**CENTRAL UNIVERSITY OF HARYANA**
**SCHOOL OF CHEMICAL SCIENCES**
**DEPARTMENT OF CHEMISTRY**

# M.Sc. (Chemistry, 2017-19)

## 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 Inorganic Chemistry | 0 | 0 | 4 | 8 | 4 |
| 5. | SCS CH 1105 DCEC 4004 | Sustainable and Green Chemistry (compulsory) | 4 | 0 | 4 | 4 | 4 |
| 6. | Elective (GEC) | ***To be taken from other department*** | 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 Organic Chemistry | 0 | 0 | 4 | 8 | 4 |
| 5 | SCS CH 1205 DCEC 4004 | Organic Chemistry of Polymers | 4 | 0 | 0 | 4 | 4 |
| 6. | Elective (GEC) | ***To be taken from other department*** | 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 | Inorganic Chemistry-III | 4 | 0 | 0 | 4 | 4 |
| 2. | SCS CH 1302 C 4004 | Organic Chemistry-III | 4 | 0 | 0 | 4 | 4 |
| 3. | SCS CH 1303 C 4004 | Physical Chemistry-III | 4 | 0 | 0 | 4 | 4 |
| 4. | SCS CH 1304 C 0084 | Practical Physical Chemistry | 0 | 0 | 4 | 8 | 4 |
| 5. | SCS CH 1305 DCEC 2002 | Seminar Paper (compulsory) | 2 | 0 | 0 | 2 | 2 |
| 6. | GEC | **To be taken from other department** | 0 | 0 | 0 | 4 | 4 |
| 7. | | ***Any one of the following two courses*** | | | | | |
| | SCS CH 1306 DCEC 2002 | Medicinal Chemistry | 2 | 0 | 0 | 2 | 2 |
| | SCS CH 1307 DCEC 2002 | Advanced Computational Chemistry | 2 | 0 | 0 | 2 | 2 |
| **Total Credits = 24** | | | | | | | |

## SEMESTER-IV

| Sl. No | Course code | Course title | L | T | P | Hrs/ week | Total Credits |
|---|---|---|---|---|---|---|---|
| 1. | SCS CH 1401 C 4004 | Organometallic Chemistry | 4 | 0 | 0 | 4 | 4 |
| 2. | SCS CH 1402 C 4004 | Bioinorganic Chemistry | 4 | 0 | 0 | 4 | 4 |
| 3. | SCC CH 1403 C 4004 | Heterocycles and Natural Products | 4 | 0 | 0 | 4 | 4 |
| 4. | SCS CH 1404 C 4004 | Organic Synthesis | 4 | 0 | 0 | 4 | 4 |
| 5. | SCC CH 1405 C 4004 | Chemical Dynamics and Catalysis | 4 | 0 | 0 | 4 | 4 |
| 6. | SCS CH 1406 C 4004 | Micelles and Electrochemistry | 4 | 0 | 0 | 4 | 4 |
| 7 | SCS CH 1407 DCEC 002216* | Dissertation | 0 | 0 | 22 | 22 | 16 |
| **OR** | | | | | | | |
| 8. | SCS CH 1408 DCEC 003024* | Dissertation | 0 | 0 | 30 | 30 | 24 |
| **Total Credits = 24** | | | | | | | |

**Skill Enhancement Elective Course*

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

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

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

# SCHOOL OF CHEMICAL SCIENCES
# DEPARTMENT OF CHEMISTRY
# CENTRAL UNIVERSITY OF HARYANA

## M.Sc. Chemistry Programme

**Total credits = 96**

| SEMESTER | CREDITS | | | | Total |
|---|---|---|---|---|---|
| | CORE COURSE | ELECTIVE COURSE | | | |
| | | Chemistry department | | Other Departments (GEC) | |
| | | DCEC | GEC | | |
| I | 16 | 4 | 0 | 4 | 24 |
| II | 16 | 4 | 0 | 4 | 24 |
| III | 16 | 4 | 0 | 4 | 24 |
| IV | 08 | 16 | 0 | 0 | 24 |
| Total | **46** | **38** | **0** | **12** | **96** |

# SEMESTER I

## SEMESTER - I

# Inorganic Chemistry-I

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

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**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. 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 $\sigma$ and $\pi$ bonding. Brief introduction of coordination polymers-1D, 2D, 3D and interpenetration.

**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: 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, interhalogens, Chlorofluorocarbons, pseudohalides and noble gas compounds.

**Unit-IV: Metal Carbonyls and Clusters**

Molecular orbital of carbonyl, classification of metal carbonyls, bonding in metal carbonyl, valence electron count (EAN rules), preparation and properties of mononuclear and polynuclearcarbonyl complexes, bond lengths and stretching frequencies, carbonylate ions, carbonyl hydride complexes, isolobal fragments, structure and important reactions of

transition metal nitrosyl. Bonding, preparation and properties of dinuclear metal cluster (dirhenium complex $[Re_2Cl_8]^{2-}$ ions), trinuclear and hexanuclear metal clusters.

**Books Suggested**

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

# SEMESTER-I
## Organic Chemistry-I

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

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

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

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

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

**Books Suggested**

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

# SEMESTER - I
## Physical Chemistry-I

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

**Unit-I: 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; 6 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 Inorganic Chemistry

**Core Course SCS CH 1104 C 0084**
**120 Hrs (8 Hrs/week)** **Credits: 4**

## Inorganic Chemistry Experiments

### I Water Analysis (Any Two)

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

### II Preparations and related complementary work and physical studies (Any Six)

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

### III Quantitative Estimation

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

### 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, 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.

## SEMESTER - I
## Sustainable and Green Chemistry

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

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**Unit-I**

Definitions of Sustainability. Principles of Green Chemistry. Biorefinery concepts. Biomass based industrial products obtained and practiced technologies in different countries: biomass fractionation of wheat straw, rice straw and sugarcane bagasse. Biomass industrial products : cellulose, hemicellulose, lignins, pectins, starch, chitosan. Lignocellulose industrial products: extractives, biofuels, syn gases, carbon dioxide

**Unit-II**

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

**Unit-III**

Cellulose, hemicellulose, lignin, glucose, lactic acid, succinic acid based biorefinery. Biochars – preparation, properties, impact on global warming.. Role of catalysis development in biomass conversion. Global impact on economics and environment.. Concepts of carbon footprints, carbon trading, Life Cycle Analysis (LCA). Biodegradable polymers: definition, natural polymers cellulose, starch, lignin and chitosan, and their derivatives in the form of bioplastics, components of plastics, components of textile fibres. Semi-synthetic biodegradable polymers (natural molecules like sugars anchored chemically onto non-degradable synthetic hydrocarbon polymers, or synthetic molecules anchored onto natural polymers like cellulose via chemical grafting). Currentlyimportant synthetic polymers like Polyvinylalcohol and Polylactic acid.Biodegradability determination. BOD, COD.Biocomposites and bionanocomposites. Geotextiles.Life cycle analysis of Biodegradable Polymers.

**Unit-IV**

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

examples. Reactions in Supercritical fluids with special reference to supercritical carbon dioxide.

**Books Suggested:**

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

## Elective Course offered by the department to students of other departments

## SEMESTER - I
## Chemistry of Materials

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

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**UNIT I: Structures and properties of solids**

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

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

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

**UNIT III: Nano Materials and Composites**

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

**UNIT IV: Analytical Methods in Chemistry**

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

**Books suggested**

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

# SEMESTER II

## SEMESTER - II

# Inorganic Chemistry –II

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

**Unit-I**

**Electronic Spectra and Magnetic Properties of Transition Metal Complexes**

Spectroscopic ground states and the evaluation of energies of various J states of free ions, splitting of S, P, D and F terms under octahedral and tetrahedral electrostatic potential, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes ($d^1$-$d^9$ states), calculations of Dq, B and 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.

**Unit-II**

**Metal-Ligand Equilibria in Solution**

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

**Unit-III**

**Reaction Mechanism of Transition Metal Complexes**

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

**Unit-IV**

**Crystal engineering and supramolecular chemistry**

Introduction to crystal engineering-synthon principle. 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.

**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. G. R. Desiraju, J. J. Vittal, A. Ramanan; Crystal Engineering, A Textbook, World Scientific, 2011.
6. J. W. Steed and J. L. Atwood; Supramolecular Chemistry, John Wiley, 2nd Ed., 2009.
7. J. M. Lehn; Supramolecular Chemistry, VCH, Wienheim, 1995.
8. J. P. Sauvage; Transition metals in supramolecular chemistry: John Wiley & sons: UK, 1st Ed., 1999.

## SEMESTER - II
## Organic Chemistry-II

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

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**UNIT I: Aromatic Substitution and Elimination Reactions**

**a) Aromatic Electrophilic Substitution**

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

**b) Aromatic Nucleophilic Substitution**

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

**c) Elimination Reactions**

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

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

**a) Addition to Carbon-Carbon Multiple Bonds**

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

**b) Addition to Carbon-Hetero Multiple Bonds**

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

**UNIT III: Free Radical Reactions and Photochemistry**

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

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

**UNIT IV: Pericyclic Reactions**

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

**Books Suggested**

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

## SEMESTER - II

## Physical Chemistry-II

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

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**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, Overton 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 Organic Chemistry

**Core Course SCS CH 1204 C 0084**
**120 Hrs (8 Hrs /week)** **Credits: 4**

**UNIT -1: Qualitative Analysis**

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

**UNIT -2: 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 -3: Solvent Extraction Technique**

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

**UNIT-4 Organic Synthesis and Characterization Techniques**

- Preparation of an organic compounds 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 (IR, NMR spectra to be provided).

**Suggested Books**

1. Vogel's Textbook of Practical Organic Chemistry, Ed. 5, Longman, 1989.
2. Experiments and Techniques in Organic Chemistry, Pasto, Johnson and Miller, Prentice Hall, 1992.
3. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath, 7th Ed., 2011.
4. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
5. Handbook of Organic Analysis-Qualitative and Quantitative, H. Clark, Adward Arnold.

## SEMESTER – II
## Organic Chemistry of Polymers

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

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**Unit I**

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

**Unit 2**

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

**Unit 3**

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

**Unit 4**

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

**Books suggested:**

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

## Elective Course offered by the department to students of other departments

### SEMESTER - II

### Environmental Chemistry

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

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**Unit-I: General aspects of environment**

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

**Unit-II: Environmental pollution and toxicology**

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

**Unit-III: Green Chemistry and Industrial Ecology**

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

**Unit-IV: Climate change**

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

**Books suggested**

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

# SEMESTER III

## SEMESTER - III

## Inorganic Chemistry-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 noumber of lines in IR and Raman Spectra. Structural studies involving IR and Raman Spectroscopy of coordination compounds containing the following molecules/ions and ligands: $NH_3$, $H_2O$, OH, $SO_4^{2-}$, $ClO_4^-$, $COO^-$, $NO_2$, $CN^-$, $SCN^-$, NO, $O_2$, $PR_3$, Halides, DMSO, azopyridine, oxime, quinine, acetylacetone, amino acids. Hydrogen bonding and infrared spectra, metal ligand and related vibrations. Application of resonance Raman spectroscopy to structural elucidation of the active sites of heme and non-heme oxygen carriers.

**UNIT-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**

**Mössebauer and Nuclear Quadrupole Resonance Spectroscopy:**

Mössebauer Spectroscopy: Introduction to Mössebauer effect - Basic principles, recoilless emission & absorption of γ-rays. Mössebauer experiment - Instrumentation, scheme of Mössebauer spectrometer, Mössebauer spectrum. Isomer shift, quadrapole splitting and hyperfine interactions, application of Mössebauer 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**

**Photochemistry**

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

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

**Books Suggested**

1. 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
## Organic Chemistry-III (Spectroscopy)

**Core Course SCS CH 1302 C 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 $^{13}C$ 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 Chemistry, William Kemp, John Wiley.
6. Organic Spectroscopy, Jag Mohan, Narosa Publishers, New Delhi
7. Rita Kakkar, Atomic and Molecule Spectroscopy: Basic Concepts and Applications, Cambridge University Press, 2015.

## SEMESTER - III
## Physical Chemistry-III

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

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**Unit-I: Principles of Quantum Mechanics**

Introduction to Quantum Mechanical Approach, Quantum Mechanical operators, Eigen values of Quantum Mechanical operators, Hermitian operator, commutation relations, postulates of quantum mechanics and Uncertainty Principle.

Schrödinger equation for finding wave function of a particle, Energy of a particle in One-Dimension box, Extension to Schrödinger equation for finding wave function in a three-dimensional box, Energy of a particle in Three-Dimension box, Energy levels, Eigen value, degeneracy and selection rules.

**Unit-II: Approximation Methods: Quantum approach**

Harmonic oscillator: Application to diatomic molecules and Energy levels; Rigid rotator: Model for a rotating diatomic molecule and Energy level; The Hydrogen atom: Schrödinger equation for hydrogen atom and shapes of atomic orbitals.

Approximate Methods: The linear variation principle, Perturbation theory (first order and non-degenerate).

**Unit-III: Surface Chemistry**

The extent of adsorption: Physorption and Chemisorptions, Adsorption isotherms, Rates of surface processes (adsorption, desorption and mobility on surfaces). BET equation.

Heterogeneous catalysis: Mechanism of heterogeneous catalysis; Langmuir–Hinshelwood mechanism.

**Unit-IV: Principles of Symmetry and Group Theory**

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

**Books Suggested:**

1. Atkins' Physical Chemistry, Peter Atkins and Julio Paula, Oxford University Press; 10th Ed. (2014)
2. Quantum Chemistry, Ira N Levine, Pearson Education, 7th Ed. (2013)
3. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw-Hill (1998)
4. Quantum Chemistry, R. K. Prasad, New Age International (2001)
5. Statistical Mechanics, RK Pathria & Paul D Beal, Elsevier III Ed. (2016)

6. An Introduction to Statistical Thermodynamics, Terrell L. Hill, Dover Publication, (2008)
7. Chemical Applications of Group Theory, F. A. Cotton, John Willey & Sons, 3rd Ed. (2008)
8. Physical Chemistry- A molecular approach, Donald Mcquarie and John Simon, Viva, 1st Ed. (2010)

## SEMESTER - III
## Practical Physical Chemistry

**Core Course SCS CH 1304 C 0084**
**120 Hrs (8 Hrs./week)** **Credits: 4**

**Physical Chemistry 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. 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.

## SEMESTER - III

## Seminar

**Core Course SCS CH 1305 C DCEC 0022**
**30 Hrs (2 Hrs./week)** **Credits: 2**

Each student must present at least one seminar (45 minutes) which will be followed by discussion session (15 minutes) with participation from other students and the concerned faculty members present. The student must also submit the slides/write-up of the presentation content to the faculty-in-charge. The seminar, participation in discussions, the submitted slides and overall attendance (as per ordinance) will form the basis of the evaluation. There will be no separate final exam for this course.

## SEMESTER – III
## Medicinal Chemistry

**Elective Course code - SCS CH 1306 DCEC 2002**
**30 Hrs (2Hrs /week)** **Credits: 2**

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

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

**UNIT III: Antibiotics and Cardiovascular Drugs**

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

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

**Books Suggested**

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

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

## SEMESTER – III
## Advanced Computational Chemistry

**Elective Course code - SCS CH 1307 DCEC 2002**
**30 Hrs (2Hrs /week)** **Credits: 2**

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

**UNIT I- Fundamentals of Molecular Dynamics (MD) simulations**
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

**UNIT II- Applications to Macroscopic properties**
**A) Topics:** Treatment of Statistical Mechanical Ensembles – Averages – Fluctuations – Time Correlation Function – Radial Distribution Function, Mean Square Displacement - Diffusion coefficient
**B) Molecular Dynamics simulations – Hands on exercise Simulations of water**
Topics: Introduction and Use of GROMACS MD Program, Visualization using Visual Molecular Dynamics (VMD)

**UNIT III- Introduction to Quantum Computational Chemistry**
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

**UNIT IV :**
**A) Basic concepts of potential energy surfaces**
Topics: Stationary Points, Geometry Optimization, Local and Global Minima, and Transition State Theory (TST)
**B) 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.

**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**
7. Essentials of Computational Chemistry: Theories and Models, 2nd Edition, Christopher J. Cramer, John Wiley & Sons Ltd, **2002**.
8. Essentials of Computational Chemistry: Theories and Models, 2nd Edition, Christopher J. Cramer, John Wiley & Sons Ltd, **2004**.
9. Exploring Chemistry with Electronic Structure Methods, 2nd Edition, James B. Foresman and Aeleen Frisch, Gaussian Inc.

## 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**

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**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
## Organometallic Chemistry

**Core Course SCS CH 1401 C 4004**
**60 Hrs (4 Hrs /week)** **Credits: 4**

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**Unit-I**

**Alkyls, Aryls, Carbenes and Carbynes of Transition Metals**

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

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

**Unit-II**

**Transition Metal π-Cyclic Complexes**

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

**Unit-III**

**Fluxional Organometallic Compounds and Coupling Reactions**

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

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

**Unit-IV**

**Catalytic Processes involving Transition Metal Organometallic Compounds:**

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

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

**Books Suggested**

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

## SEMESTER - IV

# Bioinorganic Chemistry

**Elective Course SCS CH 1402 C 4004**
**60 Hrs (4 Hrs/week)** **Credits: 4**

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**UNIT I:**

**Metal ions in Biological Systems and Bioenergetics**

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

**UNIT II:**

**Nitrogenase and Photosynthesis**

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

**UNIT III:**

**Electron Transfer, Transport and Storage of Dioxygen**

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

**UNIT IV**

**Mettaloenzymes, Metal storage Transport and Biomineralization**

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

**Books Suggested:**

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

## SEMESTER - IV
## Heterocycles and Natural Products

**Core Course SCS CH 1403 C 4004**
**60 Hrs (4Hrs /week)** **Credits: 4**

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**UNIT I: Aromatic and Non-aromatic Heterocycles**

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

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

**UNIT II: Heterocyclic synthesis and reactions**

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

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

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

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

**UNIT IV: Natural Products Chemistry (Alkaloids)**

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

**Books Suggested**

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

## SEMESTER - IV
## Organic Synthesis

**Core Course SCS CH 1404 C 4004**
**60 Hrs (4Hrs /week)** **Credits: 4**

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### 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); Common reducing agents (Dissolving metal reductions, various hydrides, catalytic/transfer hydrogenations, diimide); Common oxidising agents, oxidations of alcohols, alkenes, aldehydes, and saturated carbons; Woodward and Prevost dihydroxylations, hypervalent iodine reagents, DDQ; Organic chemistry of boron, silicon and tin; Organocatalysis

### UNIT II: Rearrangement Reactions

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

### UNIT III: Synthetic planning and retrosynthesis

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

### UNIT IV: Protecting groups and total synthesis

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

### Books Suggested

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

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

Organic Chemistry, Morrison, Boyd and Bhattcharjee, &th Edition, Pearson, 2010

## SEMESTER - IV

## Chemical Dynamics and Catalysis

**Core Course SCS CH 1405 C 4004**
**60 Hrs (4Hrs./week)** **Credits: 4**

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

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

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

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

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

## SEMESTER - IV

## Micelles and Electrochemistry

**Core Course SCS CH 1406 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: Micelles**
Micelles: Surface active agents, classification, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, phase separation, micro emulsion and reverse micelles.

**Unit-III: 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.

**Unit-IV: Advance Electroanalytical Methods**
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 – IV
## Project Work

**Core Course SCS CH 1407 DCEC 002216**
**330 Hrs (30 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
## Project Work

**Core Course SCS CH 1408 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.

## Elective Course offered by the department to students of other departments

## SEMESTER – IV

## Basics of Medicinal Chemistry

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

**UNIT I: Fundamentals**

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

**UNIT II: Drug Action**

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

**UNIT III: Drug Design and Synthesis**

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

**UNIT IV: Drugs and Society**

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

**Books Suggested**

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

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