosphilynation/-amination/-cyanation reactions; synthetic gasoline - Fischer-Tropsch process and Mobil process; polymerization, oligomerization and metatheses reaction of alkenes and alkynes, photodehydro-genation catalyst (platinum POP); metallo-fullerenes, bioorganometallics, organo-dendrimer; applications to organic syntheses: enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, reactions on inorganic functional groups

Unit-4: Materials Chemistry and Nanochemistry

Materials Chemistry: Molecules and crystals to materials, scaffold, art of synthesis, interwoven bonding, molecular aggregates and crystalline architectures, serendipity vs architectural rationale, intermolecular/inter-ion interaction, intercalation materials, dangling bond, surface functionalization, core-corona, hysteresis, robust and directional interactions, click chemistry, functional materials: conducting, superconducting, magnetic, NLO, porous, luminous, quantum dots, liquid crystals, LCD, LED, catalysts, molecular and electronic devices, molecular machine, biosensor, biomineralization, proteomics, organic soft materials, proton and hydride sponges, complex electronic oxides, ceramics, composites; clean energy - hydrogen fuel and its storage materials, biomimetics and molecular recognition; materials characterization techniques, correlation between materials structures and properties

Nanochemistry: Plenty of room at the bottom, benign synthesis under solvent free condition, in ionic liquids, microwave assisted, etc using top-down/bottom-up method for nano-structured solids; characterization of nanomaterials, properties and applications; 1D control – carbon nanotubes, inorganic nanowires; 2D control – grapheme, quantum well, 3D control – micro-/meso-porous materials, composites;

commercially useful materials, nanomachines, nanolithography, optical properties of metallic and semiconducting nanoparticles (NPs); NPs as diagnostic probes in medical science like nano-surgery, recent breakthroughs and future perspective

Unit-5: Structure-Property Relationship

An utmost need and the ultimatum, thermodynamic and kinetic parameters; diagnostic probes: spectroscopic, thermal, electrochemical, magnetic, crystallographic, computational findings; parameters – room and variable temperature: stretching frequency, chemical shift, spin-spin coupling constant, isomer shift, potential value, bond distance, bond angle, torsion angle, crystal packing and Madelung constant, magnetic moment value, rate constant, half life; correlation diagram, breakthrough and legacy – paradigm shift and a conduit of learning

Course ID: CHEM-CB43O

Unit-1: Application of MO Theory

MO theory and its applications to organic molecules, construction of MOs - linear and cyclic conjugated systems, ab initio methods; Walsh orbitals of cyclopropane and cyclobutane, stability of carbocations, pi-facial selectivities, Cieplak model, strained organic molecules, calculation of strain energies, synthesis of strained cyclic molecules

Unit-2: Natural Products-4

General methods of study and structural types, chemistry of cholesterol, hormones, bile acids, vitamins of D-group, diosgenin

General study and structural features of sesquiterpenes, diterpenes, triterpenes, carotinoids; chemistry of representative members from the diterpenoid and triterpenoid series, carotenoids

Unit-3: Nucleoside and Nucleotide

Chemical synthesis of nucleosides and oligonucleotides; biosynthesis of nucleotides and folic acids; replication, transcription - protein biosynthesis

Unit-4: Organic Name Reactions and Reagents

Name Reactions: Allan–Robinson, Appel, Balz-Schiemann, Bamford–Stevens, Barton, Baylis–Hillman, Borodine-Hunsdiecker, Finkelstein, Gombberg-Bachmann, Harger, Heck, McMurry, Schotten-Baumann. Shapiro, Simonini, Strecker, Swarts and Wittig reactions; Ley, Pfitzner-Moffat, Rubottom and Swern oxidations; Buchwald-Hartwig amination, Bergmann and Darapsky degradations, Corey–Nicolaou macrolactonization, Peterson olefination, Sharpless asymmetric epoxidation, Sonogashira coupling, Stile coupling, Suzuki coupling, Woodward and Prevost hydroxylation, Wolff aromatization, Yamaguchi esterification; Baker–Venkataraman, Brook, Neber, Stevens, Stieglitz and Tiemann rearrangements

Reagents: Hydride transfer reagent - trialkylborohydrides, diimide, trialkyltin hydride, DIBAL, $Na(CN)BH_3$; azobisisobutyronitrile (AIBN), Corey–Bakshi–Shibata reagent, Dess-Martin periodinane, Hinsberg reagent, Ley–Griffith reagent (TPAP), Petasis reagent; DCC, PCC, PDC, CuI, Zn-Cu, Pb-Na

Unit-5: Organic Reaction Mechanism

Substitution: Aliphatic nucleophilic - S_N1, S_N2, S_N1', S_N2', mixed S_N1-S_N2, S_Ni, SET mechanisms; aliphatic electrophilic - S_E1, S_E2, and S_Ei mechanisms; aromatic electrophilic - arenium ion mechanism and *ipso* attack; free radical - types and mechanisms; reactivity of aliphatic and aromatic substrates at a bridgehead; reactivity in attacking radicals; allyllic halogenation (NBS)

Elimination reactions: E1, E2 and E1CB mechanisms; pyrolytic elimination

Addition: Addition to carbon–carbon multiple bonds involving - electrophiles, nucleophiles and free radicals stressing on regio-/chemo-selectivity; addition to carbon–heteroatom multiple bonds - mechanism of metal hydride reduction of saturated/unsaturated carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds; condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions

Rearrangement: reactions involving carbocation (Wagner-Meerwein, pinacol-pinacolone), acyl cation, PPA cyclization and Fries rearrangement, carbenes (Wolff and Arndst-Eistert synthesis) and nitrenes (Hoffmann, Curtius, Schmidt, Lossen, Beckmann rearrangement); sigmatropic rearrangements

Metathesis and click: classes of reactions, catalyst used, mechanistic aspects and synthetic applications

Course ID: CHEM-CB43P

Unit-1: Solids

Crystal symmetry, glide plane and screw axis, Bravis lattice, space group and its determination, reciprocal lattice, stereographic projection, Fourier synthesis, electron density and structure factor, methods for solving the phase problems, B-zones and Fermi level in lattice, concept of particle-hole in conduction process, band theory and theory of conductors, semiconductors and insulators

Unit-2: Chemical Application of Group Theory-2

MO theory with applications to σ- and π-bonding and construction of hybrid orbitals; LFT with application in splitting of terms and levels in different coordination environments and construction of energy level diagrams, applications of symmetry principles in Woodward-Hoffman type reactions like dimerization of ethylene, Diels-Alder reaction, etc

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

Unit-4: Lasers

Principles of Maser and Laser actions; 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

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 – hyper Raman, stimulated Raman, Resonance Raman spectra

Course ID: CHEM-CB44

Review, Project Work and Grand Viva