

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

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**Ph.D. (Chemistry, 2017 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
<b>Any one of the following</b>				
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	Sustainable and Green Chemistry	6
6	SCS CH 3 106 E 6006	Elective	Medicinal Chemistry	6
7	SCS CH 3 107 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**

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**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 India, 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**

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**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 indices.

**UNIT II**

X-ray, Cu K $\alpha$  and Mo K $\alpha$  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,  $\pi$ -stacking, C-H... $\pi$  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, 3<sup>rd</sup> Ed., 2011.
2. J. D. Dunitz; X-ray analysis and the structure of organic molecules, 2<sup>nd</sup> Ed., 1995.
3. G.H. Stout and L.H. Jensen; X-ray structure determination: A practical guide, 2<sup>nd</sup> Ed., 1989.
4. J. W. Steed and J. L. Atwood; Supramolecular Chemistry, John Wiley, 2<sup>nd</sup> Ed., 2009.
5. J. M. Lehn; Supramolecular Chemistry, VCH, Weinheim, 1995.
6. J. P. Sauvage; Transition metals in supramolecular chemistry: John Wiley & sons: UK, 1<sup>st</sup> Ed., 1999.

**Elective Course**

Course Code - SCS CH 3103 E 6006

*Advance Computational Chemistry***6 hrs per week****Total Credits: 6**

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**Unit-I: Fundamentals of Molecular Dynamics simulations**

Introduction to Computer Simulation –Visual Representation of Molecular Systems, Lennard Jones potentials -- Potentials and Force-Fields, Molecular Mechanics, Periodic Boundary Conditions, Minimum Image convention. Propagation of Newton's Equation using Verlet, Velocity Verlet and Leap-Frog Algorithm.

**Unit-II: Hands on exercise Simulations of water**

Averages – Fluctuations – Time Correlation Function – Radial Distribution Function, Mean Square Displacement - Diffusion coefficient; Introduction and Use of GROMACS Molecular Dynamics Program. Visualization using Visual Molecular Dynamics (VMD).

**Unit-III: Introduction to Quantum Computational Chemistry**

Topics: Hartree-Fock Theory, 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 functions, Contractions, Polarization and Diffuse Functions, Split-valence Sets, Core-valence Sets

**Unit-IV: Basic concepts of potential energy surfaces**

Stationary Points, Geometry Optimization, Local and Global Minima, and Transition State Theory. Hands on exercise: Computations of single point energy, optimizations and transition states of polyatomic molecules, intrinsic reaction coordinates.

**Books Suggested**

1. Computer Simulations of Liquids, M. P. Allen and D. J. Tildesley.
2. Molecular Modelling: 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 Pharmaceuticals 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.

**Elective Course**

Course Code - SCS CH 3104 E 6006

*Advanced Organic Synthesis***6 hrs per week****Total Credits: 6**

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**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 Greeves, 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 3<sup>rd</sup> 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 3105 E 6006

*Sustainable and Green Chemistry*

**6 hrs per week**

**Total Credits: 6**

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Biomass based chemistry and technology, Biorefinery concepts and examples, Cellulose chemistry, Hemicellulose chemistry, Lignin chemistry, Waste to value concepts, Concepts of C footprints, water footprints, smart cities, Green chemistry, Biocatalyzed reactions, Microwave reactions, Photocatalyzed reactions, Ultrasound reactions, Phase transfer catalyzed reactions, Reactions in solid state, Ionic liquids, Supercritical fluids, Biodegradable polymers Life cycle analysis, Cradle-to-cradle analysis of chemicals and polymers, Waste management concepts.

### Books Suggested:

1. Green Chemistry – A Textbook, V.K. Ahluwalia, Narosa (New Delhi) (2013)
2. Biomass for Renewable Energy, Fuels, and Chemicals, Donald L. Klass, Elsevier (2006)
3. Cellulose science and Technology, 1<sup>st</sup> Ed., J. L. Wertz, J. P. Mercier, O. Beque, EPFL Press
4. Experiments in Green and Sustainable Chemistry, H. Rosky, D. Kenepml, J. M. Lehn, Wiley-VCH (2009)
5. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press(New York), Woodhead Publishing Ltd. (Cambridge, England) (2005)



**Elective Course**

Course Code: SCS CH 3 106 E 6006

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

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**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,  $\beta$ -lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, amoxycillin, cephalosporin, ciprofloxacin, furazolidone, dapson, gluconazole, chloroquine, primaquin, Introductory idea of tetracycline and streptomycin.

**UNIT IV: Cardiovascular Drugs**

Introduction and general mode of action. Synthesis of diltiazem, 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 3 107 E 6006

### *Spectroscopic Techniques for Chemists*

6 hrs per week

Total Credits: 6

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#### **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, hindered 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, heteroaromatic and carbonyl carbon), coupling constants and DEPT <sup>13</sup>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 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<sub>3</sub>, H<sub>2</sub>O, OH, SO<sub>4</sub><sup>2-</sup>, ClO<sub>4</sub><sup>-</sup>, COO<sup>-</sup>, NO<sub>2</sub>, CN<sup>-</sup>, SCN<sup>-</sup>, NO, O<sub>2</sub>, PR<sub>3</sub>, 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, 6<sup>th</sup> ed. Wiley, 2008.
9. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> ed. Tata McGraw Hill, 1994.
10. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5<sup>th</sup> ed. Cengage India, 2015.