

CENTRAL UNIVERSITY OF HARYANA
SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF CHEMISTRY

M.Sc. (Chemistry, 2018-20)

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 0084	Practical Organic Chemistry	0	0	4	8	4	
5.	SCS CH 1105 DCEC 4004	Physical Organic Chemistry	4	0	0	4	4	
5.	Elective (GEC)	<i>To be taken from other department</i>	4	0	0	4	4	
Total Credits = 24								

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 0084	Practical Inorganic Chemistry	0	0	4	8	4	
5	SCS CH 1205 DCEC 2002	Green and Sustainable Chemistry	2	0	0	2	2	
6.	SCS CH 1206 DCEC 2002	Seminar Paper (compulsory)	2	0	0	2	2	
7	Elective (GEC)	<i>To be taken from other department</i>	4	0	0	4	4	
Total Credits = 24								

SEMESTER-III

Sl. No	Course code	Course title	L	T	P	Hrs/week	Total Credits	
1.	SCS CH 1301 C 4004	Spectroscopy and Photoinorganic Chemistry	4	0	0	4	4	
2.	SCS CH 1302 C 4004	Reactions, Reagents and Synthesis	4	0	0	4	4	
3.	SCS CH 1303 C 4004	Chemical Bonding and Catalysis	4	0	0	4	4	
4.	SCS CH 1304 C 0084	Practical Physical Chemistry	0	0	4	8	4	
5.	SCS CH 1305 DCEC 4004	Organic Spectroscopy	4	0	0	4	4	
6.	Elective (GEC)	<i>To be taken from other department</i>	4	0	0	4	4	
Total Credits = 24								

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 C 4004	Medicinal & Pharmaceutical Chemistry	4	0	0	4	4

3.	SCS CH 1404 C 4004	Organometallic Chemistry	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
<i>Offered in Semester I</i>							
1.	SCS CH 1110 GE 4004	Chemistry of Materials	4	0	0	4	4
<i>Offered in Semester II</i>							
1.	SCS CH 1210 GE 4004	Environmental Chemistry	4	0	0	4	4
<i>Offered in Semester III</i>							
1.	SCS CH 1310 GE 4004	General Polymer Chemistry	4	0	0	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	04	00	04	24
II	16	04	00	04	24
III	16	08	00	00	24
IV	08/00	16/24	00	00	24
Total	56/48	32/40	00	08	96

SEMESTER I

SEMESTER - I

Inorganic Chemistry-I

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

Credits: 4

UNIT-I: Symmetry, Structure and Bonding in Inorganic Compounds

Symmetry elements and symmetry operations, symmetry groups with examples from inorganic compounds, groups of very high symmetry, molecular dissymmetry and optical activity. 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. Brief introduction of coordination polymers-1D, 2D, 3D and interpenetration.

UNIT-II: Chemistry of Non Transition Elements

Structures and acidic behaviour of boron halides, types and nomenclature boron hydrides (boranes), Wade's polyhedral skeleton electron pair theory (PSEPT). W. N. Lipscomb's STYX rules and semi-topological structures of boranes. Preparation, and properties of boron hydrides, carboranes, metalloboranes and metallocarboranes. Preparation, structure and properties of borazines, phosphazenes, sulphur-nitrogen compounds, silicates, pseudohalides and noble gas compounds.

UNIT-III: Reaction Mechanism of Transition Metal Complexes

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.

Reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, mechanism and kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reaction in square planar complexes, trans effect, redox reactions, mechanism of inner-outer sphere type reactions, cross reactions and Marcus-Hush theory.

UNIT-IV: Bioinorganic Chemistry

a) 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 processes. Na^+/K^+ Pump.

b) 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.

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, 6th ed. John Wiley, 2006.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.
3. N. N. Greenwood and E. A. Earnshaw; Chemistry of elements, 2nd ed. Butterworth-Heinemann, 1997.
4. Magnetochemistry, R.L. Carlin, Springer Verlag. Heidelberg, New York, Tokyo, 1986.
5. Magnetochemistry, A. Earnshaw. 1st ed. Academic Press, 1968.
6. Inorganic chemistry, G. Wulfsburg. University Science Books, 2000.
7. Introduction to ligand fields, B.N. Figgis, 2nd ed. Wiley Eastern, 1966.
8. Principles of Bioinorganic Chemistry. S. J. Lippard, J. M. Berg. University Science Books, 1994.
9. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books, 1994.

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, 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; fullerenes. Fundamentals of Supramolecular Chemistry, 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 principles, 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: Aliphatic Nucleophilic Substitution and Elimination Reactions

a) 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_Ni 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, ambidentnucleophile, regioselectivity.

b) 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 IV: Aromatic Substitution 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, Vilsmeier reaction, Gattermann-Koch reaction.

b) Aromatic Nucleophilic Substitution:

The S_NAr , diazonium salts and benzyne mechanisms. Reactivity–effect of substrate structure, leaving group and attacking nucleophile. The *von Richter*, *Sommelet-Hauser* and *Smiles* rearrangements.

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. Greeves 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 Bhattacharjee, 7th 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: Introduction to Physical Chemistry and Classical Thermodynamics

Logarithmic relations, Curve sketching and linear graphs, calculation of slopes, terms of mean and median, Precision and accuracy in chemical analysis, types of error, standard deviation, Numerical Problems.

Classical Thermodynamics Laws, state and path functions and their applications. Thermodynamic description of several 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: Solutions & Colligative Properties

Methods of Expressing the Concentration of a Solution, Activity & Activity Coefficient, Raoult's Law, Ideal and Non-Ideal Solution, Vapour pressure of Ideal Solution, Deviation from Ideal Behaviour, Thermodynamic properties of ideal solution and Azeotropes. Colligative properties of dilute solutions, Lowering of Vapour Pressure, Elevation in Boiling Point, Depression in Freezing Point & Osmotic Pressure.

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: 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 & Tafel plot.

Books Suggested

1. Atkins' Physical Chemistry, Peter Atkins and Julio Paula, Oxford University Press; 10th ed. (2014)
2. Physical Chemistry- A molecular approach, Donald Mcquarie and John Simon, Viva, 1st ed. (2010).
3. Physical Chemistry, Ira N Levine, Tata Mcgraw-Hill Education; 6th ed. (2011).
4. Chemical Kinetics, Keith J. Laidler, Pearson Education, 3rd ed. (1997)
5. Modern Electrochemistry Vol-I and Vol-IIA/B, J. O. M. Bockris and A. K. N. Reddy, Plenum.

SEMESTER - I
Practical Organic Chemistry

Core Course SCS CH 1104 C 0084
120 Hrs (8 Hrs /week)

Credits: 4

UNIT-I: Qualitative Analysis

- Qualitative analysis of common organic compounds having (aromatic rings, unsaturation, alcohols, phenols, carboxylic acids, carbonyl compounds, nitro, amine, amide and sugars)

UNIT-II: Separation and Purification Techniques

- Recrystallisation, vacuum distillation and sublimation.
- Thin Layer Chromatography: Separation of a mixture of organic compounds by TLC. Measurement of R_f values.
- Column chromatography, separation of coloured and colourless mixtures.

UNIT-III: Solvent Extraction Technique

- Separation of an organic mixture containing two solid components using solvent extraction
- Extraction of caffeine from tea leaves

UNIT-IV: Organic Synthesis and Characterization Techniques

- Preparation of an organic compound involving one step.
- Preparation of an organic compound involving two steps.
- Characterization of compounds with the help of chemical analysis and confirmation of their structures with the help of IR/NMR/UV-Vis spectral data (Measure and interpret IR and UV spectra, NMR spectra to be provided to the students).

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 - I
Physical Organic Chemistry

Elective Course SCS CH 1105 DCEC 4004
60 Hrs (4Hrs /week)

Credits: 4

UNIT-I: Reactive Intermediates

Introduction to structure, formation, stability and reactions of carbocations, carbanions, free radicals, radical anions, radical cations, arynes, carbenes and nitrenes. Photochemically excited species.

UNIT-II: Chemical Equilibria and Chemical Reactivity

Thermodynamic and kinetic control of reactions, Correlation of reactivity with structure, linear free energy relationships, Hammond's postulate, Curtin-Hammett principle, substituent constants and reaction constants.

UNIT-III: Chemical Kinetics and Isotope Effects

Various types of catalysis and isotope effects, importance in the elucidation of organic reaction mechanisms, Intermolecular forces and its impact on reactivity.

UNIT-IV: Stereoelectronic Effects in Organic Chemistry

Role of stereoelectronic effects in the reactivity of acetals, esters, amides and related functional groups, Anomeric effect, Reactions at sp^3 , sp^2 , and sp carbons, Cram, Felkin-Ahn, Zimmermann-Traxler, Houk, Cieplek, Allylic strain ($A^{1,2}$ and $A^{1,3}$) and other strains.

Books suggested

1. N. S. Isaacs., Physical Organic Chemistry, 2nd ed. (1995) Longman Scientific & Technical.
2. P. Deslongchamps., Stereoelectronic Effects in Organic Chemistry, (1983) Pergamon.
3. F. A. Carey and R. J. Sundberg., Advanced Organic Chemistry, Part A 5th ed. (2012) Springer.
4. E. V. Anslyn and D. A. Dougherty., Modern Physical Organic Chemistry, (2005) University Science Books.
5. J. March, Advanced Organic Chemistry, Reactions, Mechanisms and Structure, 4th ed. (1999) John-wiley.
6. P. Sykes, A guide book to Mechanism in Organic Chemistry, 5th ed. (1985) Longman Scientific Technical.
7. Warren, S.; Greeves, N.; J. Clayden and P. Wothers, Organic Chemistry, 2nd ed. (2001) Oxford University Press.

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

Introduction, crystalline and amorphous solids, Unit cell, Bravais lattices, structure of NaCl and KCl, point defects – Frenkel, Schottky defects and non-stoichiometric defects.

Conductors, variation of conductivity with temperature, semiconductors, p and n types, photo voltaic cell. Piezoelectric and pyro-electrics. Photoluminescence.

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: 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.

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.

UNIT-III: Radioactivity and Nuclear Chemistry

Nuclear binding energy, nuclear emissions, nuclear transformations, kinetics of radioactive decay, bombardment of nuclei, nuclear fission, nuclear fusion, kinetic isotope effects, radiocarbon dating, chemical separation, Szilard–Chalmer’s effect, effects of radiation on life, radioactivity in medicines.

UNIT-IV: Photo Physical Phenomena

Interaction of electromagnetic radiation with matter, Grotthus-Draper law, Stark-Einstein law of photochemical equivalence, Frank-Condon principle, quantum yield, electronically excited singlet states, life time of electronically excited state, construction of Jablonski diagram, electronic transitions and intensity of absorption bands, types of photophysical

pathways, radiationless transitions, fluorescence emission, phosphorescence emission, Fluorescence quenching, chemiluminescence.

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, An Introduction, 9th ed. (2014) Callister, Wiley.
3. L. V. Azaroff, Introduction to Solids, (1977) Tata McGraw-Hill, New Delhi.
4. H. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1988.
5. K. K. Rohatgi and K. K. Mukherjee; Fundamentals of Photochemistry, 3rd ed. (2014) New Age International (P) Ltd.
6. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed. (2006) Springer, New York.

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 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, mechanism of exchange interaction, reduced magnetization, magnetic anisotropy, magnetic hysteresis, Single Molecule Magnets (SMMs) and mononuclear SMMs or Single Ion Magnets (SIMs).

UNIT-II: Transition Elements, Lanthanides and Actinides-General Aspects

Elements of first transition series and their comparison with the second and third series, general periodic trends, chemistry of the various oxidation states of first row transition metals and their comparison based on electronic configuration. The splitting of f -orbitals in octahedral field, Lanthanide contraction, Lanthanide shift reagent, oxidation states complexes, magnetic and optical properties of lanthanides and actinides.

UNIT-III: Supramolecular chemistry

Origin of supramolecular chemistry - "Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry. Nature and types of supramolecular interactions (Hydrogen bonding, van der Waal 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-IV: Bioinorganic Chemistry**a) Electron Transfer, Transport and Storage of Dioxygen:**

Structure and function of metalloproteins in electron transport processes- cytochromes and iron-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.

b) 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 B₁₂, Ferritin, transferrine and siderophores.

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. J. W. Steed and J. L. Atwood; Supramolecular Chemistry, John Wiley, 2nd Ed., 2009.
6. J. M. Lehn; Supramolecular Chemistry, VCH, Wienheim, 1995.
7. J. P. Sauvage; Transition metals in supramolecular chemistry: John Wiley & sons: UK, 1st Ed., 1999.
8. Principles of Bioinorganic Chemistry. S. J. Lippard, J. M. Berg. University Science Books, 1994.
9. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentne, University Science Books, 1994.

SEMESTER - II

Organic Chemistry-II

Core Course SCS CH 1202 C 4004

60 Hrs. (4Hrs /week)

Credits: 4

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

a) Addition to Carbon-Carbon Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Woodward and Prevost dihydroxylations, 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/nitriles. Wittig reaction. Mechanism of condensation reactions involving enolates; Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Modern Aldol reactions. Hydrolysis of esters, amides and nitriles.

UNIT-II: Common Heterocycles

a) Introduction:

Nomenclature, General chemical behaviour of aromatic heterocycles, criteria of aromaticity (bond length, ring current and chemical shifts in ^1H NMR spectra). 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 and pyramidal inversion.

b) Synthesis and reactivity:

Three, four, five and six membered heterocycles (aziridine, oxirane, thiirane, azetidine, oxetane, thietane, furan, thiophene, pyrrole, imidazole and pyridine)..

UNIT-III: Free Radical Reactions and Photochemistry

a) Free radicals:

Generation of free radicals, structure and stability, persistent radicals, common initiators and uses, types of free radical reactions, radical scavengers, Role of oxygen, Radical dimerisation-Pinacol, McMurry and acyloin reactions, Chain Reactions- Allylic halogenation (NBS), reduction of alkyl halides, auto-oxidation of aldehydes, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical cyclizations, Hunsdiecker reaction.

b) Organic Photochemistry:

Fundamentals of photochemistry, photochemical reactions of alkenes (2+2 cycloaddition, Paterno-Buchi reaction, di-pi-methane rearrangement) aromatic compounds (cycloadditions), carbonyl compounds and other systems (Norrish types I and II, oxa-di-pi methane rearrangement), 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, allyl and pentadienyl systems. Classification of pericyclic reactions. FMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, $4n$, $4n + 2$, allyl and pentadienyl systems, Nazarov cyclization. Cycloadditions–antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, 2+2 addition of ketenes, Detailed treatment of Diels-Alder reactions, 1,3-dipolar cycloadditions. Sigmatropic rearrangements–suprafacial and antarafacial shifts of H and alkyl groups, 3,3- 5,5 and 2,3-sigmatropic rearrangements. Variants of Claisen, Cope and aza-Cope rearrangements. Ene reaction. Chelotropic reactions.

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. Greeves and S. Warren, Oxford University Press, 2012.
4. Organic Chemistry, Morrison, Boyd and Bhattacharjee, 8th 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: 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-II: 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. Heat capacity, Fermi-Dirac statistics, distribution law and Bose-Einstein statistics - distribution law and applications.

UNIT-III: Molecular Spectroscopy- Rotational Spectroscopy

The Born-Oppenheimer Principle, Rotational Spectroscopy-Rigid Rotator, Selection rule for rotational/microwave spectrum, determination of bond-length, intensity of spectral lines, effects of isotopes on rotational spectra, Non-rigid rotator, Stark effect, Nuclear spin interactions, application of microwave spectroscopy.

UNIT-IV: Molecular Spectroscopy- Vibrational Spectroscopy

Infrared/Vibrational Spectroscopy- Vibration in Diatomic molecules, Harmonic Oscillator Model, Zero-point Energy, Selection Rule, An-harmonic Oscillator, Population of Vibrational Energy level, Diatomic Vibrating Rotator, P-Q-R Branches of Spectra, Breakdown of Born-openheimer approximation, Fundamental Vibration and Symmetry, Overtone and combination frequency.

Books Suggested:

1. Atkins' Physical Chemistry, Peter Atkins and Julio Paula, Oxford University Press; 10th Ed. (2014)
2. Statistical Mechanics, RK Pathria & Paul D Beal, Elsevier III Ed. (2016)
3. An Introduction to Statistical Thermodynamics, Terrell L. Hill, Dover Publication, (2008)

4. Physical Chemistry- A molecular approach, Donald Mcquarie and John Simon, Viva, 1st Ed. (2010)
5. Physical Chemistry, Ira N Levine, Tata Mcgraw-Hill Education; 6 Ed. (2011)
6. Fundamentals of Molecular & Spectroscopy, C N Banwell, Tata McGraw-Hill Education IV Ed. (2013)
7. Rita Kakkar, Atomic and Molecule Spectroscopy: Basic Concepts and Applications, Cambridge University Press, 2015.
8. Molecular Spectroscopy, J L McHale, Pearson Education India (2008)

SEMESTER - II

Practical Inorganic Chemistry

Core Course SCS CH 1204 C 0084
120 Hrs (8 Hrs /week)

Credits: 4

UNIT-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 nephelometer.

UNIT-II: Preparations and related complementary work and physical studies (Any Six)

1. Reinecke Salt
2. $\text{VO}(\text{acac})_2$
3. $\text{Mn}(\text{acac})_3$
4. Prussian Blue/Turnbull's Blue
5. $\text{Hg}[\text{Co}(\text{NCS})_4]$
6. Potassium trioxalatoferate (III) Trihydrate
7. Dichlorobis (hydroxylamine) Zinc(II)
8. Pentathioureadicuprous nitrate
9. Potassium trioxaltochromate (III)
10. Cis, trans-dichloro bis(ethylenediamine) cobalt(III)chloride.

UNIT-III: Quantitative Estimation

Quantitative estimation (involving volumetric-redox and complexometry, gravimetric) of constituents in two and three component mixtures.

UNIT-IV: Spectroscopic Studies

Data plotting, analysis and characterization of coordination compounds using Infrared and UV-Visible Spectroscopy.

Books Suggested:

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, 5th ed. ELBS, 1989.

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2. Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, revised, G. Svehla, 5th ed. Longman, 1979.
3. Practical Inorganic Chemistry, Marr and Rocket, Van Nostrand Reinhold, 1972.

SEMESTER - II
Green and Sustainable Chemistry

Elective Course SCS CH 1205 DCEC 2002
30 Hrs (2Hrs /week)

Credits: 2

UNIT-I: Principles and concepts of Green chemistry

Chemistry in the context of sustainable development, Current status and future perspective. The twelve principles of Green Chemistry.

UNIT-II: Catalysis and Renewable raw materials

Introduction to catalysis. Homogeneous and Heterogeneous catalysis, Phase-transfer catalysis and Biocatalysis. Chemical products based on renewable sources.

UNIT-III: Alternative solvents

Volatile organic compounds (VOCs) Supercritical fluids. Alternatives in extraction and chromatography. Ionic liquids as solvents: its types, properties and applications.

UNIT-IV: Green technology and sources of alternative energy

Photochemical and Electrochemical reactions. Reactions under Microwave, sonication and ball milling. Flow techniques.

Books suggested

1. S. E. Manahan, Fundamentals of Environmental Chemistry, 3rd ed. (2009) CRC Press.
2. R. A. Sheldon, I. Arends and U. Hanefeld, Green Chemistry and Catalysis, 1st ed. (2007) Wiley-VCH.
3. V. K. Ahluwalia and M. Kidwai, New Trends in Green Chemistry, 1st ed. (2004) Springer.
4. T. Clifford, Fundamentals of Supercritical Fluids, 1st ed. (1999) Oxford press.
5. C. -J. Li, T. -K. Chan, Organic Reactions in Aqueous Media, 1st ed. (1997) Wiley-Interscience, Newyork.
6. Recent review articles relevant to above topics (reprints to be handed over to students).

SEMESTER - II
Seminar

Elective Course SCS CH 1206 DCEC 2002
30 Hrs (2Hrs /week)

Credits: 2

Each student must present at least two seminars (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.

Elective Course offered by the department to students of other departments

SEMESTER - II

Environmental Chemistry

Elective Course 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 and acid rain. Ozone depletion and its consequences. Technologies to alleviate Global warming.

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: Sustainable Energy

Nature of energy, Sources of energy used in the anthrosphere, Energy devices and conversions, Energy conservation and renewable energy sources, Nuclear energy, Solar energy, Energy from moving air and water, Biomass energy and Hydrogen as a means to store and utilize energy.

UNIT-IV: Chemical analytical methods

Nature and importance of chemical analysis, Chemical analysis process, Major categories of chemical analysis, Error and treatment of data, Spectrophotometric methods, Electrochemical method of analysis, Chromatography, Mass spectrometry, Automated analysis and Immunoassay screening.

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

Spectroscopy and Photoinorganic Chemistry

Core Course SCS CH 1301 C 4004

60 Hrs. (4Hrs /week)

Credits: 4

UNIT-I: Infrared and Raman Spectroscopy:

Molecular vibrations, force constants, molecular vibrations and absorption of Infrared radiations. Raman spectroscopy, polarized Raman lines. Use of symmetry considerations to determine the number 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-II: Electron Spin Resonance Spectroscopy:

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.

UNIT-III: Mössbauer and Nuclear Quadrupole Resonance Spectroscopy:

Mössbauer Spectroscopy: Introduction to Mössbauer effect - Basic principles, recoilless emission & absorption of γ -rays. Mössbauer experiment - Instrumentation, scheme of Mössbauer spectrometer, Mössbauer spectrum. Isomer shift, quadrupole splitting and hyperfine interactions, application of Mössbauer effect to the investigations of compounds of iron and tin.

Nuclear Quadrupole Resonance Spectroscopy: Principle, nuclear quadrupole resonance experiment, structural information from NQR spectra, Interpretation of nuclear quadrupole coupling constants.

UNIT-IV: Photoinorganic chemistry

Interaction of electromagnetic radiation with matter, 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. electronic transition, Frank-Condon principle, selection rules, electronically excited singlet states, life time of electronically excited state, construction of Jablonski diagram, electronic transitions and intensity of absorption bands, photophysical pathways of excited molecular system (radiative and non-radiative), chemiluminescence, phosphorescence and fluorescence.

Books Suggested

1. K. Nakamoto; Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A and B, 6th ed. Wiley, 2008.
2. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4th ed. Tata McGraw Hill, 1994.
3. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.
4. K. K. Rohatgi and K. K. Mukherjee; Fundamentals of Photochemistry, 3rd ed. New Age International (P) Ltd., 2014.
5. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed. Springer, New York, 2006.
6. N. J. Turro, V. Ramamurthy and J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, 1st ed. University Science, Books, CA, 2010.
7. I. Ninomiya, T. Naito, Photochemical Synthesis, 1st ed. Academic Press, New York, 1989.

SEMESTER - III

Reactions, Reagents and Synthesis

Core Course SCS CH 1302 C 4004
60 Hrs (4 Hrs /week)

Credits: 4

UNIT I: Reagents and methods 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); Modern oxidation/reduction reagents and methods (Dissolving metal reductions, various hydrides, catalytic/transfer hydrogenations, diimide); (oxidations of alcohols, alkenes, aldehydes, and saturated carbon, hypervalent iodine reagents, DDQ) Modern dihydroxylation methods, Organic chemistry of boron, silicon and tin; Organocatalysis, Transition-metal mediated reactions, Olefin metathesis.

UNIT-II: Named Reactions and Rearrangements

Rearrangements: Wagner-Meerwein, Pinacol, Wolff, Beckmann, Baeyer-Villiger, Curtius, Lossen, Schmidt, Favorskii, Benzilic acid, Payne, Dienone-Phenol, Fries, Neber, Brook.
Fragmentations: Eschenmoser, Grob. Reactions: Fischer Indole synthesis, Pictet-Spengler reaction, Mitsunobu reaction, Passerini and Ugi reactions.

UNIT III: Synthetic planning and retrosynthesis

Retrosynthesis, synthons and synthetic equivalents, disconnection approach, functional group inter-conversions; 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 protecting groups (exemplified for hydroxyl, amino and carbonyl groups), Stork's total synthesis of quinine as a case study.

UNIT- IV: Chemistry of Natural Products

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, isoprene rule. Biosynthesis and chemical synthesis of the following representative molecules: α -Terpeneol, Farnesol and β -carotene.

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, introductory idea of testosterone and oestrone, biosynthesis of cholesterol and biomimetic synthesis of progesterone.

Alkaloids: Definition, nomenclature, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring. Stereochemistry, biosynthesis, synthesis of the following: nicotine and atropine.

Carbohydrates: Types of naturally occurring sugars, deoxysugars, aminosugars, polysaccharides of industrial and biological importance.

Lipids: Classification and biological importance of fatty acids and lipids

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-Inter 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, Bantrophe 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

Chemical Bonding and Catalysis

Core Course SCS CH 1303 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: 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-III: 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-IV: 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.

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
Practical Physical Chemistry

Core Course SCS CH 1304 C 0084

120 Hrs (8 Hrs./week)

Credits: 4

Experiments

1. Determine the Energy of Activation for a 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. Determination of the equivalent conductance of strong electrolytes such as HCl, KCl, KNO_3 , $AgNO_3$, and NaCl at different concentration and the validity of Onsager equation.
8. Study conductometric/ pH titration of (1) HCl / NaOH (2) CH_3COOH / NaOH and comment on nature of graph.
9. Study conductometric/ pH titration of (1) HCl / NH_4OH (2) CH_3COOH / NH_4OH and comment on nature of graph.
10. Determine the equivalent conductance, degree of dissociation and dissociation constant of acetic acid.
11. Determination of relative viscosities of acids/solvents and polymers.
12. To determine the strength of acids including polybasic acids by titrating against base pH meter and potentiometrically.

Books Suggested:

1. Experimental Physical Chemistry: A Laboratory Textbook, A. Halpern & G. McBane III Ed. W. H. Freeman (2006)
2. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.
3. Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, revised, G. Svehla, Longman.
4. Practical Chemistry, A. M. James and F. E. Prichard, 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.

SEMESTER - III

Organic Spectroscopy

Elective Course SCS CH 1305 DCEC 4004
60 Hrs (4Hrs /week)

Credits: 4

UNIT I: 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.

UNIT II: 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.

UNIT III: 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 ¹³C NMR spectra. General introduction to two-dimensional NMR spectroscopy-COSY, HETCOR, INADEQUATE and NOESY.

UNIT IV: 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 Spectroscopy, William Kemp, Mac publishers, 3rd Edition, 2011.
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. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4th ed. Tata McGraw Hill, 1994.
9. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.

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).
4. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press (new York, Woodhead Publishing Co., (Cambridge) (2005).

SEMESTER IV

SEMESTER – IV
Dissertation

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
Dissertation

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 C 4004

60 Hrs (4 Hrs /week)

Credits: 4

UNIT-I: Drug Targets

Introduction to medicinal chemistry intermolecular binding forces, Introduction to various drug targets; **Proteins**- primary, secondary and tertiary structure, protein function, proteomics; **Enzymes**- catalytic role, active site, allosteric binding, feedback control, binding interactions, isozymes, co-factors; **Receptors**- types of receptors, their roles, neurotransmitters, hormones, receptor activation and regulation, signal transduction; **Nucleic acids**- DNA, primary and secondary structure of DNA, function of DNA < molecular biology and genetic engineering.

UNIT-II: Drug-target binding

Introduction to Pharmacodynamics and pharmacokinetics, Enzymes as drug targets- types of enzyme inhibitors, medicinal use of enzyme inhibitors with examples; Receptors as drug targets- agonists, antagonists, allosteric modulators, partial agonists, inverse agonists, desensitization, tolerance and dependence, affinity and efficacy; Nucleic acids as drug targets- Intercalating agents, topoisomerase poisons, alkylating/metallating agents, chain cutters, chain terminators, examples of medicinal use. Miscellaneous drug targets-

UNIT-III: Drug discovery, design and development

Development of new drugs, concept of lead compounds and lead modifications, bioassays, in vitro, in vivo and in silico tests, HTS, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism. Theories of drug activity, Quantitative structure activity relationship, Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric factors, toxicity studies, clinical trials, regulatory process of getting drugs into markets.

UNIT-IV: Types of Medicinal Agents

Antibacterial agents-history, bacterial cell, classification of antibacterial agents, examples; Antiviral agents- introduction to viruses, life cycle, vaccination, classification of antiviral drugs; Anticancer agents- Introduction to cancer and cancer treatment, classification of anticancer drugs; Cardiovascular drugs, Psychoactive drugs, Synthesis of the following drugs- ciprofloxacin and cisplatin.

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 Organometallic Chemistry

Core Course SCS CH 1401 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 carbynes: synthesis, reactivity, structure and bonding considerations of Fischer and Schrock carbyne complexes.

UNIT-II: Transition Metal Fluxional and π -Cyclic complexes

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).

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,

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, asymmetric and supported organometallic catalysis.

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 polynuclear carbonyl 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 $[\text{Re}_2\text{Cl}_8]^{2-}$ ions), trinuclear and hexanuclear metal clusters.

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. 1987.
2. The Organometallic Chemistry of the Transition Metals, Crabtree, R. H. John Wiley. 6th ed. 2014.
3. Organometallic Chemistry, Mehrotra R.C. and Singh, A. New Age International. 1999.
4. Reaction Mechanism of Inorganic and Organometallic systems; Robert .B. Jordan. 3rd ed. Oxford University Press, 2007.
5. Inorganic Chemistry, 3rd edn,; Miessler ,G. L., Donald, A. T. 3rd ed. Pearson, 2004.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.