CENTRAL UNIVERSITY OF HARYANA
SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF CHEMISTRY

M.Sc. (Chemistry)

SEMESTER-I

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.	SCS CH 1 1 01 C 4004	Inorganic Chemistry-I	4	0	0	4	4
2.	SCS CH 1 1 02 C 4004	Organic Chemistry-I	4	0	0	4	4
3.	SCS CH 1 1 03 C 4004	Physical Chemistry-I	4	0	0	4	4
4.	SCS CH 1 1 04 C 0044	Chemistry Laboratory-I	0	0	4	8	4
5.		***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 1 2 05 C 4004	Inorganic Chemistry-II	4	0	0	4	4
2.	SCS CH 1 2 06 C 4004	Organic Chemistry-II	4	0	0	4	4
3.	SCS CH 1 2 07 C 4004	Physical Chemistry-II	4	0	0	4	4
4.	SCS CH 1 2 08 C 0044	Chemistry Laboratory-II	0	0	4	8	4
5	SCS CH 1 1 03 GE 2002	Basic Techniques in Chemical Sciences (compulsory)	0	2	0	2	2
6.		***Any one of the following three courses***	4	0	0	4	
	SCS CH 1 1 01 DCEC 4004	Analytical Chemistry-I	4	0	0	4	4
	SCS CH 1 1 02 DCEC 4004	Materials Chemistry	4	0	0	4	4
	SCS CH 1 1 03 DCEC 4004	Biosciences for Chemists	4	0	0	4	4
							Total Credits = 22

SEMESTER-III

Sl. No	Course code	Course title	L	T	P	Hrs/ week	Total Credits
1.	SCS CH 1 3 09 C 4004	Applications of Spectroscopy	4	0	0	4	4
2.	SCS CH 1 3 10 C 4004	Specialization paper-I (Inorg./Org./Phy.)	4	0	0	4	4
3.	SCS CH 1 3 11 C 4004	Specialization paper-II (Inorg./Org./Phy.)	4	0	0	4	4
4.	SCS CH 1 1 04 DCEC 4004	Seminar Paper (compulsory)	0	2	0	2	2
		To be taken from other department					
5.		***Any one of the following three courses***					
	SCS CH 1106 DCEC 4004	Medicinal Chemistry	4	0	0	4	4
	SCS CH 1305 DCEC 4004	Advanced Computational Chemistry	4	0	0	4	4
	SCS CH 1306 DCEC 4004	Organic Chemistry of Polymers	4	0	0	4	4
Total Credits from Chemistry Department = 18							

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 1101 DCEC 002424	Dissertation	0	0	24	24	24

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 1 1 01 GE 4004	Chemistry of Materials	4	0	0	4	4
2.	SCS CH 1 1 02 GE 4004	Bioorganic Chemistry	4	0	0	4	4
3.	SCS CH 1 1 05 GEC 4004	Environmental Friendly Processes for Sustainable Development	4	0	0	4	4
Offered in Semester III							
1.	SCS CH 1 3 04 GE 4004	General Polymer Chemistry	4	0	0	4	4
2.	SCS CH 1 3 05 GE 4004	Environmental 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

Total required credits = 88

SEMESTER	CREDITS				Total
	CORE COURSE	ELECTIVE COURSE			
		Chemistry department		Other departments	
		DCEC	GEC		
I	16	0	0	4	20
II	16	4	2	0	22
III	14	4	0	4	22
IV	24	0	0	0	24
Total	**70**	**8**	**4**	**8**	**88**

SEMESTER - I
Inorganic Chemistry-I

Core Course SCS CH 1 1 01 C 4004
60 Hrs. (4Hrs. /week) **Credits: 4**

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.

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.

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.

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 1 1 02 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

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.

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.

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.

Aliphatic Nucleophilic Substitution

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

Bimolecular mechanisms S_E2 and S_E^i. 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. Advanced Organic Chemistry-Reactions, Mechanism and Structure, March and Smith, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundburg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, CBC Publisher & Distributors.
5. Organic Chemistry, Morrison, Boyd and Bhattcharjee, Prentice-Hall.
6. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
7. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
8. Stereochemistry of Organic Compounds, E. L. Eliel and S. H. Wilen, Wiley Interscience.

SEMESTER - I
Physical Chemistry-I

Core Course SCS CH 1 1 03 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

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. 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.

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.

Electrochemistry
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. Electrochemistry-by Glasstone
4. Modern Electrochemistry vol.1 and vol IIA/B J. O. M. Bockris and A. K. N. Reddy, Plenum.
5. Thermodynamics for Chemists, S. Glasstone, Affiliated East-West Press.
6. Chemical Thermodynamics, I.M. Klotz and R.M. Rosenberg, Benzamin.

SEMESTER - I

Chemistry Laboratory-I

Core Course SCS CH 1 1 04 C 0044
120 Hrs (8Hrs /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 1 1 01 GE 4004
60 Hrs (4Hrs /week) **Credit: 4**

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1. **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.

2. **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.

3. **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.

4. **Chromatography**
   1) Classification, principle and efficiency of the technique.
   2) Mechanism of separation.

Books suggested

1. A. R. West, Solid State Chemistry and its Applications, (**1984**) John Wiley and Sons, Singapore.
2. L. V. Azaroff, Introduction to Solids, (**1977**) Tata McGraw-Hill, New Delhi.
3. D. A. Skoog and D.M. West, Fundamental of Analytical Chemistry, International Edition, 7th Edition (**1996**), Saunders College Publishing, Philadelphia, Holt, London.
4. E. Heftmann, Chromatography Fundamentals and applications of chromatography and related differential migration methods - Part A: Fundamentals and techniques, (**2004**).

Elective Course offered by the department to students of other departments

SEMESTER - I

Bio-Organic Chemistry

Course Code - SCS CH 1 1 02 GE 4004
60 Hrs (4Hrs /week) **Credits: 4**

Enzymes
Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification (suitable examples of reactions), extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling. Enzyme kinetics, reversible and irreversible inhibition.

Mechanism of Enzyme Action
Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, and carboxypeptidase A.

Biotechnological Applications of Enzymes
Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes.

Books Suggested

1. Understanding Enzymes, Trevor Palmer, Prentice Hall.
2. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.
3. Enzyme Mechanisms Ed, M. I. Page and A. Williams, Royal Society of Chemistry.
4. Immobilized Enzymes: An Introduction and Applications in Biotechnology, M. D. Trevan, John Wiley.
5. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman.
6. Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
7. Bioorganic Chemistry, Bertini G. and Lippard V, VIVA Low Priced Student Edition.

Elective Course offered by the department to students of other departments

SEMESTER - I

Environmental Friendly Processes for Sustainable Developments

Course Code: SCS CH 1105 GEC 4004
(4 hrs per week) **Credits: 4**

Biorefinery concepts and examples, Waste to value concepts, Concepts of C footprints, water footprints, smart cities, Biocatalyzed reactions, Microwave reactions, Ultrasound reactions, Ionic liquids, Biodegradable polymers Life cycle analysis, Cradle-to-cradle analysis of chemicals and polymers, Waste management concepts.

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
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)**

SEMESTER - II
Inorganic Chemistry –II

Core Course SCS CH 1 2 05 C 4004
60 Hrs. (4Hrs /week) **Credits: 4**

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 β 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.

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin.

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, the 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.

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.

SEMESTER - II
Organic Chemistry-II

Core Course SCS CH 1 2 06 C 4004
60 Hrs. (3Hrs /week) **Credits: 4**

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.

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.

Free Radical Reactions
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.

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.

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.

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.

Pericyclic Reactions
Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. FMO and PMO 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. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundburg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, CBC Publisher & Distributors.
5. Organic Chemistry, Morrison, Boyd and Bhattacharjee, Prentice-Hall.
6. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
8. Advanced Organic Chemistry: Reaction Mechanism, R Bruckner, Harcourt (India) Pvt. Ltd.

SEMESTER - II
Physical Chemistry-II

Core Course SCS CH 1 2 07 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Quantum Chemistry
Introduction to Quantum Mechanical Approach, Hermition operators and their properties, commutation relations, postulates of quantum mechanics, uncertainty principle, Schrodinger equation and its interpretation. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, simple harmonic oscillator, selection rules, expectation values, hydrogen atom, rigid rotator, shapes of atomic orbital.

Approximate Methods: The linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

Symmetry and Group Theory in Chemistry
Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. Groups to be worked out explicitly). Character of a representation. Determination of point groups of molecules reducible and irreducible representations. The Great Orthogonality theorem (without proof) and its importance.

Chemical Dynamics
Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), kinetics of enzyme reactions, dynamics of unimolecular reactions-Lindemann Theory.

Books Suggested
1. Physical Chemistry, P. W. Atkins, Oxford University Press.
2. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, I. M. Levine, Prentice Hall.
4. Physical Chemistry, G. W. Castellan, Narosa. Publishers, New Delhi.
5. Quantum Mechanics, M. L. Strause, Prentice – Hall.
6. Quantum Chemistry, R. K. Prasad, New Age International

SEMESTER - II
Chemistry Laboratory-II

Core Course SCS CH 1 2 08 C 0044
120 Hrs (8Hrs /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 Organic Synthesis

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

IV Extraction of caffeine from tea leaves

IV Qualitative Analysis

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

V. 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.
2. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
3. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H. Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A. R. Tatchell, John Wiley.

SEMESTER - II
Analytical Chemistry-I

Course code - SCS CH 1 1 01 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

Analytical chemistry forms the back bone for the research in academics as well as in industries. Analytical Chemistry is a measurement science consisting of set of powerful ideas and methods that are useful in all fields of Sciences. It is the investigation of the separation, detection, identification and quantification of atomic, molecular, and ionic species.

1. Introduction:

Analytical Chemistry and its interdisciplinary nature. Classification of analytical methods and Method selection. Sample preparation and processing. Steps involve in quantitative analysis. Importance of accuracy, precision and Standard Deviation, methods of expressing them. Sources of error in analytical measurements, Normal error curve and its equation, Propagation of error. Statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least-square method for linear plots), Concept of sensitivity and detection limit. Presentation of experimental data and results, from the point of view of significant figures. Use of computer in data analysis.

2. Introduction to Volumetric Method of Analysis

Primary and secondary standards. Preparation of standard solutions (concept of Molarity, Normality, Molality, Formality etc.) Visual method of detection of end point, theory of indicators and their classification. Classification of titration, theory of indicators and their selection: Neutralisation titration, Redox titrations, Complexometrie titrations, precipitation titrations etc. Concept of titration error and its determination/calculation.

3. Introduction to Gravimetric Analysis

Theory of Gravimetric Analysis: Estimations of metals and metal oxides, sulphates etc.

4. Modern Separation Methods:

Gas Chromatography: Theory and Instrumentation, Column types, Solid/Liquid Stationary phases, Column switching techniques, Basic and specialized detectors. Applications of the technique. **High Performance Liquid Chromatography:** Theory and instrumentation, Adsorption chromatography, Liquid-Liquid partition chromatography, Size exclusion, Ion pair separations, Applications of the technique. **Electrophoresis:** Separation by Adsorption-Affinity techniques, Affinity elution from Ion exchangers

polyacrylamide gel electrophoresis, Isoelectric focusing, Two-dimensional gel electrophoresis, capillary zone electrophoresis.

5. Electro analytical Methods of Analysis.

Polarography: Principle and instrumentation of polarography using dropping mercury electrode, DME (advantages and disadvantages of DME). Concept of residual, migration and diffusion current. Importance of half – wave potential, $E_{1/2}$. Ilkovic equation, qualitative and quantitative aspect of the technique. Principle and instrumentation using hanging dropping mercury electrode, HMDE. (advantages and disadvantages of HMDE). **Pulse polarography, differential pulse polarography, square wave polarography. Amperometric titrations:** Principle, instrumentation and application of amperometric titration (chrono-amperometry and chrono-potentiometry). **Coulometric Analysis:** Principles of coulometric analysis, applications of coulometric methods of analysis. Instrumentations, coulometric titrations, advantages and limitations.
Nanoscience: Synthesis of Nanomaterial by electrochemical deposition method, general applications of nanomaterial.

6. Role of Computers and Microprocessors in Analytical Chemistry:

Use of computer in data analysis. Computers and microprocessors: instrument – computer interfaces. The scope of microprocessor control to various laboratory instruments.

Books Recommended

1. Vogel's Textbook of Quantitative Chemical Analysis by J. Menham, R. C. Denney, J. D. Barnes and M. J. K. Thomas, 6th Edn, Low Price Edn, Pearson Education Ltd, New Delhi (**2000**).

2. Principles of Instrumental Analysis by D. A. Skoog, F. J. Holler and T. A. Nieman, 5th Edn, Thomson Brooks/Cole, Bangalore (**2004**).

3. Fundamentals of Analytical Chemistry by D. A. Skoog, D. M West, F. J. Holler and S. L. Crouch, 8th Edn, Thomson Brooks/Cole, Bangalore (**2004**).

4. Analytical Chemistry by G. D. Christian, 6th Edn, John Wiley & Sons Inc, Singapore (**2003**).

5. Principles and Practice of Analytical Chemistry by F. W. Fifield and D. Kealey, 5th Edn, Blackwell Science Ltd, New Delhi (**2004**).

6. Handbook of Instrumental Techniques for Analytical Chemistry, Editor, F. Settle, Low Price Edn, Pearson Education Inc, New Delhi (**2004**).

7. Instrumental Methods of Chemical Analysis by G.W. Ewing, 5th Edn, Mc-Graw Hill Singapore (**1985**).

8. Instrumental Methods of Analysis by H. H. Willard, l. L. Merritt, J. A. Dean & F. A. Seattle CBS Publishers & Distributors, New Delhi (**1986**).

SEMESTER - II
Materials Chemistry

Course code - SCS CH 1 1 02 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

Nano Materials Composites and organic solids

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. Composite materials: Introduction, types of fillers and matrix, classification of composite materials based on distribution and nature of fillers. Particulate and fibrous metal/non-metal composites, polymer nanocomposites and their applications. Organic solids, electron transfer conductors (conducting polymers) electron transfer salt based one and two dimensional organic conductors. Fullerenes and their applications

Glasses, ceramics and composites

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories characterizations, properties and applications.

Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, nanocrystalline phase, preparation procedures, special properties, applications. Band structures of insulators and semiconductors. Intrinsic semiconductors, hole formation in intrinsic semiconductors. Extrinsic semiconductors, p&n-type semiconductors. Concept of donar and acceptor lebvel, Fermi energy levels of carriers in intrinsic donar and extrinsic semiconductors.

Thin films and Langmuir-Blodgett films

Preparation, techniques, Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Liquid crystals

Mesmorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals, dielectric susceptibility and dielectric constants, lyotropic phases and their description of ordering in liquid crystals.

Semiconductors and High Tc materials

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization od 1-2-3 and 2-1-4 materails, normal state properties; anisotropy;

temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications.

Corrosion: Introduction, cost of corrosion, units and conversion rate expression. Modern theory of corrosion, electro-chemical reactions, free energy, cell potential, EMF series. Corrosion kinectics (Electrode Kinetics) exchange current density, activation and concentration polarization, mixed potential theory. Potentiostat Techniques for corrosion rate measurements: Tafel extrapolation and linear polarizations

Books suggested

1. Material science and engineering, an introduction, Callister, Wiley
2. Principles of the solid states, Keer, Wiley Eastern.
3. Thermotropic liquid crystals, Ed, Gray, John Wiley
4. Material science, Anderson, Leaver, Alexander and Rawlings, ELBS
5. Corrosion Science and engineering. Mars and Fontana.
6. Chemistry of Advanced Materials by Leonard V. Interrante, Mark J. Hampden–Smith. Wiley-VCH.

SEMESTER – II

Biosciences for Chemists

Course code - SCS CH 1 1 03 DCEC 4004
60 Hrs. (4Hrs /week) **Credits: 4**

Cell Structure and Functions

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of prokaryotic and eukaryotic cells, plant and animal cells. Overview of metabolism–catabolism and anabolism. ATP–the biological energy currency. Photosynthetic pigments, light & dark reactions, Biological N-fixation.

Carbohydrates

Types of carbohydrates**,** Conformation of monosaccharides, structure and functions of glycosides, deoxy sugars and myoinositol, *N*-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides–cellulose and chitin. Storage polysaccharides–starch and glycogen. Glycoproteins and glycolipids. Carbohydrate metabolism - Aerobic and anaerobic respiration, Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway, Cori cycle.

Lipids

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes and their functions. Fluid mosaic model of membrane structure. Lipid metabolism, β-oxidation of fatty acids.

Proteins and Nucleic acid

Introduction, amino acids, peptide linkage: Levels of organization in proteins-Primary, secondary, tertiary and quaternary structures, binding forces involved. Biological functions of proteins. Enzymes and their mechanism of action.

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Nucleotides and Nucleosides, Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it.

Books Suggested

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W. H. F. Freeman.

3. Biochemistry, J. David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.

SEMESTER - III

Inorganic Chemistry- Specialization paper-I

Core Course SCS CH 1 3 10A C 4004
60 Hrs (4 Hrs /week) **Credits: 4**

Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Transition Metal π-Complexes

Transition metal π-complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, cyclopentadienyl (nature of bonding of ferrocene, MO description and aromatic character), arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^2-olefins, η^3-allyl and dienyl complexes.

Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

Transition metal compounds with bonds to hydrogen.

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, R. H. Crabtree, John Wiley.
3. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New Age International.
4. Organometallics, A. Salzer, Ch. Elschenbrioch. VCH Publications.

SEMESTER - III

Organic Chemistry-Specialization paper-I

Heterocyclic and Natural Products Chemistry

Core Course SCS CH 1 3 10B C 4004
60 Hrs (4 Hrs /week) **Credits: 4**

Heterocyclic Chemistry

Aromatic Heterocycles

General chemical behaviour of aromatic Heterocycles, classification (structural type), criteria of aromaticity (bond length, ring current and chemical shifts in ^{1}H NMR spectra, empirical resonance energy, delocalization energy and Dewar resonance energy.

Non-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. Stereoelectronic effect-anomeric and related effects. Attractive interactions–hydrogen bonding and intermolecular nucleophilic – electrophilic interactions.

Heterocyclic synthesis (three, four and benzofused five membered)

Three-membered and four-membered Heterocycles–synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes. Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes.

Six-membered Heterocycles with one, two or more heteroatoms

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.

Natural Products Chemistry

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.

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.

Steroids

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

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

Physical Chemistry- Specialization paper-I

Core Course SCS CH 1 3 10 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Kinetics of polymerization
Introduction, kinetics to step growth polymerization, free radical addition polymerization, ionic polymerization, copolymerization; random walk and emergent properties, 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.

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.

Substitution reactions
Substitution reactions, classification of ligand substitution mechanism, inner and outer sphere electron transfer reactions and mechanism, adjacent and remote attack linkage isomerism, Marcus-Cross relation in outer sphere reactions and its applications, bridged outer-sphere electron transfer mechanism.

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

SEMESTER - III

Inorganic Chemistry- Specialization paper-II
Bio-inorganic Chemistry

Elective Course SCS CH 1 3 11A C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Metal ions in Biological Systems and Na^+/K^+ Pump

Essential and trace metals. Role of metals ions in biological processes.

Bioenergetics and ATP Cycle

DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.

Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes– cytochromes and ion-sulphur proteins, synthetic models.

Mettaloenzymes

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}

Metal storage Transport and Biomineralization

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.

SEMESTER - III

Organic Chemistry- Specialization paper-II

Core Course SCS CH 1 3 11B C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Reagents in Organic Synthesis

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details. Lithium diisopropylamide (LDA), Dicyclohexylcarbodimide (DCC), 1,3-Dithiane (reactivity umpoloung), trimethylisilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ, phase transfer catalysts (crown ethers and quaternary ammonium salts), Oxidation with Ruthenium tetraoxide, iodobenzene diacetate and thallium nitrate.

Rearrangements

A detailed study of the following rearrangements Demyanov, Favorskii, Arndt-Eistert synthesis, Neber, Baeyer-Villiger, Shapiro reaction, Hoffmann-Loffer-Fretag reaction, Chichibabin reaction.

Disconnection Approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X disconnections and two-group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

Protecting Groups

Principles of protection of alcohol, amine, carbonyl and carboxyl groups.

One Group C-C Disconnections

Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two Group C-C Disconnections

Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1.5-difunctionalised compounds. Michael addition and Robinson annelation.

Books Suggested

1. Modern Synthetic Reactions, H. O. House, W. A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Foundation Books.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.

4. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F. A. Carey and R. J. Sandburg, Plenum Press.
6. Designing Organic Synthesis, S. Warren, Wiley.
7. Organic Synthesis-concept, Methods and Starting Materials, Fhrhop and Penzillin, Verlage VCH.
8. New Horizons in Organic Synthesis, Nair V., New Age International.
9. Reagents in Organic Synthesis, Fieser and Fieser, Wiley.

SEMESTER - III

Physical Chemistry- Specialization paper-II

Core Course SCS CH 1 3 11C C 4004
60 Hrs (4Hrs /week) **Credits: 4**

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.

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, The Eley-Rideal Mechanism; Catalytic activity at surfaces- molecular beam reactive scattering studies.

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

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 1 3 09 C 4004
60 Hrs (4Hrs /week) **Credits: 4**

Ultraviolet and Visible Spectroscopy

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.

Infrared Spectroscopy

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.

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.

Mass Spectrometry

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).

Combined problems

Combined problems relating to structure elucidation by UV, IR, NMR Spectroscopy and Mass Spectrometry.

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

SEMESTER – III
Medicinal Chemistry

Elective Course code - SCS CH 1 1 06 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

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: occupancy theory, rate theory, induced fit theory. 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.

Antineoplastic Agents

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer.

Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil and 6-mercapto purine, Recent development in cancer chemotherapy.

Antibiotics

Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis, Synthesis of penicillin G, amoxycillin, cephalosporin, ciprofloxacin. Introductory idea of tetracycline and streptomycin.

Cardiovascular Drugs

Introduction and general mode of action. Synthesis of ditiazem, verapamil, methyldopa and atenolol.

Local Antiinfective Drugs

Introduction and general mode of action. Synthesis of furazolidone, naldixic acid, dapsone, isoniazid, ethambutol, gluconazole, chloroquin and primaquin.

Psychoactive Drugs – The Chemotherapy of Mind

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, G. L. Patrick, Oxford University Press.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F Dorge.
3. An Introduction to Drug Design, S. S. Pandeya and J. R. Dmmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1, Ed. M E Wolff, John Wiley.
5. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.

SEMESTER – III
Organic Chemistry of Polymers

Elective Course code - SCS CH 1 1 06 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

Introduction to polymer structures, Different classes of polymers, Synthesis of polymers by radical, emulsion, suspension, and ionic mechanisms, Copolymers, Functionalization of polymers, Crosslinking of polymers, Stereochemistry of polymers, Natural Polymers, Biodegradable Polymers

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**).

SEMESTER – III
Advanced Computational Chemistry

Elective Course code - SCS CH 1305 DCEC 4004
60 Hrs (4Hrs /week) **Credits: 4**

This course will introduce theoretical concepts of Molecular Dynamics and Quantum Mechanics. Experiments based on the theory will be part of the course. Students interested in computational chemistry will benefit from the course.

Section #1- Fundamentals of Molecular Dynamics (MD) simulations (8 hrs)
Topics: Introduction to Computer Simulation –Visual Representation of Molecular Systems, Lennard-Jones potentials -- Potentials and Force-Fields, Phase Space, Periodic Boundary Conditions, Minimum Image convention. Propagation of Newton's Equation, Time Step and Energy Minimization

Section #2- Applications to Macroscopic properties (2 hrs)
Topics: Treatment of Statistical Mechanical Ensembles – Averages – Fluctuations – Time Correlation Function – Radial Distribution Function, Mean Square Displacement - Diffusion coefficient

Section #3- Molecular Dynamics simulations – Hands on exercise Simulations of water (2 hrs instructions + 12 hrs lab)
Topics: Introduction and Use of GROMACS MD Program, Visualization using Visual Molecular Dynamics (VMD)

Section #4- Introduction to Quantum Computational Chemistry (8 hrs)
Topics: Scope of Computational Chemistry, Restricted and Unrestricted Hartree-Fock, Density Functional Theory: Exchange-Correlation Functional, Local Density Approximation, Generalized Gradient Approximation, Hybrid Density Functional Methods and Basis Sets: Slater and Gaussian Type Orbitals, Polarization and Diffuse Functions, Split-valence Sets, Core-valence Sets

Section #5 Basic concepts of potential energy surfaces (2 hrs)
Topics: Stationary Points, Geometry Optimization, Local and Global Minima, and Transition State Theory (TST)

Section #6- Hands on exercise (2 hrs instructions + 12 hrs lab)
Topics: Computations of Single Point Energy, Optimizations and Transition States of Polyatomic Molecules, Intrinsic Reaction Coordinate Analysis

Evaluation /assessment (evaluation components with weightage)

1. End - Sem examination: 40 %
2. Sessional I (Section 1-3) examination: 15 %
3. Sessional II (Section 4-6) examination: 15 % Assignment + Labs etc - 30 %

Suggested reading

1. Computer Simulations of Liquids, M. P. Allen and D. J. Tildesley.
2. Molecular Modeling: Principles and Applications, Andrew R. Leach, Addison Wesley Publishing Company (March **1997**).
3. Introduction to Computational Chemistry, Frank Jensen, John Wiley & Sons, **2007**
4. Electronic Structure: Basic Theory & Practical Methods, by Richard M. Martin, Cambridge University Press
5. A Practical Guide for Applying Techniques to Real-World Problems by David C. Young, Cytoclonal Pharmaceutics Inc. **2001**
6. Introduction to the Theory and Applications of Molecular and Quantum Mechanics, by Errol Lewars, Kluwer Academic Publishers, New York, Boston, Dordrecht, London, Moscow, **2004**

SEMESTER – IV
Project Work

Core Course SCS CH 1 1 01 DCEC 002424
450 Hrs (30 Hrs /week) **Credits: 24**

The topic for the project work is to be decided by the supervisor/guide concerned. The project report is to be submitted within six month of the date of start of fourth semester. 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.