SYLLABUS FOR

M. Sc. COURSE IN CHEMISTRY

(CBCS SYSTEM)

Department of Chemistry

Diamond Harbour Women's University

Sarisha, West Bengal

743368

(Modified and Effective from the Academic Session 2024-25)

Syllabus for Two-Year Four-Semester PG Course in Chemistry
DHWU
COURSE STRUCTURE

Grand Total Marks – 1000

SEMESTER WISE DIVISION OF MARKS AND CREDITS

SEMESTER	Theoretical (Core course) (CC)	Practical (Core course) (CC)	Discipline Centric Elective (CE)		Open Elective (OE) (Theory)	Total Marks	Total Credits
			Theory	Practical			
SEMESTER-I	150	100	--	--	--	250	20
SEMESTER-II	150	100	--	--	--	250	20
SEMESTER-III	50		50	50	100	250	20
SEMESTER-IV	--		150	100		250	20
Total	**350**	**200**	**200**	**150**	**100**	**1000**	**80**

FIRST YEAR (FIRST SEMESTER)

Paper	Subject/Topics	Marks		Total Marks in End semester	Total Credits End semester
		Internal	Semester exam		
CHEM/CC/4101	General Inorganic Chemistry	10	40	50	4
CHEM/CC/4102	General Organic Chemistry	10	40	50	4
CHEM/CC/4103	General Physical Chemistry	10	40	50	4
CHEM/CC/4104	Practical Inorganic Chemistry	10	40	50	4
CHEM/CC/4105	Practical Physical Chemistry-I	10	40	50	4
Total		50	200	250	20

FIRST YEAR (SECOND SEMESTER)

Paper	Subject/Topics	Marks		Total Marks in End semester	Total Credits End semester
		Internal	Semester exam		
CHEM/CC/4201	Advanced Inorganic Chemistry	10	40	50	4
CHEM/CC/4202	Advanced Organic Chemistry	10	40	50	4
CHEM/CC/4203	Advanced Physical Chemistry	10	40	50	4
CHEM/CC/4204	Practical Organic Chemistry	10	40	50	4
CHEM/CC/4205	Practical Physical Chemistry-II	10	40	50	4
Total		50	200	250	20

SECOND YEAR (THIRD SEMESTER)

Paper	Subject/Topics	Marks		Total Marks in End semester	Total Credits End semester
		Internal	Semester exam		
CHEM/CC/5101	General Spectroscopy	10	40	50	4
CHEM/CE/5102A	Inorganic Chemistry Special Theory-I	10	40	50	4
CHEM/CE/5102B	Organic Chemistry Special Theory-I				
CHEM/CE/5102C	Physical Chemistry Special Theory-I				
CHEM/CE/5103A	Inorganic Chemistry Special Practical	10	40	50	4
CHEM/CE/5103B	Organic Chemistry Special Practical				
CHEM/CE/5103C	Physical Chemistry Special Practical				
CHEM/OE/5104	Concepts in Modern Chemistry-I	10	40	50	4
CHEM/OE/5105	Concepts in Modern Chemistry-II	10	40	50	4
Total		50	200	250	20

SECOND YEAR (FOURTH SEMESTER)

Paper	Subject/Topics	Marks		Total Marks in End semester	Total Credits End semester
		Internal	Semester exam		
CHEM/CC/5201	Thermal Analysis, Applied Spectroscopy & Magnetochemistry	10	40	50	4
CHEM/CC/5202	Nanoscience and Biochemistry	10	40	50	4
CHEM/CE/5203A	Inorganic Chemistry Special Theory-II	10	40	50	4
CHEM/CE/5203B	Organic Chemistry Special Theory-II				
CHEM/CE/5203C	Physical Chemistry Special Theory-II				
CHEM/CE/5203D	Inorganic Chemistry Special Theory-III				
CHEM/CE/5203E	Organic Chemistry Special Theory-III				
CHEM/CE/5203F	Physical Chemistry Special Theory-III				
CHEM/CE/5203G	Electrochemistry, Green chemistry, Drug synthesis and Biophysical chemistry				
CHEM/CC/5204	Literature Review and presentation	10	40	50	4
CHEM/CC/5205	Project/Dissertation	10	40	50	4
Total		50	200	250	20

SEMESTER – I

Course ID: CHEM/CC/4101

Unit-1: Coordination Chemistry 1

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

Unit-2: Organometallics 1

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, isolobal and isoelectronic relationships with examples. Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and -cyclopentadienyl complexes. Structure and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples; structure and bonding of $K[Pt(C_4H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$ 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-3: Bioinorganic Chemistry 1

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

Unit-4: Inorganic Reaction Mechanisms

Mechanistic labels A, D, I_a, I_d: compare with SN_1 and SN_2; 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.

Reference Books:

1. Concepts and Models of Inorganic Chemistry, 3rd ed (B. Douglas, D. Mcdaniel, J. Alexander)

2. General and Inorganic Chemistry (Vol I and II). (R. P. Sarkar)

3. Inorganic Chemistry: Principles of Structure and Reactivity (J. E. Huheey, E. A. Keiter, R. L. Keiter)

4. Basic Inorganic Chemistry (Cotton & Wilkinson) 6

5. Inorganic Chemistry (Shriver, Atkins & Langford)

6. Elements of Bioinorganic Chemistry (G. N. Mukherjee & A. Das)

7. Bioinorganic Chemistry (A. K. Das)

8. Inorganic Chemistry (G. Wulfsberg)

9. Fundamentals of Analytical Chemistry (Skoog, West, Holler & Crouch)

Course ID: CHEM/CC/4102

Unit-1: General Organic Reaction Mechanism

Reactive Intermediates**:** Formation, Stability and Reactivity of Carbocation, Carbanion, Carbenes, Nitrenes, free radicals and arynes with reference to basic type of reaction. Ring closer reactions; Baldwin rules and exceptions, Thorp Ingold effect. Interconversion of ring system (Contraction and expansion). Determination of reaction mechanism; Hammett equation and its modification.

Unit-2: Stereochemistry 1

Concept of centre and plane of chirality, axial chirality and symmetry, point groups. Topicity relationship (homotopic, diastereotopic and enantiotopic), Topicity descriptor (Pro-R/Pro-S, Re/Si), determination of relative configuration: Prelog's rule, Cram's rule (Felkin modification), allylic strain, reactions of 5/6- membered ring containing one or more trigonal carbon(s).

Unit-3: Pericyclic Reactions

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

Unit-4: NMR Spectroscopy

Basics of NMR spectroscopy. 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. Classification of ABX, AMX, ABC, A_2B_2 in proton NMR.

Unit-5: Natural Products-1

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

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

Reference Books:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen, Wiley India Ed, 2008.

2. Stereochemistry of Organic Compounds: Principles and Applications – D. Nassipuri, New Age International, 1994. 3. Advanced Organic Chemistry (Part A & B) - F.A. Carey and R. J. Sundberg, Springer Science + Business Media, 5th Ed, 2007. 7

4. Organic Chemistry - J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Ed, 2012.

5. The Conservation of Orbital Symmetry - R.B. Woodward and R. Hoffmann, Academic Press, 1971

6. Organic Reactions and Orbital Symmetry - P. L. Gilchrist and R. C. Storr, Cambridge [Eng.] University Press, 1972. 7. Pericyclic Chemistry -Orbital Mechanisms and Stereochemistry -D. K. Mandal, Elsevier, 2018.

8. Pericyclic Reaction - I. Fleming, Oxford University Press, 1998.

9. Molecular Orbitals and Organic Chemical Reactions - I. Fleming, John Wiley and Sons, Ltd.

10. Orbital Symmetry- A Problem-Solving Approach – R. E. Lehr, Alan P. Marchand, Academic Press INC, 1972.

11. Pericyclic Reactions - A Text Book: Reactions, Applications and Theory – S. Sankararaman, Wiley-VCH, 2005

12. Organic Spectroscopy - W. Kemp, ELBS

13. Introduction to Spectroscopy - D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Cengage Learning India Pvt. Ltd.

14. Applications of Absorption Spectroscopy of Organic Compounds – J. R. Dyer, Prentice Hall India Learning Pvt. Ltd.

15. Spectrometric Identification of Organic Compounds by R. M. Silverstein and G. C. Bassler, and T. C. Morrill, Spectrometric identification of Organic compounds, John Wiley & Sons, 5th Ed, 1991

16. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming, Tata McGraw Hill Education.

17. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Günther, Wiley

18. Organic Structure Determination – J. H. Simpson, Elsevier 19. NMR Spectroscopy Explained – N. E Jacobsen, Wiley, 20. I.L Finar Vol-1 and 2.

Course ID: CHEM/CC/4103

Unit-1: Thermodynamics and Statistical Mechanics 1

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

Unit-2: Atomic Structure and Spectra

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

Unit-3: Quantum Mechanics 1

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

Unit-4: Kinetics 1

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

Unit-5: Polymer chemistry

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

Reference Books:

1. Introduction to Quantum Mechanics- D. J. Griffiths

2. Quantum Mechanics-Bransden, Joachen

3. Chemical Kinetics – K.J.Laidler

4. Statistical Mechanics – R.K. Pathria

5. Thermodynamics and Introduction to Thermostatics – H.B. Callen

6. Modern Spectroscopy – J.M. Hollas

7. Principles of Polymer Chemistry, P.J. Flory

Course ID: CHEM/CC/4104

1. Semi-micro qualitative analysis for selected uncommon elements.

2. Stability constants of coordination complexes and analysis of drugs

Reference Books: Semi-micro qualitative inorganic analysis, G. N. Mukherjee

Course ID: CHEM/CC/4105

1. Use of standard commands to write elementary programs.

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

Reference Books: Fortran 77 and Numerical Methods, C.L Xavier

SEMESTER – II

Course ID: CHEM/CC/4201

Unit-1: Coordination Chemistry 2

Electronic spectra of transition metal complexes – determination of free ion terms of d^1 to d^9, microstates, determination of ground and all excited state terms of d^n terms in octahedral and tetrahedral fields, Orgel diagrams (qualitative approach), hole formalism, inversion and equivalence relations, selection rules for spectral transitions, d-d spectra and crystal field

parameters, Nephelauxetic series, qualitative idea of Tanabe–Sugano diagrams, charge transfer spectra. Magnetic properties – elementary idea. Charge transfer spectra, CD, ORD, and MCD spectra and absolute configuration of coordination compounds. Cotton effect and Faraday effect.

Unit-2: Chemical Bonding

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

Unit-3: Clusters and Boranes

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

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

Unit-4: Complex Equilibria

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

Unit-5: Solid-state Chemistry

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

Reference Books:

1. Concepts and Models of Inorganic Chemistry, 3rd ed (B. Douglas, D. Mcdaniel, J. Alexander)

2. General and Inorganic Chemistry (Vol I and II). (R. P. Sarkar)

3. Inorganic Chemistry: Principles of Structure and Reactivity (J. E. Huheey, E. A. Keiter, R. L. Keiter)

4. Inorganic Chemistry (C. Housecroft& A. Sharpe)

5. Inorganic Chemistry, 3rd ed (Miessler&Tarr)

6. Inorganic Chemistry (G. Wulfsberg)

7. Solid state chemistry and its applications (A. R. West) 8. Solid state chemistry: An introduction, 3rd ed (L. E. Smart & E. A. Moore)

Course ID: CHEM/CC/4202

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.

Unit-2: Synthetic Methodology 1

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

Unit-3: Heterocyclic Chemistry 1

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

Unit-4: Synthetic Methodology 2

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

Unit-5: Natural Products -II

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

Reference Books:

1. Modern Methods of Organic Synthesis - W. Carruthers, I. Coldham, CUP

2. Organic Chemistry -J. Clayden, N. Greeves, S. Warren and P. Wothers, OUP

3. Principle of Organic Synthesis - R.O.C. Norman and J.M. Coxon, Blackie

4. Organic Synthesis: The Disconnection Approach - S. Warren, Wiley

5. Organic Synthesis - M.B. Smith, McGraw – Hill

6. The Logic in Organic Synthesis - E.J. Corey and X. Cheng, Wiley

7. Organic Chemistry, Vol. II - I. L. Finar, ELBS

8. Mechanism and Theory in Organic Chemistry by Lowry and Richardson

9. Advanced Organic Chemistry: reactions, Mechanism and Structures (8th Edn) by J. March

10.Heterocycles in Organic Synthesis - A.I. Meyers, Wiley

11.Heterocyclic Chemistry - J.A. Joule and K. Mills, Blackwell

12.Heterocyclic Chemistry - T.L. Gilchrist, Wiley

13.Classics in Total Synthesis (Vol I) - K.C. Nicolaou and E.J. Sorensen, Wiley- VCH

14.Classics in Total Synthesis II - K.C. Nicolaou and S.A. Snyder Wiley-VCH

15. Photochemistry and Pericyclic Reactions, Jagdamba Singh, New Age International 16. Organic Photochemitry Coxon & Halton, Chembridge

Course ID: CHEM/CC/4203

Unit-1: Quantum Mechanics 2

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

Unit-2: The H-atom Problem

Cartesian and polar coordinates. Centre of mass and relative coordinates. General forms of solutions for stationary states with orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constants of motion like L2, Lz, etc. 10

Unit-3: Group theory 1

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

Unit-4: Interfacial Chemistry

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

Unit-5: Kinetics 2

PE surface, reaction coordinates and reaction paths. Idea of the BEBO method. Absolute rate

theory. Sample case-studies using partition functions. Comparison with collision theory. Ionic reactions in solutions.

Reference Books:

1. Chemical Application of Group Theory- F. A. Cotton

2. Quantum Mechanics-Bransden, Joachen

3. Physical Chemistry of Surfaces – A.W. Adamson

4. Chemical Kinetics – K.J.Laidler

Course ID: CHEM/CC/4204

1. Identification of organic compounds in a binary mixture (solid/liquid).

2. Two step organic preparations, including methods of purification.

Reference Books:

1. Systematic Organic Qualitative Analysis – H. Middleton

2. Hand Book of Organic Analysis – H.T. Clarke

3. Qualitative Organic Analysis – A.I. Vog

Course ID: CHEM/CC/4205

1. Selected equilibrium/kinetics experiments (analytical).

2. Selected equilibrium/kinetics experiments (instrumental).

Reference Books: 1. Practical Physical Chemistry – B.P. Levitt

SEMESTER – III

Course ID: CHEM/CC/5101

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 non-equivalent 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, O2, CO, HCl, etc. Principles of electron, neutron and X-ray diffraction methods in determining the structure of molecules – a comparative approach.

Unit-3: Mass Spectroscopy

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

Applications of mass spectroscopy to simple structural and mechanistic problems.

Unit-4: Absorption Spectroscopy and Molecular Interactions

$\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and $d \rightarrow d$ transitions. Solvent effects on spectra. Weak and CT interactions. Vibronic and spin-orbit coupling: detection from spectral data.

Unit-5: Emission Spectroscopy

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

Reference Books:

1. Modern spectroscopy, 4th ed (J. M. Hollas)
2. Principles of Fluorescence Spectroscopy, J. Lakowicz
3. Fundamental of photochemistry- Rohatgi and Mukherjee
4. Introduction to Spectroscopy - Pavia, Lampman
5. Applications of Absorption Spectroscopy of Organic Compounds – Dyer
6. Spectrometric Identification of Organic Compounds - R. M. Silverstein and G. C. Bassler
7. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming.
8. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Gunther, Wiley
9. Organic Structure Determination - Jeffrey H Simpson 8. NMR Spectroscopy Explained - Neil E Jacobs

Course ID: CHEM/CE/5102A

Unit-1: X-ray Crystallography

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

Unit-2: 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: 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-4: Inorganic Spectroscopy

Application of IR, Raman 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.

Unit-5: Inorganic Photochemistry

Introduction to Inorganic photochemistry: Photophysical and photochemical processes, laws of photochemistry, 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, relevance of Ruthenium polypyridine complexes in solar energy conversion and storage, photochemistry of iron complexes, photosplitting of water; inorganic photochemistry of biological processes and their model studies.

Reference Books:

1. Elements of Magnetochemistry, 2nd ed (Dutta & Shyamal)

2. Elements of Bioinorganic Chemistry (G. N. Mukherjee & A. Das)

3. Bioinorganic Chemistry (A. K. Das)

4. Inorganic Chemistry (G. Wulfsberg)

5. Chemistry of the elements (N.N. Greenwood & A. Earnshaw)

6. Advanced Inorganic Chemistry (F. A. Cotton)

Course ID: CHEM/CE/5102B

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.

Unit-2: 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.

Unit 3: Synthetic Methodology 3

Chemistry of organosilicon compounds, Synthetic uses of silyl ethers, silylenol ethers, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon BaeyerVilliger rearrangement. Ionic hydrogenation, synthetic use of TMSCN, TMSNCO, TMSI, TMSNHCOMe, TMSN3 etc.

Unit-4: Medicinal Chemistry 1

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

Unit 5: Name reactions and Methods of Ring Formation

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

Reference Books:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.

2. Stereochemistry of Carbon Compounds - E.L. Eliel and S. H. Wilen.

3. Stereochemistry of Organic Compounds: Principles and Applications - D. Nasipuri.

4. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Gunther, Wiley

5. Organic Structure Determination - Jeffrey H Simpso

6. NMR Spectroscopy Explained - Neil E Jacobsen5. Lehninger Principles of Biochemistry: David L. Nelson, Michael M. Cox.

7. Burger's Medicinal Chemistry, Drug Discovery and Developments (Vol 1-8) by Burger and Burger

8. The Organic Chemistry of Drug Design and Drug Action - R. B. Silverman

9. Top Drugs: Their History, Pharmacology and Synthesis - Ji Jack Li 15

10.Beta lactams (Vol I and II) - A.K. Bose and M. S. Manhas

11.Medicinal Chemistry - G. L. Patrick

12. Fundamentals of Biochemistry: Life at the Molecular Level: Donald Voet, Judith G. Voet, Charlotte W. Pratt.

Course ID: CHEM/CE/5102C

Unit-1: 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-2: Reaction Dynamics

Properties of electronically excited molecules; potential energy diagram for donor-acceptor system. Nonradiative intramolecular electronic transition; crossing of potential energy surfaces (Franck-Condon factor). Adiabatic-nonadiabatic

cross-over. Kasha's rule. Study of molecular energy transfer and state-to-state reactions. Macroscopic rate from microscopic rate coefficients.

Unit 3: Theoretical Spectroscopy

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: 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-5: 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.

Reference Books:

1. Quantum Chemistry-I. N. Levine

2. Molecular Quantum Mechanics-P.W.Atkins

3. Modern Molecular Photochemistry - Nicholas J. Turro

4. Spectra of Atoms and Molecules - Peter F. Bernath

5. Statistical Mechanics- Pathria

Course ID: CHEM/CE/5103A

1. Ion-exchange studies.

2. Preparation and characterization of some coordination complexes.

Reference Books:

1. Advanced Experiments in Inorganic Chemistry (G. N. Mukherjee)

Course ID: CHEM/CE/5103B

1. Extraction and purification of selected natural products.

2. Multistep organic preparations and Identification using Chromatographic separation spectroscopic methods.

Reference Books:

1. Systematic Organic Qualitative Analysis – H. Middleton

2. Hand Book of Organic Analysis – H.T. Clarke

3. Qualitative Organic Analysis – A.I. Vogel

Course ID: CHEM/CE/5103C

1. Numerical analysis and programming.

2. Selected equilibrium/kinetics experiments (analytical/Instrumental).

Reference Books:

1. Fortran-77 and numerical methods-Xavier
2. 1. Practical Physical Chemistry – B.P. Levitt

Course ID: CHEM/OE/5104

Unit-1: Green Chemistry

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

Unit 2: Basic idea of crystal field theory

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

Unit 3: Essential of Inorganic chemistry

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

Unit 4: Thermodynamics

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

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

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

Reference Books:

1. General and Inorganic Chemistry (Vol II). (R. P. Sarkar)

2. Fundamental Concepts of Inorganic Chemistry, Vol 1-7 (A. K. Das)

3. A Guidebook to Mechanism in Organic Chemistry sixth edn Peter Skyes Pearson

4. Physical Chemistry- G. Castellan

Course ID: CHEM/OE/5105

Unit-1: Nanoscience

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

Unit 2: Drugs & Pharmaceuticals

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

Unit 3: Biomolecules

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

Unit 4: Rotational and Vibrational Spectroscopy

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

Unit 5: Atomic Structure and Spectra Atomic spectra:

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

Reference Books:

1. General and Inorganic Chemistry (Vol II). (R. P. Sarkar)

2. Fundamental Concepts of Inorganic Chemistry, Vol 1-7 (A. K. Das)

3. Nanoscience & Technology (Shah & Ahmad)

4. Principles of nanoscience and nanotechnology (Shah & Ahmad)

5. The Organic Chemistry of Drug Design and Drug Action - R. B. Silverman

6. Top Drugs: Their History, Pharmacology and Synthesis - Ji Jack Li

7. Fundamentals of Molecular Spectroscopy-C.N. Banwell

SEMESTER – IV

Course ID: CHEM/CC/5201

Unit 1: 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 2: Rotational and vibrational spectroscopy

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

Unit 3: Group Theory 2

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

Unit 4: Magnetochemistry 1

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

Unit 5: 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: Hückel theory for conjugated systems (linear and cyclic). Resonance energy and bond order

Reference Books:

1. Modern Spectroscopy – J.M. Hollas

2. Quantum Chemistry-I. N. Levine

3. Applications of Group Theory F.A. Cotton

Course ID: CHEM/CC/5202

Unit 1: Chemical Biology

Molecular models of biological receptors, design, synthesis and binding studies of synthetic receptors. Enzyme models, micelles, biopolymers, remote functionalization reactions, catalytic antibodies, principle of gene synthesis. Proteins, peptides and amino acids. 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. Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Amino-acids-protein biosynthesis. Interactions of nucleic acids with small molecules. Structural features of DNA and RNA.

Unit 2: **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).

Unit 3: Carbohydrate Chemistry

Basic structure and type of sugars. Chemistry of sucrose, maltose and gentiobiose. Glycosides, protection and deprotection. O-glycocylation and C-glycocylation. Deoxy-sugars, amino sugars, glycal sugars and their synthetic and biological aspects. Carbohydrates as chiral pools in organic synthesis. Chemistry of naturally occurring oxygen heterocyclic compounds, polyphenolics and other antioxidants.

Unit 4: Bioinorganic Chemistry 2

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

Unit 5: 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, Membrane mimetics, Nucleic acid mimics.

Reference Books:

1. Lehninger Principles of Biochemistry – D.L. Nelson and M. Cox
1. Harper's Illustrated Biochemistry (32nd edition)
2. Basic Organometallic Chemsitry- B.D. Gupta and A.J. Elias
3. Principles of Bioinorganic Chemsitry- Stephen J. Lippard and Jeremy M. Berg
4. Bioinorganic Chemistry- Bertini, Gray, Lippard, Valentine

Course ID: CHEM/CE/5203A

Unit-1: Electrochemical methods

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

Unit-2: Bioinorganic Chemistry 3

Metal storage and transport proteins: transferring, ferritin, ceruloplasmin, calmodulin. Electron transport proteins: cytochromes, ferredoxins and rubredoxins, blue copper proteins. Redox metalloenzymes: catalase (both Fe and Mn), Ascorbate oxidase, peroxidase, superoxide dismutase, cytochrome c oxidases. Nitrogen fixation. Cobalamins including vitamin and coenzyme B12. Structural/functional models of some of the above-mentioned systems. DNA – Metal complexes interactions. Antitumor activities of metal complexes and structure-activity relationship.

Unit-3: Magnetochemistry 2

Introduction: Magnetic properties of substances, orbital and spin angular momentum of electrons. Quantum theory of paramagnetic susceptibility – Van Vleck equation. 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. Single molecule magnet, Single ion magnet, Single chain magnet.

Unit-4: 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.

Unit-5: 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.

Reference Books:

1. Concepts and Models of Inorganic Chemistry, 3rd ed (B. Douglas, D. Mcdaniel, J. Alexander)

2. Inorganic Chemistry: Principles of Structure and Reactivity (J. E. Huheey, E. A. Keiter, R. L. Keiter)

3. Inorganic Chemistry (G. Wulfsberg)

4. Basic Inorganic Chemistry (Cotton & Wilkinson)

5. Inorganic Chemistry (Shriver, Atkins & Langford)

Course ID: CHEM/CE/5203B

Unit 1: Asymmetric Synthesis

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

Unit 2: Heterocyclic Chemistry-II

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

Unit 3: Medicinal Chemistry 2

Total synthesis of Taxol, Prostaglandin, Cholesterol
Classification and mechanism of action of antibiotics. Gram positive and gram negative microorganisms. Synthesis of penicillin-G, penicillin-V, amoxycillin, chloramphenicol, norfloxacins, cephalosphorins and other new generation antibiotics. Introduction to cardiovascular drugs, cardiovascular diseases, lipoproteins (LDL, HDL etc.) and their role in atherosclerosis. Mechanism of action of some cardiovascular and antianginal drugs (Statins and other nitrate drugs). Chemistry and mode of action of some important antihistamines and anti-ulcer agents (ranitidine, famotidine, omeprazole, lansoprazole, etc.). Local anti-infective drugs. Antineoplastic agents. Antimalarial, anticholenergic and psychotic drugs (diazepam, oxazepam, chlorpromazine, librium, alprazolam, barbiturates etc.).

Unit 4: Retrosynthetic approach in total synthesis

Protection and Deprotection of Oxygen and Nitrogen containing common functional groups; Use of blocking groups, use of activating groups, alkylation of anions from 1,3–dithiane, alkylation of dihydro-1,3–oxazines. Umpolung reactions. Retrosynthetic approach.

Unit 5: NMR Spectroscopy II

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.

Reference Books:

1. Modern Methods of Organic Synthesis - W. Carruthers, I. Coldham, CUP

2. Organic Chemistry -J. Clayden, N. Greeves, S. Warren and P. Wothers, OUP

3. Principle of Organic Synthesis - R.O.C. Norman and J.M. Coxon, Blackie

4. Organic Synthesis: The Disconnection Approach - S. Warren, Wiley

5. Organic Synthesis - M.B. Smith, McGraw – Hill

6. The Logic in Organic Synthesis - E.J. Corey and X. Cheng, Wiley

7. Organic Chemistry, Vol. II - I. L. Finar, ELBS

8. Mechanism and Theory in Organic Chemistry by Lowry and Richardson

9. Advanced Organic Chemistry: reactions, Mechanism and Structures (8th Edn) by J. March

Course ID: CHEM/CE/5203C

Unit 1: **Angular Momentum**

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

Unit 2: Quantum Chemistry 2

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

Unit 3: 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 4: FT Spectroscopy: FT NMR and FTIR

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

Unit 5: 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.

Reference Books:

1. Modern Spectroscopy – J.M. Hollas

2. Pulse & Fourier Transform NMR -T. C. Farrar & E. D. Becker

3. Elementary Quantum Chemistry-F. L. Pilar

4. Quantum Chemistry-I. N. Levine

5. Statistical Mechanics – R.K. Pathria

6. Introduction to Quantum Mechanics- D. J. Griffiths

7. Introduction to Quantum Mechanics – L.Pauling, E.B.Wilson

8. Quantum Chemistry – I.N.Levine Coulson's Valence- R. McWeen

Course ID: CHEM/CE/5203 D

Unit 1: 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.

Unit 2: 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-3: 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, et

Unit 4: Inorganic 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: Inorganic 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.

References:

1. Infrared and Raman Spectra of Inorganic and Coordination Compounds – Nakamoto and Kazuo
2. Spectroscopy of Inorganic Compounds – Jagadamba Singh, M.D. Pandey, Jaya Singh
3. Inorganic Chemistry – Greenwood
4. Advanced Inorganic Chemistry – Cotton and Wilkinson

Course ID: CHEM/CE/5203 E

Unit 1: Huckle Molecular Orbital Theory

MO treatment of acyclic and cyclic conjugated systems; Hückel'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. Hückel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene.

Unit 2: 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 3: Bio-organic Chemistry

Molecular models of biological receptors, design, synthesis and binding studies of synthetic receptors. Enzyme models, micelles, biopolymers, remote functionalization reactions, catalytic antibodies, principle of gene synthesis. Structure, function, purification, analysis and modern applications of proteins, peptides and amino acids. Nucleic acids and their biological role. Strategies to improve micelle stability for drug delivery.

Unit 4: 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 5: Nucleoside and Nucleotide

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

References:

1. Lehninger Principles of Biochemistry – D.L. Nelson and M. Cox
2. Biochemistry – Lubert Stryer
3. Organic Chemistry – Morrison Boyd and Bhattacharjee

4. Advanced Organic Chemistry – Jerry March
5. Advanced Organic Chemistry (Part A and B) – F.A. Carey and R. J. Sundberg
6. Organic Chemistry – Clayden, Greeves, Warren

Course ID: CHEM/CE/5203 F

Unit 1: 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 2: Statistical Mechanics 2

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

Unit 3: Electronic Spectroscopy

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

Unit 4: 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 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.

Reference Books:
1. Modern Spectroscopy – J.M. Hollas
2. Quantum Chemistry-I. N. Levine
3. Introduction to Quantum Mechanics- D. J. Griffiths
4. Introduction to Quantum Mechanics – L.Pauling, E.B.Wilson
5. Principles of Fluorescence Spectroscopy-J. Lakowicz
6. Statistical Mechanics – R.K. Pathria
7. Chemical Kinetics – K.J.Laidler

Course ID: CHEM/CE/5203 G

Unit 1: 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.

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: Electrochemistry

Debye-Hückel theory, Debye-Hückel-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 4: Natural Products as Lead Drug

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

Unit 5: 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.

References:

1. Lehninger Principles of Biochemistry – D.L. Nelson and M. Cox
2. Biochemistry – Lubert Stryer
3. An Introduction to Electrochemistry – S. Glasstone
4. Organic Chemistry Natural products (Vol I and II) – O.P. Agarwal

Course ID: CHEM/CC/5204

1. Write-up of review/literature survey

2. Continuous assessment and grand viva-voce

Course ID: CHEM/CC/5205

1. Write-up of project report

2. Oral presentation and discussion around the project work

Appendix

Detailed Chemistry Practical Worksheet

CHEM/CC/4104: 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/CC/4105: Practical Physical Chemistry-I

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/CC/4204: Practical Organic Chemistry

A. Identification of organic compound in a binary mixture (solid/liquid) through preparation of derivatives.

B. Organic preparations including methods of purification (e.g.,crystallization, steam distillation, vacuum distillation, sublimation, etc.).

CHEM/CC/4205: Practical Physical Chemistry-II

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: E0 of Ag/Ag+ and $[Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$, pKa of AcOH. Colorimetry: Job's method, iodination of acetone.

CHEM/CE/5103A: Inorganic Chemistry Special Practical

1. Ion-exchange experiments (to determine strength/concentration of Metal ion or anion)
2. Synthesis and characterization of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands

CHEM/CE/5103B: Organic Chemistry Special Practical

1. Multistep organic preparations of various organic compounds. Chromatographic separation with TLC monitoring, and identification of the components via spectroscopic method.
2. Extraction and purification of selected natural products (any two: Caffine, Nicotine, Protein, beta-Carotene, Eucalyptus, etc.).

CHEM/CE/5103C: Physical Chemistry Special Practical

1. Formatting statements, uses of data files (r/w), subroutines and function subprograms. Use of 'RAND()': diffusion and the random walk problem, variants of the problem.
   Numerical integration and differentiation; position-momentum uncertainty products for the box and oscillator problems with given wave functions, etc.
   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; Interpolations (Newton, cubic spline, etc)

2. Autocatalysis by Mn2+ 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)
   Quenching of fluorescence (fluorimetric)