CENTRAL UNIVERSITY OF HARYANA
SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF CHEMISTRY

M.Sc. (Chemistry, 2016-18)

SEMESTER-I

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.	SCS CH 1101 C 4004	Inorganic Chemistry-I	4	0	0	4	4
2.	SCS CH 1102 C 4004	Organic Chemistry-I	4	0	0	4	4
3.	SCS CH 1103 C 4004	Physical Chemistry-I	4	0	0	4	4
4.	SCS CH 1104 C 0044	Chemistry Laboratory-I	0	0	4	8	4
5.	Elective (GEC)	***To be taken from other department***	4	0	0	4	4
							Total Credits = 20

SEMESTER-II

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.	SCS CH 1201 C 4004	Inorganic Chemistry-II	4	0	0	4	4
2.	SCS CH 1202 C 4004	Organic Chemistry-II	4	0	0	4	4
3.	SCS CH 1203 C 4004	Physical Chemistry-II	4	0	0	4	4
4.	SCS CH 1204 C 0044	Chemistry Laboratory-II	0	0	4	8	4
5	SCS CH 1205 DCEC 4004	Sustainable and Green Chemistry (compulsory)	4	0	0	4	4
6.	SCS CH 1206 DCEC 2002	Seminar Paper (compulsory)	2	0	0	2	2
7	Elective (GEC)	***To be taken from other department***	4	0	0	4	4
							Total Credits = 26

SEMESTER-III

Students opt for two specialisation courses from Nos 1-6 (Inorganic/Organic/Physical Chemistry). Courses numbered 7-10 are compulsory for all students.

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.	SCS CH 1301 C 4004	Organometallic Chemistry	4	0	0	4	4
2.	SCS CH 1302 C 4004	Bioinorganic Chemistry	4	0	0	4	4
3.	SCS CH 1303 C 4004	Heterocycles and Natural Products	4	0	0	4	4
4.	SCS CH 1304 C 4004	Organic Synthesis	4	0	0	4	4
5.	SCS CH 1305 C 4004	Chemical Dynamics and Catalysis	4	0	0	4	4
6.	SCS CH 1306 C 4004	Surface Chemistry and Electrochemistry	4	0	0	4	4
7.	SCS CH 1307 C 4126	Applications of Spectroscopy	4	1	2	7	6
8.	SCS CH 1308 DCEC 4004	Seminar Paper (compulsory)	4	0	0	4	4
9.	GEC	**To be taken from other department**	0	0	0	4	4
10.	SCS CH 1309 DCEC 4004	Organic Chemistry of Polymers	4	0	0	4	4
							Total Credits = 26

SEMESTER-IV

Skill Enhancement Elective Course (Compulsory and exclusively for Chemistry students)

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.*	SCS CH 1401 DCEC 003024	Dissertation	0	0	30	30	24
OR							
1.*	SCS CH 1402 DCEC 002216	Dissertation	0	0	22	22	16

2.	SCS CH 1403 DCEC 4004	Medicinal & Pharmaceutical Chemistry	4	0	0	4	4
3.	SCS CH 1404 DCEC 4004	Materials and Photochemistry	4	0	0	4	4
							Total Credits = 24

***** For students who opt to do their dissertation at other institutes, course code SCS CH 1401 DCEC 003024 applies. They **need not take** the theory DCECs numbered 2 and 3.
Students who carry out their dissertation in Central University of Haryana, course SCS CH 1402 DCEC 002216 applies. They **must take** the theory DCECs numbered 2 and 3.

List of Generic Elective Course (GEC) offered by the department to students of other departments*

S. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
Offered in Semester I							
1.	SCS CH 1110 GE 4004	Chemistry of Materials	4	0	0	4	4
Offered in Semester II							
1.	SCS CH 1210 GE 4004	Environmental Chemistry	4	0	0	4	4
Offered in Semester III							
1.	SCS CH 1310 GE 4004	General Polymer Chemistry	4	0	0	4	4
Offered in Semester IV							
1.	SCS CH 1410 GE 4004	Basics of Medicinal Chemistry	0	0	4	4	4

**These courses will be offered subject to availability of Faculty.*

SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF CHEMISTRY
CENTRAL UNIVERSITY OF HARYANA

M.Sc. Chemistry Programme (2016-18)

Total credits = 96

SEMESTER	CREDITS				Total
	CORE COURSE	ELECTIVE COURSE			
		Chemistry department		Other Departments (GEC)	
		DCEC	GEC		
I	16	0	0	4	20
II	16	6	0	4	26
III	14	8	0	4	26
IV	00	24	0	0	24
Total	**46**	**38**	**0**	**12**	**96**

SEMESTER I

SEMESTER - I
Inorganic Chemistry-I

Core Course SCS CH 1101 C 4004
60 Hrs. (4Hrs. /week) **Credits: 4**

UNIT I: Theories of Bonding in Coordination Complexes

Valence bond theory, electro neutrality principle and limitations, Crystal field theory, splitting of d-orbitals in cubic, octahedral, tetragonal, tetrahedral and square planar ligand environments. Structural consequences of splitting of d-orbitals, Jahn Teller theorem, trends in ionic radii, lattice energy and heat of ligation. Structure of spinels. MOT with σ and π bonding.

UNIT II: Chemistry of Lanthanides and Actinides

Lanthanides

Extraction & applications, colour and spectra, magnetic properties, Binary & Ternary compounds, oxo salts, compound containing oxygen, nitrogen, sulphur & phosphorus ligands, cyclopentadienyl compounds, Low oxidation state compounds, Lanthanide contraction, Use of lanthanide compounds as shift reagents.

Actinides

General properties, oxidation states, Dioxoions, chemistry of Actinium, Thorium, Protactinium, Uranium, Compounds containing oxygen, nitrogen, sulphur, phosphorus ligands, uranyl & cyclopentadienyl compounds, Transuranic elements, Later actinide elements.

UNIT III: Chemistry of Non Transition Elements

General discussion on the properties of the non-transition elements, special features of individual elements, synthesis, properties and structure of their halides and oxides, polymorphism of carbon, phosphorus and sulphur, Synthesis, properties and structure of boranes, carboranes, borazines, silicates, phosphazenes, sulphur-nitrogen compounds, peroxo compounds of boron, carbon and sulphur, oxy acids of nitrogen, phosphorus, sulphur and halogens, interhalogens, pseudohalides and noble gas compounds.

UNIT IV: Non-aqueous Solvents

Solvent system definition, Reactions in non-aqueous media with respect to H_2SO_4, BrF_3, N_2O_4, HF, thionyl chloride and phosphoryl chloride. Mechanism of coordination reactions in non-aqueous media.

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, HarperCollins.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
4. Magnetochemistry, R.L. Carlin, Springer Verlog.
5. Magnatochemistry, A. Earnshaw.
6. Inorganic chemistry, G. Wulf'sburg.
7. Introduction to ligand fields, B.N. Figgis, Wiley Eastern-IIed.

SEMESTER-I
Organic Chemistry-I

Core Course SCS CH 1102 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

UNIT I: Nature of Bonding in Organic Molecules
Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism; Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Hückel's rule, energy level of π–molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity; Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

UNIT II: Stereochemistry
Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding; Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, asymmetric synthesis (basic principle, auxiliary, substrate, reagent and catalyst controlled). Methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes); Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

UNIT III: Reaction Mechanism: Structure and Reactivity
Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms. Generation, structure, stability and reactivity of carbocations, carbanions free radicals, carbenes and nitrenes; Effect of structure on reactivity–resonance and field effects, steric effect. The Hammett equation and linear free energy relationship, substituent and reaction constants.

UNIT IV: Aliphatic Substitution Reactions
Aliphatic Nucleophilic Substitution Reactions: The S_N2, S_N1, mixed S_N1 and S_N2 and SET Mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. The S_N^i mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nuleophile, regioselectivity.

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms S_E2 and S_Ei. The S_E1 mechanism, electrophilic substitution accompanied by double bound shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books Suggested

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edition, Michael B. Smith, WILEY, 2013.
2. Advanced Organic Chemistry PART A., F. A. Carey and R. J. Sundburg, Springer 2007.
3. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
4. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, 1985.
5. Organic Chemistry, Morrison, Boyd and Bhattcharjee, &th Edition, Pearson, 2010.
6. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan, 1984.
7. Stereochemistry of Organic Compounds, Second Ed., D. Nasipuri, New Age International, 2005.
8. Stereochemistry of Organic Compounds, E. L. Eliel and S. H. Wilen, Wiley India, 2008.

SEMESTER - I
Physical Chemistry-I

Core Course SCS CH 1103 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit-I: Classical Thermodynamics and applications
Classical Thermodynamics Laws, state and path functions and their applications. Thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; free energy, chemical potential, and entropies.

Unit-II: Partial molar properties and applications
Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. The concept of fugacity and determination of fugacity. Thermodynamics of ideal and non-ideal gases, and solutions. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Unit-III: Statistical Thermodynamics
The concept of distribution, ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions– translational, rotational, vibrational, and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, applications of partition functions.

Unit-IV: Electrochemistry and structure of electrified interfaces
Electrochemistry of solutions. Nernst equation, redox systems, electrochemical cells; Debye-Hückel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria Debye-Hückel–Onsager treatment and its extension, ion-solvent interactions. The structure of electrified interfaces: Guoy-Chapman, Stern, Devanathan models. Over potentials, Exchange current density, Tafel plot.

Books Suggested

1. Physical Chemistry, P. W. Atkins, Oxford University Press
2. Physical Chemistry, G. W. Castellan, Narosa Publishers, New Delhi
3. Thermodynamics for Chemists, S. Glasstone, Affiliated East-West Press
4. Chemical Thermodynamics, I.M. Klotz and R.M. Rosenberg, Benzamin
5. Modern Electrochemistry Vol-I and Vol-IIA/B, J. O. M. Bockris and A. K. N. Reddy, Plenum
6. Physical Chemistry- A molecular approach, Donald Mcquarie and John Simon, Viva
7. Physical Chemistry, Ira N Levine, Tata McGraw-Hill

SEMESTER - I

Chemistry Laboratory-I

Core Course SCS CH 1104 C 0044
120 Hrs (8 Hrs /week) **Credits: 4**

Inorganic Chemistry Experiments

I Water Analysis (Any Two)

1. Determination of DO, COD and BOD of a waste water sample.
2. Determination of total suspended solids and total dissolved solids.
3. Determination of turbidity of a water sample by nephlometer.

II Preparations (Any Four)

Preparation of selected compounds and their spectroscopic studies.

1. $VO(acac)_2$
2. $Mn(acac)_3$
3. Prussian Blue/ Turnbull's Blue
4. $Hg[Co(NCS)_4]$
5. Potassium trioxalatoferate (III) Trihydrate
6. Dichlorobis (hydroxylamine) Zinc (II)
7. Pentathioureadicuprous nitrate
8. Potassium trioxaltochromate (III)

III Quantitative Analysis (Any Three)

Separation of the metal ions and determination of any one of them use volumetric methods:

Cu-Ni, Cu-Zn, Fe-Mg, Fe-Ni, Ag-Ni, Cu-Ba, Ag-Mg, Cu-Mg, Ag-Zn, Ag-Cu

IV Chromatographic Separations (Two)

Thin- layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of R_f values.

Physical Chemistry Experiments

1. Determination of the equivalent conductance of strong electrolytes such as HCl, KCl, KNO_3, $AgNO_3$, and NaCl and the validity of Onsager equation.
2. Study conductometeric titration of (**1**) HCl / NaOH (**2**) CH_3COOH / NaOH and comment on nature of graph.
3. Study conductometeric titration of (**1**) HCl / NH_4OH (**2**) CH_3COOH / NH_4OH and comment on nature of graph
4. Determine the equivalent conductance, degree of dissociation and dissociation constant of acetic acid.
5. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
6. To determine the strength of acids including polybasic acids by titrating against base pH meter and potentiometrically.

Books Suggested:

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.
2. Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, revised, G. Svehla, Longman.
3. Practical Inorganic Chemistry, Marr and Rocket.
4. Practical Chemistry, A. M. James and F. E. Pricherd, Longman.
5. Practical Physical Chemistry, B. P. Levitt and Zindley's, Longman.
6. Practical Physical Chemistry, S. R. Palit and S. K. De, Science Book Agency.
7. Experimental Physical Chemistry, R. C. Das and B. Behra, McGraw Hill.
8. Experiments in Physical Chemistry, Shoemaker and Gailand McGraw Hill.

Elective Course offered by the department to students of other departments

SEMESTER - I

Chemistry of Materials

Course Code - SCS CH 1110 GE 4004
60 Hrs (4Hrs /week) **Credit: 4**

UNIT I: Structures and properties of solids

1) Introduction, crystalline and amorphous solids, Unit cell, Bravais lattices, structure of NaCl and KCl, point defects – Frenkel, Schottky defects and non-stoichiometric defects.
2) Conductors, variation of conductivity with temperature, semiconductors, p and n types, photo voltaic cell. Piezoelectric and pyro-electrics. Photoluminescence.
3) Diamagnetic, paramagnetic, anti-ferromagnetic, ferro- and ferrimagnetic materials. Magnetic susceptibility, variation with temperature – Curie-Wiess law, Curie temperature and Neel temperature. Permanent and temporary magnets.

UNIT II: Hazardous and nonhazardous materials, treatment and disposal to these types of wastes

1) Identify the physical hazards of chemicals, and categorize chemicals according to their hazards and physical characteristics.
2) Define toxicity as it relates to humans and hazardous chemicals and list the elements of risk assessment.
3) Explain the pathways for transport of hazardous materials in various environments.

UNIT III: Nano Materials and Composites

1) Nano scale Regime, gas phase clusters, condensed phase, Nanoparticles. Classification of nanomaterials.
2) Methods of preparation. Top to down and Bottom up approach, Reduction of metal ions, Zeolite and inverse micelles and co-precipitation methods.
3) Composite materials: Introduction, types of fillers and matrix, classification of composite materials based on distribution and nature of fillers.
4) Particulate and fibrous metal/non-metal composites, polymer nanocomposites and their applications.

UNIT IV: Analytical Methods in Chemistry

1) Qualitative and quantitative aspects of analysis: Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression.
2) Analysis of soil, Composition of soil, Concept of pH and pH measurement, Analysis of water, Definition of pure water, sources responsible for contaminating water, water purification methods.
3) Food Analysis, food adulteration.

Books suggested

1. A.R. West, Solid State Chemistry and its Applications, 2nd ed. (**2014**) John Wiley and Sons, Singapore.
2. W. D. Callister, D. G. Rethwisch,Material Science and Engineering, AnIntroduction, 9th ed. (**2014**) Callister, Wiley.
3. L. V. Azaroff, Introduction to Solids, (**1977**) Tata McGraw-Hill, New Delhi.
4. D. A. Skoog and D.M. West, Fundamental of Analytical Chemistry, International Edition, 7th Edition (**1996**), Saunders College Publishing, Philadelphia, Holt, London.

SEMESTER II

SEMESTER - II
Inorganic Chemistry –II

Core Course SCS CH 1201 C 4004
60 Hrs. (4Hrs /week) **Credits: 4**

Unit-I
Electronic Spectra and Magnetic Properties of Transition Metal Complexes
Spectroscopic ground states and the evaluation of energies of various J states of free ions, splitting of S, P, D and F terms under octahedral and tetrahedral electrostatic potential, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and □ parameters, charge transfer spectra of complexes (both metal to ligand and ligand to metal), spectroscopy method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Unit-II
Metal-Ligand Equilibria in Solution
Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors influencing stability of metal complexes dependent on size and charge, metal class, ligand preference, nature of transition metal ions,basic strength, chelate effect, ring size, steric strain, macrocyclic effect, thermodynamic and kinetic stability, determination of formation constants by pH-metry and spectrophotometry.

Unit-III
Reaction Mechanism of Transition Metal Complexes
Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reaction in square planar complexes, trans effect, mechanism of the substitution reactions. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Unit-IV
Metal Carbonyls and Clusters
Molecular orbital of carbonyl, classification of metal carbonyls, bonding in metal carbonyl, valence electron count (EAN rules), preparation and properties of mononuclear and polynuclearcarbonyl complexes, bond lengths and stretching frequencies, carbonylate ions, carbonyl hydride complexes, isolobal fragments, structure and important reactions of transition metal nitrosyl.
Bonding, preparation and properties of dinuclear metal cluster (dirhenium complex $[Re_2Cl_8]^{2-}$ ions), trinuclear and hexanuclear metal clusters.

Books Suggested

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.
2. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. John Wiley, 1999.
3. N. N. Greenwood and E. A. Earnshaw; Chemistry of elements, 2nd ed. Butterworth-Heinemann, 1997.
4. B. E. Douglas, D. H. McDaniel, J. J. Alexander; Concepts and Models of Inorganic Chemistry, 3rd ed. John Wiley, 1993.
5. P. Atkins, T. Overtone, J. Rourke, M. Weller, F. Amstrong; Inorganic Chemistry, 5th ed. Oxford University Press, 2010.

SEMESTER - II
Organic Chemistry-II

Core Course SCS CH 1202 C 4004
60 Hrs. (3Hrs /week) **Credits: 4**

UNIT I: Aromatic Substitution and Elimination Reactions

a) Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity. The *ortho/para* ratio, *ipso* attack, orientation in other ring systems. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

b) Aromatic Nucleophilic Substitution

The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity–effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

c) Elimination Reactions

The E2, E1 and E1cB mechanisms. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium.

UNIT II: Chemistry of carbon-carbon and carbon-heteroatom multiple bonds

a) Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophilies, nucleophiles and free radicals. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

b) Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of carbonyl compounds, acids and esters. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates; Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides.

UNIT III: Free Radical Reactions and Photochemistry

a) Free radicals: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

b) Organic Photochemistry: Fundamentals of photochemistry, photochemical reactions of alkenes, aromatic compounds, carbonyl compounds and other systems, synthetic applications of photochemical reactions, modern methods in organic photochemistry.

UNIT IV: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. FMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n +2 and allyl systems. Cycloadditions–antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes. Sigmatropic rearrangements–suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Ene reaction.

Books Suggested

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edition, Michael B. Smith, WILEY, 2013.
2. Advanced Organic Chemistry PART A and PART B., F. A. Carey and R. J. Sundburg, Springer 2007.
3. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
4. Organic Chemistry, Morrison, Boyd and Bhattcharjee, &th Edition, Pearson, 2010.
5. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, 1985.
6. Pericyclic Reactions, S. M. Mukherji, Macmillan, India, 1980.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan., 1984.
8. Advanced Organic Chemistry: Reaction Mechanism, R Bruckner, Harcourt (India) Pvt. Ltd., 2001.

SEMESTER - II
Physical Chemistry-II

Core Course SCS CH 1203 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit-I: Principles of Quantum Mechanics

Introduction to Quantum Mechanical Approach, Quantum Mechanical operators, Eigen values of Quantum Mechanical operators, Hermitian operator, commutation relations, postulates of quantum mechanics and Uncertainty Principle.
Schrödinger equation for finding wave function of a particle, Energy of a particle in One-Dimension box, Extension to Schrödinger equation for finding wave function in a three-dimensional box, Energy of a particle in Three-Dimension box, Energy levels, Eigen value, degeneracy and selection rules.

Unit-II: Approximate Methods: Quantum approach

Harmonic oscillator: Application to diatomic molecules and Energy levels; Rigid rotator: Model for a rotating diatomic molecule and Energy level; The Hydrogen atom: Schrödinger equation for hydrogen atom and shapes of atomic orbitals.
Approximate Methods: The linear variation principle, Perturbation theory (first order and non-degenerate).

Unit-III: Chemical Kinetics and Theory of Unimolecular Reactions

Methods of determining rate laws, Arrhenius equation and the activated complex; Steady-State kinetics; Steady state approximation- Dynamic of chain reactions: hydrogen-bromine reaction, pyrolysis of acetaldehyde, Decomposition of Ethane; Kinetics of One-Enzyme-One-Substrate reactions: Michaelis-Menten Mechanism, Theory of Unimolecular reactions-Lindemann Mechanism.

Unit-IV: Principles of Symmetry and Group Theory

Symmetry elements and symmetry operations; Definitions of groups, subgroups, and classes; Improper Axes and Improper Rotations, General relations among symmetry elements and operations; Symmetrical Point Groups; Linear Molecules, Symmetry elements in Allene, H_2O_2, Benzene and Ferrocene; Determination of point groups of small molecules and Schönflies Symbols; Representations of groups by matrices; The Great Orthogonality theorem and its consequences. Character table for point group C_n, C_{nh}, C_{nv}, D_n, D_{nh} (n=2, 3 and 4), T_d and O_h.

Books Suggested:

1. Quantum Chemistry, Ira N Levine, Pearson Education, 7th Ed. (2013)
2. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw-Hill (1998)
3. Quantum Chemistry, R. K. Prasad, New Age International (2001)
4. Chemical Kinetics, Keith J. Laidler, Pearson Education, 3rd Ed. (1997)

5. Chemical Applications of Group Theory, F. A. Cotton, John Willey & Sons, 3rd Ed. (2008)
6. Atkins' Physical Chemistry, Peter Atkins and Julio Paula, Oxford University Press; 10th Ed. (2014)
7. Physical Chemistry- A molecular approach, Donald Mcquarie and John Simon, Viva, 1st Ed. (2010)
8. Physical Chemistry, Ira N Levine, Tata Mcgraw-Hill Education; 6 Ed. (2011)

SEMESTER - II
Chemistry Laboratory-II

Core Course SCS CH 1204 C 0044
120 Hrs (8 Hrs /week) **Credits: 4**

I Separation and Purification Techniques

Recrystallisation, Distillation: simple, fractional, steam and vacuum distillation, sublimation, extraction.

II Qualitative Analysis

Analysis of an organic mixture containing two solid components using water, $NaHCO_3$, NaOH, HCl and ether for separation and preparation of suitable derivatives.

III Extraction of caffeine from tea leaves

IV Organic Synthesis

1. Preparation of an organic compounds involving one step.
2. Preparation of organic compound involving two steps.

V Qualitative Analysis

Characterization of compounds with the help of chemical analysis and confirmation of their structures with the help of IR/NMR/UV-Vis spectral data (IR, NMR spectra to be provided).

VI. Physical Chemistry Experiments:

1: Determine the Energy of Activation for the reaction.
2: Study the nature of salt effect on the $(S_2O_8)^{2-}$ I^- reaction and calculate overall order of the reaction and w.r.t. each reactant species.
3: Study the kinetics of saponification conductometrically and determine the rate constant.
4: Verify Beer's law for the solution of potassium permanganate.
5: Determine the Half wave potential for the cation like Cd^{2+}, Pb^{2+} and Cu^{2+}.
6: Phase diagram of three component system: water-acetic acid-chloroform.
7: Determine the equivalent conductance of strong electrolyte (KCl, NaCl, HNO_3, HCl) at different concentration and verify Onsagar's equation.

Books Suggested

1. Experiments and Techniques in Organic Chemistry, Pasto, Johnson and Miller, Prentice Hall, 1992.

2. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath, 7th Ed., 2011.
3. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H. Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, Ed. 5, Longman, 1989.

SEMESTER - II
Sustainable and Green Chemistry

Elective Course SCS CH 1205 E 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit-I

Definitions of Sustainability. Principles of Green Chemistry. Biorefinery concepts. Biomass based industrial products obtained and practiced technologies in different countries: biomass fractionation of wheat straw, rice straw and sugarcane bagasse. Biomass industrial products : cellulose, hemicellulose, lignins, pectins, starch, chitosan. Lignocellulose industrial products: extractives, biofuels, syn gases, carbon dioxide. Cellulose, hemicellulose, lignin, glucose, lactic acid, succinic acid based biorefinery. Biochars – preparation, properties, impact on global warming.. Role of catalysis development in biomass conversion. Global impact on economics and environment.. Concepts of carbon footprints, carbon trading, Life Cycle Analysis (LCA)

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Unit-II

Cellulose chemistry: structure, types, sources, and grades of cellulose; functionalization of cellulose; nanocelluloses and their preparation, structure and applications. Hemicellulose chemistry, structures, commercial products obtained from hemicellulose and their potential. Lignin structure, industrial sources of lignins, sodium lignosulfonate, lignosulfonates in oil-well drilling, industrial scale lignin derivatives, diverse applications of lignin, potential of lignin, nanolignins and their potential.

Unit-III

Biocatalyzed reactions with examples of cellulase and lipase catalyzed reactions, microbial oxidation and reductions. Microwave reactions with examples of reactions in water, organic solvents, and in solid state, with representative examples. Photo-induced reactions with representative examples. Ultrasound assisted reactions with representative some examples. Phase transfer catalyzed reactions with representative examples. Reactions in solid state with representative examples. Reactions in Ionic liquids with representative examples. Reactions in Supercritical fluids with special reference to supercritical carbon dioxide

Unit-IV

Biodegradable polymers: definition, natural polymers cellulose, starch, lignin and chitosan, and their derivatives in the form of bioplastics, components of plastics, components of textile fibres. Semi-synthetic biodegradable polymers (natural molecules like sugars anchored chemically onto non-degradable synthetic hydrocarbon polymers, or synthetic molecules anchored onto natural polymers like cellulose via chemical grafting). Currently important synthetic polymers like Polyvinylalcohol and Polylactic acid. Biodegradability

determination. BOD, COD. Biocomposites and bionanocomposites. Geotextiles. Life cycle analysis of Biodegradable Polymers.

Books Suggested:

1. Green Chemistry – A Textbook, V.K. Ahluwalia, Narosa (New Delhi) (**2013**)
2. Biomass for Renewable Energy, Fuels, and Chemicals, Donald L. Klass, Elsevier (**2006**)
3. Cellulose Science and Technology, 1st Ed., J. L. Wertz, J. P. Mercier, O. Beque, EPFL Press, Distributed by CRC Press, Taylor and Francis Group, (**2010**)
4. Experiments in Green and Sustainable Chemistry, H. Rosky, D. Kenepml, J. M. Lehn, Wiley-VCH (**2009**)
5. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press(New York), Woodhead Publishing Ltd. (Cambridge, England) (**2005)**
6. Biorefineries - Industrial Processes and Products: Status Quo and Future Directions, Birgit Kamm (Editor), Patrick R. Gruber (Editor), Michael Kamm (Editor), Wiley (**2010**)
7. Lignin and Lignans as Renewable Raw Materials: Chemistry, Technology and Applications, Francisco G. Calvo-Flores, Jose A. Dobado, JoaquínIsac-García, Francisco J. Martín-Martínez, Wiley (**2015**)

Elective Course offered by the department to students of other departments

SEMESTER - II
Environmental Chemistry

Course Code - SCS CH 1210 GE 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit-I: General aspects of environment

Environmental segments: Atmosphere, Hydrosphere, Lithosphere and Biosphere. Vertical structure of the atmosphere. Green house effect: global temperature and acid rain. Ozone depletion: ozone layer formation, reactions, role and ozone depletion processes. Consequences of ozone depletion.

Unit-II: Environmental pollution and toxicology

Types and classification of pollutions. Pollution control techniques. Contaminants and their natural pathways into atmosphere. Toxicology of inorganic and organic compounds. Reactions and fate of Hazardous waste. Chemical methods of treatment for hazardous waste.

Unit-III: Green Chemistry and Industrial Ecology

Principle of green chemistry. Waste prevention. Renewable feedstocks. Industrial ecology: Major components of industrial ecosystem, Environmental impact in industrial ecology, Industrial waste reduction and minimization methods.

Unit-IV: Climate change

Consequences, predications and adapting to climate change. International response to climate change: Montreal protocol, Rio de Janeiro summit, Kyoto protocol, ONG Earth summit, Copenhagen summit and Paris climate accord.

Books suggested

1. Environmental Chemistry, Manahan S. E., 3rd edition, CRC Press, 2009.
2. Environmental Science, Technology, and Chemistry, Manahan S. E., CRC Press, 2000.
3. Fundamentals of Environmental Chemistry, Manahan S. E., CRC Press, 2001.
4. Understanding Our Environment An Introduction to Environmental Chemistry and Pollution, Harrison, R. M., 3rd edition, RSC, 1999.
5. Environmental Chemistry, De A.K.; Fourth Edition; New Age International Pvt. Ltd., New Delhi, 2003.

SEMESTER III

SEMESTER - III
Organometallic Chemistry

Core Course SCS CH 1301 C 4004
60 Hrs (4 Hrs /week) **Credits: 4**

Unit-I

Alkyls, Aryls, Carbenes and Carbynes of Transition Metals

Synthesis, structure and bonding considerations of Zeise's salt; synthesis, stability and decomposition pathways of organocopper in organic synthesis; synthesis and reactivity of alkyl lithium; synthesis and reactivity of organozinc compounds.

Metal carbenes: preparation, reactivity, structure and bonding considerations of Fischer and Schrock carbene complexes, Tebbe's reagent, Grubb's reagent, Petasis reagent, Metal carbines: synthesis, reactivity, structure and bonding considerations of Fischer and Schrock carbyne complexes.

Unit-II

Transition Metal π-Cyclic Complexes

Half and bent sandwich compounds, molecular orbitals of metallocenes, structures of cyclopentadienyl compounds, covalent versus ionic bonding, 18 electron rule, synthesis, structure, aromatic behaviour of Ferrocene, reactions such as metallation, Friedal Craft, Mannich reaction, sulphonation, nitrations, halogenations reactions, Synthesis, structure and reactions of other metallocenes (with Cr, Ni and Zr metals).

Unit-III

Fluxional Organometallic Compounds and Coupling Reactions

Rates of rearrangement and techniques of study, NMR study of Fluxional behavior, Classification of fluxional organometallic Compounds, Mechanism of fluxionality in compounds of η^1- Cyclopentadienyls and η^3–allyls. Stereochemical non rigidity in case of coordination numbers- 4 & 5 (*cis-trans*, atomic inversion, Berry Pseudorotation).

Tsuji-Trost, Mizoroki-Heck, Miyaura-Suzuki, Stille, Negishi, Sonogashira, Kumada, Hiyama, Buchwald-Hartwig amination or coupling reactions

Unit-IV

Catalytic Processes involving Transition Metal Organometallic Compounds:

Oxidative addition, reductive elimination, insertion-migration reactions, C-H bond activation catalytic mechanism of hydrogenation, hydroformylation, oxidation and isomerization of alkenes, Monsanto acetic acid synthesis, olefin metathesis, Fischer-

Tropsch synthesis and Ziegler-Natta polymerization of alkenes, water gas shift reaction, asymmeteric and supported organometallic catalysis.

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J. P. Collman, L.S. Hegsdus, J. R. Norton and R. G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, Crabtree, R. H. John Wiley.
3. Organometallic Chemistry, Mehrotra R.C. and Singh, A. New Age International.
4. Organometallics, Salzer, A. Ch. Elschenbrioch.VCH Publications.
5. Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan.
6. Inorganic Chemistry, 3rd edn,; Miessler ,G. L., Donald, A. T.
7. Inorganic Chemistry ; 4th edn.; Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K.; Pearson Education, Inc.

SEMESTER - III

Bioinorganic Chemistry

Elective Course SCS CH 1302 C 4004
60 Hrs (4 Hrs/week) **Credits: 4**

UNIT I:

Metal ions in Biological Systems and Bioenergetics

Essential and trace metals. Role of metals ions in biological processes. Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processe. Na^+/K^+ Pump DNA polymerisation, glucose storage, metal complexes in transmission of energy.

UNIT II:

Nitrogenase and Photosynthesis

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems. Chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.

UNIT III:

Electron Transfer, Transport and Storage of Dioxygen

Structure and function of metalloproteins in electron transport processes– cytochromes and ion-sulphur proteins, synthetic models. Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

UNIT IV

Mettaloenzymes, Metal storage Transport and Biomineralization

Zinc enzymes- carboxypeptidase and carbonic anhydrase. Iron enzymes- catalase, peroxidase and cytochrome P-450. Copper enzymes- superoxide dismutase. Molybednum oxatransferase enzymes- xanthine oxidase. Coenzyme vitamin B_{12}, Ferritin, transferrine and siderophores.

Books Suggested:

1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentne, University Science Books.
3. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.

SEMESTER - III

Heterocycles and Natural Products

Core Course SCS CH 1303 C 4004
60 Hrs (4 Hrs /week) **Credits: 4**

UNIT I: Aromatic and Non-aromatic Heterocycles

- General chemical behaviour of aromatic heterocycles, criteria of aromaticity (bond length, ring current and chemical shifts in 1H NMR spectra, empirical resonance energy, delocalization energy and Dewar resonance energy). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

- Strain-bond angle and torsional strain and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction.

UNIT II: Heterocyclic synthesis and reactions

- Synthesis and reactions of three and four membered heterocycles (aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes).
- Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes.
- Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrirylium salts and pyridones.
- Synthesis and reactions of quinolinizium and benzopyrylium salts.

UNIT III: Chemistry of Natural Products (Terpenoids and Steroids)

- **Terpenoids and Carotenoids**
  Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Stereochemistry, synthesis and biosynthesis of the following representative molecules: Citral, α-Terpeneol, Farnesol, Santonin, Phytol and β-carotene.

- **Steroids**
  Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation and synthesis of Cholesterol, Testorosterone, Progesterone, Oestrone.

UNIT IV: Natural Products Chemistry (Alkaloids)

Definition, nomenclature, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen Heterocyclic ring. Stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Atropine and Quinine.

Books Suggested

1. The chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
2. Heterocyclic Chemistry, J. A. Joule, ELBS.
3. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical.
4. Contemporary Heterocyclic Chemistry, G. R. Newkome and W. W. Paudler, Wiley-Iter Science.
5. An Introduction to Heterocyclic Chemistry, R. M. Acheson, John Wiley.
6. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, eds. Pergamon Press.
7. Natural products: Chemistry and Biological Significance, Mann, Davidson, Hobbs, Banthrope and Harborne, Longman, Essex.
8. Organic Chemistry, *Vol. 2*, I. L. Finar, ELBS.
9. Rodd's Chemistry of Carbon Compounds, Ed. S Coffey, Elsevier.
10. Introduction to Flavonoids, B. A. Bohm, Harwood Academic Publishers.
11. Chemistry, Atta-ur-Rahman and Choudhary, Harwood Academic Publishers.

SEMESTER - III
Organic Synthesis

Core Course SCS CH 1304 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

UNIT I: Reagents in Organic Synthesis

Modern alkali metal reagents (LDA, LiHMDS. KHMDS); Enamines and modern aldol chemistry; Olefination reactions and reagents (Wittig, Wadsworth, Peterson, Julia and McMurry); Amide coupling reagents (DCC, DIC, EDC, HOBt); Common reducing agents (Dissolving metal reductions, various hydrides, catalytic/transfer hydrogenations, diimide); Common oxidising agents, oxidations of alcohols, alkenes, aldehydes, and saturated carbons; Woodward and Prevost dihydroxylations, hypervalent iodine reagents, DDQ; Organic chemistry of boron, silicon and tin; Organocatalysis

UNIT II: Rearrangement Reactions

A detailed study of the following rearrangements: Wagner-Meerwein, Pinacol, Tiffeneau–Demjanov, Wolff, Beckmann, Baeyer-Villiger, Curtius, Lossen, Schmidt, Favorskii, Baker-Venkataraman and Neber and variants of Pericyclic (Cope, Claisen) rearrangements.

UNIT III: Synthetic planning and retrosynthesis

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions; chemoselectivity, reversal of polarity (Umpolung exemplified by 1,3-dithianes, benzoin condensations and N-heterocyclic carbenes); the importance of the order of events in organic synthesis. Use of carbonyl compounds, acetylenes and nitro compounds. Basics of asymmetric synthesis

UNIT IV: Protecting groups and total synthesis

Protecting Groups in total synthesis for alcohol, amine, carbonyl and carboxyl groups; Total synthesis, semi synthesis and formal total synthesis; Classical and modern total syntheses any two of the following natural products; Prostaglandin, Reserpine, Strychnine and Quinine

Books Suggested

1. Modern Synthetic Reactions, H. O. House, W. A. Benjamin, 1972.
2. Some Modern Methods of Organic Synthesis, W. Carrutheoldham, Cambridge University Press, 2004.
3. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional, 1993.

4. Organic Synthesis: The Disconnection Approach- 2nd Edition, Stuart Warren and Paul Wyatt, WILEY, 2008.
5. New Horizons in Organic Synthesis, V. Nair & S. Kumar, New Age International, 1996.
6. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edition, Michael B. Smith, WILEY, 2013.
7. Advanced Organic Chemistry PART A and PART B., F. A. Carey and R. J. Sundburg, Springer 2007.
8. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2012.
9. Organic Chemistry, Morrison, Boyd and Bhattcharjee, &th Edition, Pearson, 2010

SEMESTER - III

Chemical Dynamics and Catalysis

Core Course SCS CH 1305 C 4004
60 Hrs (4Hrs./week) **Credits: 4**

Unit-I: Kinetics of polymerization & Enzyme Inhibitions
Introduction, kinetics to step growth polymerization, free radical addition polymerization, calculation of radius of gyration.
Enzymes and Inhibitions
Enzyme catalysed models of 1:2 type enzyme substrate systems, kinetics of one enzyme – two substrate systems and their experimental characteristics, enzyme inhibitors and their experimental characteristics, kinetics of enzyme inhibited reactions.

Unit-II: Transition State Theory
A brief aspect of statistical mechanics and transition state theory, application on calculation of second order rate constant for reactions with collision for (atom + atom), (atom + molecule), and (molecule + molecule) reactions, static solvent effect and thermodynamic formulation, adiabatic electron transfer reaction and energy surfaces.

Unit-III: Kinetics of Substitution reactions
Substitution reactions, classification of ligand substitution mechanism, inner and outer sphere electron transfer reactions and mechanism, adjacent and remote attack linkage isomerism.

Unit-IV: Metal ion catalysis and induced Phenomena
Metal ion catalysed reactions and reaction mechanism, induced reactions and their characteristics, applications, kinetics and mechanism of induced reaction in metal complexes, kinetics of hydroformylation reactions.

Books Suggested
1. H. Taube, Electron Transfer Reactions, Oxford Press.
2. Basolo and Pearson, Inorganic Reaction Mechanism, Wiley.
3. N. L. Bender, Mechanism of Homogenous catalysis, Wiley.
4. A. G. Sykes, Kinetics in Inorganic reactions, Academic Press.

SEMESTER - III

Surface Chemistry and Electrochemistry

Core Course SCS CH 1306 C 4004
60 Hrs (4Hrs./week) **Credits: 4**

Unit-I: Molecular Orbital Theory

Molecular Orbital theory, effective Hamiltonian, Hückel theory of conjugated system, application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene, benzene etc. introduction to Extended Hückel theory.

Unit-II: Surface Chemistry

The extent of adsorption: Physorption and Chemisorptions, Adsorption isotherms, Rates of surface processes (adsorption, desorption and mobility on surfaces). BET equation.
Heterogeneous catalysis: Mechanism of heterogeneous catalysis; Langmuir–Hinshelwood mechanism.

Unit-III: Micelles

Micelles: Surface active agents, classification, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, phase separation, micro emulsion and reverse micelles.

Unit-IV: Fuel Cells and Batteries

Electrochemical storage, theoretical consideration of fuel cells, maximum intrinsic efficiency, Hydrogen–Oxygen cell, alkaline fuel cell, phosphoric acid fuel cell, direct methanol fuel cell, Hydrocarbon–Air cells, Natural gas.

Battery characteristics specification, components, battery systems, Lead storage battery, Dry cell, Silver-Zinc cell, Sodium–Sulphur cell and Ni-Cd battery.

Potential Sweep Method: Linear Sweep voltammetry, cyclic voltammetry, controlled current techniques- chronopotentiometry: theory and applications, Polarography: theory and applications.

Books suggested

1. Quantum Chemistry, I. M. Levine, Prentice Hall.
2. Micelles, Theoretical and applied aspects, V. Moroi, Plenum
3. Physical Chemistry, P. W. Atkins, ELBS.
4. Fuel cells from fundamentals to applications, S. Srinivasan, Springer, New York, 2006.

SEMESTER - III
Applications of Spectroscopy

Core Course SCS CH 1307 C 4126
105 Hrs (7Hrs /week) **Credits: 6**

UNIT I: Ultraviolet and Visible Spectroscopy, Infrared Spectroscopy and Mass Spectrometry

Various electronic transitions, Beer-Lambert law, visible spectrum & colour, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds.

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

Introduction, ion production–EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry (HRMS).

UNIT II: Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding and deshielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindred rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents. Fourier transform technique, nuclear Overhauser effect (nOe). Resonance of other nuclei-F, P. **Carbon-13 NMR Spectroscopy:** General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroarmatic and carbonyl carbon), coupling constants and DEPT ^{13}C NMR spectra. General introduction to two-dimensional NMR spectroscopy-COSY, HETCOR, INADEQUATE and NOESY.

UNIT III: Infrared and Raman Spectroscopy of inorganic compounds

Molecular vibrations, force constants, molecular vibrations and absorption of Infrared radiations. Raman spectroscopy, polarized Raman lines. Use of symmetry considerations to determine the noumber of lines in IR and Raman Spectra. Structural studies involving IR and Raman Spectroscopy of coordination compounds containing the following molecules/ions and ligands: NH_3, H_2O, OH, SO_4^{2-}, ClO_4^-, COO^-, NO_2, CN^-, SCN^-, NO, O_2, PR_3,

Halides, DMSO, azopyridine, oxime, quinine, acetylacetone, amino acids. Hydrogen bonding and infrared spectra, metal ligand and related vibrations. Application of resonance Raman spectroscopy to structural elucidation of the active sites of heme and non-heme oxygen carriers.

UNIT-IV: Electron Spin Resonance Spectroscopy of inorganic compounds

Basic principle, selection rules, presentation of spectra, origin and interpretation of Lande's factor(g), factor affecting 'g-value', isotropic and anisotropic hyperfine coupling, super hyperfine coupling, spin-orbit coupling, line shape, zero field splitting, Kramer's degeneracy, quadrupolar interactions, ESR analysis of organic compounds, transition metal complexes of vanadium, chromium, manganese, iron, copper, cobalt and iron.

Application of ESR spectroscopy: structure determination, interpretation of ESR spectra of simple organic radicals like benzene, naphthalene, toluene and xylene radical ions, study of unstable paramagnetic species.

Books Suggested

1. Spectrometric Identification of Organic Compounds, Silverstein, Bassler and TMorrill, John Wiley.
2. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
3. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
4. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
5. Organic Chemistry, William Kemp, John Wiley.
6. Organic Spectroscopy, Jag Mohan, Narosa Publishers, New Delhi
7. Rita Kakkar, Atomic and Molecule Spectroscopy: Basic Concepts and Applications, Cambridge University Press, 2015.
8. K. Nakamoto; Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A and B, 6th ed. Wiley, 2008.
9. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4th ed. Tata McGraw Hill, 1994.
10. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.

SEMESTER - III
Seminar

Core Course SCS CH SCS CH 1308 DCEC 4004
60 Hrs (4 Hrs./week) **Credits: 4**

Each student must present at least two seminar (30 minutes each) which will be followed by discussion session (10 minutes) with participation from other students and the concerned faculty members present. The student must also submit the slides/write-up of the presentation contents to the faculty-in-charge. The seminars, participation in discussions, the submitted slides and overall attendance (as per ordinance) will form the basis of the evaluation. There will be no separate final exam for this course.

SEMESTER – III
Organic Chemistry of Polymers

Elective Course code - SCS CH 1309 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit I

Classification of polymers by properties (morphological, elastomeric, thermoplastic, thermoset, emulsion polymers, suspension polymers), and structures (aliphatic hydrocarbons, aromatic hydrocarbons, polysaccharides, polyesters, polyamides, polyurethanes, polyphosphazenes, silicones, glasses, phenol-formaldehyde resins)

Unit 2

Applications of polymers (elastomeric, adhesives, membranes, agricultural mulch films. Introduction to polymer structures. Synthesis of different classes of polymers (condensation polymers, free radical polymers, coordination polymers). Mechanisms of polymerizations by anionic, cationic, free radical and coordination catalysis.

Unit 3

Synthesis of polymers by radical, emulsion, suspension, and ionic mechanisms, Copolymers, Functionalization of synthetic (hydrocarbons) and natural polymers (cellulose, lignin) by use of chemical reactions, Crosslinking of polymers, Stereochemistry of polymers, cis trans rubbers, poly(methylmethacrylate) polymers.

Unit 4

Natural Polymers (cellulose, starch, lignin, galactomannans, xanthan gum, alginic acid). Biodegradable Polymers, with special reference to Polyvinyl alcohol, polylactic acid, and cellulose esters. Applications of biodegradable polymers.nn

Books suggested:

1. Principles of Polymerization, George Odian, 4th. Edition, Wiley-Interscience (**2004**).
2. Textbook of Polymer Science, Fred W. Billmeyer, 3rd. Ed., John Wiley and Sons (Asia) (**2013**).
3. A Textbook of Polymer Chemistry, M.S.Bhatnagar, S.Chand& Co., (New Delhi) (**2014** reprint).
4. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press (new York, Woodhead Publishing Co., (Cambridge) (**2005**).

Elective Course offered by the department to students of other departments

SEMESTER – III

General Polymer Chemistry

Elective Course code - SCS CH 1310 GE 4004
60 Hrs (4Hrs /week) **Credits: 4**

Unit I: Introduction to polymers

Nomenclature of polymers: names based on source, structure (IUPAC and Non-IUPAC) and trade names. Exposure to important terminologies and definitions used in polymer chemistry such as molecular weight, size, glass transition temperature and morphology.

Unit II: Types of polymerization

Step polymerization, Chain transfer for polymerization, Anionic & Cationic polymerization, Coordination polymerization, Solution & Template polymerization, Bulk & Block polymerization, Radical polymerization, Ring opening polymerization.

Unit III: Application of synthetic polymers

(i) In medicinal field as artificial heart, artificial skin, contact lenses and dental resins. (ii)Electrical properties: Conducting polymers (polyacetylenes), polymer electronics (polymer based LED, solar cells, transistors, and sensors).

Unit IV: Natural and Biodegradable polymers

Naturally occurring Polymers (polysaccharides, cellulose, starch, proteins, nucleic acid, lignin, melanins). Biodegradable Polymers, with special reference to polyvinyl alcohol, polylactic acid, and cellulose esters. Application of biodegradable polymers.

Books suggested:

1. Introduction to Polymer Chemistry, Charles E. Carraher, Jr., 3rd. Edition, CRC press (**2013**).
2. Introduction to Polymers, Robert J. Young and Peter A. Lovell, 3rd. Edition, CRC press (**2011**).
3. A Textbook of Polymer Chemistry, M.S.Bhatnagar, S.Chand& Co., (New Delhi) (**2014** reprint).
1. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press (new York, Woodhead Publishing Co., (Cambridge) (**2005**).

SEMESTER IV

SEMESTER – IV
Project Work

Core Course SCS CH 1401 DCEC 003024
450 Hrs (30 Hrs /week) **Credits: 24**

For students who opt for out-station dissertation projects

The aim of the dissertation project work is to familiarize the students with advanced research. This course applies to students who opt to go to other institutes for their dissertation work. The topic for the project work is to be decided by the supervisor/guide concerned. The project report is to be evaluated by a committee constituted by the Head, Department of Chemistry/School of Chemical Sciences having at least one external member.

SEMESTER – IV
Project Work

Core Course SCS CH 1402 DCEC 002216
330 Hrs (22 Hrs /week) **Credits: 16**

For students who opt for dissertation projects in Central University of Haryana

The aim of the dissertation project work is to familiarize the students with advanced research. This course applies to students who opt to carry out their dissertation work in Central University of Haryana. The topic for the project work is to be decided by the supervisor/guide concerned. The project report is to be evaluated by a committee constituted by the Head, Department of Chemistry/School of Chemical Sciences having at least one external member.

SEMESTER – IV
Medicinal & Pharmaceutical Chemistry

Elective Course code - SCS CH 1403 DCEC 4004
60 Hrs (4 Hrs /week) **Credits: 4**

UNIT I: Drug Design
Development of new drugs, concept of lead compounds and lead modifications, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism. Theories of drug activity, Quantitative structure activity relationship, Concepts of drugs receptor, Elementary treatment of drug receptor interactions, Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric factors.

UNIT II: Antineoplastic Agents
Introduction, cancer chemotherapy, targets of cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Synthesis of any three representative anticancer drugs, Recent development in cancer chemotherapy.

UNIT III: Antibiotics and Cardiovascular Drugs
Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis, Synthesis of penicillin G, amoxycillin, cephalosporin, ciprofloxacin. Introductory idea of tetracycline and streptomycin. Introduction and general mode of action. Synthesis of ditiazem, verapamil, methyldopa and atenolol.

UNT IV: Local Antiinfective Drugs and Psychoactive Drugs
Introduction and general mode of action. Synthesis of furazolidone, naldixic acid, dapsone, isoniazid, ethambutol, gluconazole, chloroquin and primaquin. Introduction, neurotransmitters, CNS depressants, general anaesthgetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazopines, buspirone. Antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones. Synthesis of diazepam, alprazolam, phenyltoin and glutethimide.

Books Suggested

1. An Introduction to Medicinal Chemistry, 5th Edition, G. L. Patrick, Oxford University Press, 2013.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge, 12th Edition, 2010.
3. An Introduction to Drug Design, 1st Edition, S. S. Pandeya and J. R. Dmmock, New Age International, 1999.

4. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1, 7th Edition, Ed. M E Wolff, John Wiley, 2010.
5. The Organic Chemistry of Drug Design and Drug Action, 3rd Edition, R. B. Silverman, Academic Press, 2014.

SEMESTER - IV
Materials and Photochemistry

Course Code: SCS CH 1404 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

UNIT I: Nano Materials and Composites

Nano scale regime, gas phase clusters, condensed phase, nanoparticles. Classification of nanomaterials.Methods of preparation.Top to down and bottom up approach, Reduction of metal ions, Zeolite and inverse micelles and co-precipitation methods. Porous materials: design, structure, property and applications. Composite materials: Introduction, types of fillers and matrix, classification of composite materials based on distribution and nature of fillers.

UNIT II: Supramolecular Materials

"Chemistry beyond the molecules".Concepts and terminology insupramolecular chemistry. Nature and types of supramolecular interactions (Hydrogen bonding, van der Waals interactions, π-stacking, C-H···π interactions etc.).Molecular recognition- Information and complementarity. Different types of receptors with special reference of Crown ethers, cryptates and Calix[4]arene. Anion recognition and anion coordination chemistry.Molecular self-assembly formation and examples.Supramolecular chemistry of life, application of supramolecular chemistry in drug design.Application in material science-molecular machines.

UNIT III: Introduction to Photochemistry and Basic Photochemical Reactions

Interaction of electromagnetic radiation with matter, electronic transition, Frank-Condon principle, selection rules, Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law, quantum yield, photodissociation, predissociation, photochemical reactions: photoreduction, photooxidation, photodimerization, photochemical substitution, photoisomerization.

UNIT IV: Photophysical Phenomena

Electronic structure of molecules, molecular orbital, electronically excited singlet states, life time of electronically excited state, construction of Jablonski diagram, electronic transitions and intensity of absorption bands, photphysical pathways of excited molecular system (radiative and non-radiative), chemiluminescence, phosphorescence and fluorescence.

Books Suggested

1. W. D. Callister, D. G. Rethwisch, MaterialScience and Engineering, AnIntroduction, 9th ed. (**2014**) Callister, Wiley.
2. J. W. Steed & J. L. Atwood. Supramolecular Chemistry, John Wiley (2002)
3. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995
4. Lehn, J.M. Transition metals in supramolecular chemistry: John Wiley & sons: New York, 1999.
5. N. J. Turro, V. Ramamurthy and J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, 1st ed. University Science, Books, CA, 2010.
6. I. Ninomiya, T. Naito, Photochemical Synthesis, 1st ed. Academic Press, New York, 1989.

Elective Course offered by the department to students of other departments

SEMESTER – IV

Basics of Medicinal Chemistry

Elective Course code - SCS CH 1410 GEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

UNIT I: Fundamentals

Historical development of systems of medicine, Basic chemical and biochemical principles, Key definitions, drug, target, receptors, enzymes, common drugs and their classification, anti-inflammatory drugs, antihistamines, antacids, antibiotics, narcotics, antivirals, and antineoplastics.

UNIT II: Drug Action

Chemistry of drug-target interactions, bioavailability, drug absorption, distribution, metabolism, excretion (ADME), pharmacokinetics and pharmacodynamics, toxicity, side effects, lipophilicity and hydrophilicity, blood-brain barrier and its significance, routes of drug administration

UNIT III: Drug Design and Synthesis

Development of new drugs, concept of lead compounds and lead modifications, structure-activity relationship (SAR), isosterism, bio-isosterism, important chemical principles behind design of drugs, natural products and their uses, chemical synthesis of drugs, drug formulation, drug delivery, photodynamic therapy.

UNIT IV: Drugs and Society

Regulatory processes for drug approval, regulatory agencies, intellectual property, patents, drug misuse, drug abuse, abuse of antibiotics, fraud practices in treatment, historically important drugs and vaccines

Books Suggested

1. An Introduction to Medicinal Chemistry, 5th Edition, G. L. Patrick, Oxford University Press, 2013.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge, 12th Edition, 2010.

3. An Introduction to Drug Design, 1st Edition, S. S. Pandeya and J. R. Dmmock, New Age International, 1999.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1, 7th Edition, Ed. M E Wolff, John Wiley, 2010.
5. The Organic Chemistry of Drug Design and Drug Action, 3rd Edition, R. B. Silverman, Academic Press, 2014.