CENTRAL UNIVERSITY OF HARYANA
SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF CHEMISTRY

Ph.D. (Chemistry, 2018 admission)

Structure and curriculum for course work for PhD degree

Sl. No.	Course code	Course type	Course title	Credits
1	SCS CH 3101 C 6006	Core	Research Methodology, Quantitative methods and Computer Applications for Chemistry	6
Any one of the following				
2	SCS CH 3102 E 6006	Elective	Solid State and Supramolecular Chemistry	6
3	SCS CH 3 103 E 6006	Elective	Advanced Computational Chemistry	6
4	SCS CH 3 104 E 6006	Elective	Advanced Organic Synthesis	6
5	SCS CH 3 105 E 6006	Elective	Medicinal Chemistry	6
6	SCS CH 3 106 E 6006	Elective	Spectroscopic Techniques for Chemists	6

Core Course

Course Code SCS CH 3101 C 6006

Research Methodology, Quantitative methods and Computer Applications for Chemistry

6 hrs per week **Total Credits: 6**

A. RESEARCH METHODOLOGY

UNIT I

Research problems: Meaning, Motivation" Objectives and types of research. Significance of research, Research proposals and aspects, Criteria of good research, Research formulation and hypotheses. Selection and necessity of defining the problem, Literature review, Primary and secondary sources- Reviews, Treatise, Mono graphs, Patents

UNIT II

Research Design: Need. Problem Definition, Variables, Research design concepts, Research design process, Research Modeling: Types of models, Model building and stages, Data collection, processing and analysis, Simulation techniques using computer software(s).

UNIT III

Design and planning of Experiments: Aims and objectives, expected outcome, methodology to be adopted, importance of reproducibility of research work, Interpolation, Extrapolation, Types of errors (rounding. truncation, machine and random), Error analysis and least square curve fitting Analysis of Variance components (ANOVA) for fixed effect model, Objectives and basic principles of designs of experiments. Complete randomized design (CRD), Randomized block design (RBD) and Latin square design (LSD)

UNIT IV

Data mining and Report Writing: Library resources, Internet, Scientific search engines, Introduction to Latex/Google docs, Structure and component of research paper, Presenting the research paper/thesis, Journal impact factor, Citation index, References and bibliography, Copyright. Plagiarism and ethics in research, Communication and presentation

UNIT V

Research design and methods as applied to Chemical Sciences: Experiment design-monitoring- laboratory safety- Laboratory notebook keeping- data collection-coding of samples and experiments- storage of samples- Use of Chemistry Software like ChemDraw and MNova.

Teaching Assistance: Tutorials

Suggested Readings:

1. Kothari. C. R and Garg Gaurav (2014). Research Methodology: Methods and Techniques, 3rd Edition, New Age International Publishers, New Delhi.
2. Pannerselvan, R. (2009). Research Methodology, Prentice Hall of lndia, New Delhi.
3. Singh. Y. K. (2008). Fundamental of research Methodology and Statistics, New Age International Publishers" New Delhi.
4. Montgomery, D.C. (2013). Design and Analysis of Experiments, 8th Edition. Wiley India.
5. Prathapan. K, Research Methodology for Scientific Research. IK International, New Delhi.
6. Leedy, P.D. and Ormrod, J.E., Practical Research: Planning and Design, Prentice Hall, 2004

Elective Course

Course Code - SCS CH 3102 E 6006

Solid State and Supramolecular Chemistry

6 hrs per week **Total Credits: 6**

Symmetry and Structure in Solid State:

UNIT I

Crystal symmetry – (i) point group elements and (ii) space group elements; 32 crystal classes, HM notations, distribution in different systems and stereographic projections.

Space group – HM notation, space groups in triclinic and monoclinic systems.

Indexing of lattice planes; Miller indeces.

UNIT II

X-ray, Cu Kα and Mo Kα radiation; X-ray diffraction; Bragg equation; Reciprocal lattice and its relation to direct lattice; Bragg reflection in terms of reciprocal lattice – sphere of reflection and limiting sphere; relation between d_{hkl} and lattice parameters.

Supramolecular Chemistry:

UNIT III

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.)

UNIT IV

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. C. Giacavazzo; Fundamentals of crystallography, 3rd Ed., 2011.
2. J. D. Dunitz; X-ray analysis and the structure of organic molecules, 2nd Ed., 1995.
3. G.H. Stout and L.H. Jensen; X-ray structure determination: A practical guide, 2nd Ed., 1989.
4. J. W. Steed and J. L. Atwood;SupramolecularChemistry, John Wiley, 2nd Ed., 2009.
5. J. M. Lehn;Supramolecular Chemistry, VCH, Wienheim, 1995.
6. J. P. Sauvage; Transition metals in supramolecular chemistry: John Wiley & sons: UK, 1st Ed., 1999.

Elective Course

Course Code - SCS CH 3103 E 6006

Advanced Computational Chemistry

6 hrs per week **Total Credits: 6**

UNIT-I: Introduction to Computational Chemistry

Computational chemistry map, Scope of Computational Chemistry, Born-Oppenheimer approximation, Restricted and Unrestricted Hartree-Fock.

Density Functional Theory: Exchange-Correlation Functional, Local Density Approximation, Generalized Gradient Approximation, Hybrid Density Functional Methods.

UNIT-II: Basis Sets

Definition, Slater and Gaussian Type Orbitals, Minimal, Double-zeta, Split-valence, Core-valence, Pople style basis sets, Polarization and Diffuse Functions, Calculation of Basis Functions for with suitable examples, Pseudopotentials or Effective Core Potentials.

UNIT-III: Basic concepts of potential energy surfaces

Stationary Points, Geometry Optimization, Local and Global Minima, and Transition State Theory (TST).

UNIT-IV: Hands on exercise

Computations of Single Point Energy, Formation Energy, Optimizations and Transition States of Polyatomic Molecules, Intrinsic Reaction Coordinate Analysis, Natural Bond Order, Electron Decomposition Analysis.

Books Suggested

1. Introduction to Computational Chemistry, Frank Jensen, John Wiley & Sons, **2007**
2. Essentials of Computational Chemistry: Theories and Models, 2nd Edition, Christopher J. Cramer, John Wiley & Sons Ltd, **2002**.
3. Essentials of Computational Chemistry: Theories and Models, 2nd Edition, Christopher J. Cramer, John Wiley & Sons Ltd, **2004**.
4. Exploring Chemistry with Electronic Structure Methods, 2nd Edition, James B. Foresman and Aeleen Frisch, Gaussian Inc.

Elective Course

Course Code - SCS CH 3104 E 6006

Advanced Organic Synthesis

6 hrs per week **Total Credits: 6**

UNIT I: Transition metal catalysis in synthesis

Overview of modern catalytic methods in organic synthesis, transition metal catalysis, details of homogeneous catalysis by palladium, copper, silver, gold, rhodium and ruthenium complexes. Olefin and alkyne metathesis reactions.

UNIT II: Organocatalysis and biocatalysis

Asymmetric catalysis. Organocatalysis. Iminium and enamine catalysis. N-heterocyclic carbenes (NHC). Enzyme catalysis and biocatalysis. Light mediated reactions..

UNIT III: Modern Organic Reactions

Modern methods of carbonyl olefinations. Boron, Tin and Silicon based reagents. Modern oxidation reactions. Hypervalent iodine reagents. Sharpless asymmetric epoxidation and dihydroxylation reactions. New methods of reduction. Super hydride. Selectrides. Catalytic asymmetric hydrogenations and hydrogen transfer reductions. CH- and C-C activations.

UNIT IV: Total Synthesis

Strategies and tactics in total synthesis. Classical examples. Woodward synthesis of Strychnine. Stork synthesis of reserpine. Corey synthesis of longifolene. Overman synthesis of morphine. Vollhardt synthesis of estrone. Baran synthesis of vinigrol.

Suggested Reading

1. Advanced Organic Chemistry; Parts A and B; by Carey and Sundberg, Springer 2007.
2. Organic Chemistry, By Jonathan Clayden, Nick Geeves, Stuart Warren, OUP.
3. The logic of Chemical Synthesis, By E. J. Corey and X.-M. Cheng, Wiley
4. Classics in Total Synthesis, by K. C. Nicolaou, E. J. Sorensen, Wiley
5. Principles of Organic Synthesis 3rd Ed., R. O. C. Norman and J. M. Coxon, CRC Press
6. Organic Synthesis, by M. B. Smith, Academic Press.

Elective Course

Course Code: SCS CH 3 105 E 6006

Medicinal Chemistry

6 hrs per week **Total Credits: 6**

UNIT I: Drug Design

Introduction, Development of new drugs, Concept of lead compounds and lead modifications, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship, Concepts of drugs receptor, Elementary treatment of drug receptor interactions, Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric factors.

UNIT II: Anticancer Agents

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Synthesis of 6-mercapto purine, melphalan, mechlorethamine, cyclophosphamide and uracil, Recent development in cancer chemotherapy.

UNIT III: Anti-infective Drugs

Introduction and general mode of action of antibiotic and antibacterial-, antiviral-, antifungal- and antiprotozoan drugs. Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, amoxycillin, cephalosporin, ciprofloxacin, furazolidone, dapsone, gluconazole, chloroquine, primaquin, Introductory idea of tetracycline and streptomycin.

UNIT IV: Cardiovascular Drugs

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

Books Suggested

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

Elective Course

Course Code: SCS CH 3 106 E 6006

Spectroscopic Techniques for Chemists

6 hrs per week **Total Credits: 6**

UNIT I: UV-Visible, IR and Mass Spectroscopic techniques for Organic Compounds

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

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

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

UNIT II: Nuclear Magnetic Resonance Spectroscopy

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

UNIT III: Infrared and Raman Spectroscopy of inorganic compounds

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

and infrared spectra, metal ligand and related vibrations. Application of resonance Raman spectroscopy to structural elucidation of the active sites of heme and non-heme oxygen carriers.

UNIT-IV: Electron Spin Resonance Spectroscopy of inorganic compounds

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

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

Books Suggested

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