**CENTRAL UNIVERSITY OF HARYANA**

**SCHOOL OF CHEMICAL SCIENCES**

**DEPARTMENT OF CHEMISTRY**

**Ph.D. (Chemistry, 2019 admission)**

**Structure and curriculum for course work for Ph.D. degree**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sl. No.** | **Course code** | **Course type** | **Course title** | **Credits** |
| 1 | SCS CH 3101 C 5016 | Core | Research Methodology and Computer Applications for Chemistry | 6 |
| **Any one of the following** |
| 2 | SCS CH 3102 E 5016 | Elective | Solid State and Supramolecular Chemistry | 6 |
| 3 | SCS CH 3 103 E 5016 | Elective | Advanced Computational Chemistry | 6 |
| 4 | SCS CH 3 104 E 5016 | Elective | Advanced Organic Synthesis | 6 |
| 5 | SCS CH 3 105 E 5016 | Elective | Medicinal Chemistry | 6 |
| 6 | SCS CH 3 106 E 5016 | Elective | Spectroscopic Techniques for Chemists | 6 |
| 7 | SCS CH 3 107 E 5016 | Elective | Chemistry of toxicity and detoxification  | 6 |
| **Total Credits** | **12** |

**Core Course**

Course Code SCS CH 3101 C 5016

*Research Methodology and Computer Applications for Chemistry*

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

1. **RESEARCH METHODOLOGY**

**Chapter I: Methods and types of Research**

Research methods vs Methodology. Types of research – Descriptive vs. Analytical, Applied vs. Fundamental, Quantitative vs. Qualitative, Conceptual vs. Empirical. Research proposals- design and components.

**Chapter II: Literature review**

Defining and formulating the research problem - Selecting the problem - Necessity of defining the problem - Importance of literature review in defining a problem – Literature review – Primary and secondary sources – reviews, treatise, monographs-patents – web as a source – searching the web - Critical literature review – Identifying gap areas from literature review - Development of working hypothesis.

**Chapter-III - 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- Hypothesis-testing - Generalization and Interpretation.

**Chapter IV: Reporting, documentation and presentation**

Structure of research reports- technical reports and thesis-publication writing-presentation of raw and processed data-Bibliography- Plagiarism - Citation and acknowledgement Oral presentations-visual aids

**Seminar and Teaching Assistance**

**References**

1. Garg, B. L., Karadia, R., Agarwal, F. and Agarwal, U.K. An introduction to Research Methodology, RBSA Publishers, 2002.
2. Kothari, C.R., Research Methodology: Methods and Techniques. New Age International. p 418, 1990.
3. Trochim, W.M.K. Research Methods: the concise knowledge base, Atomic Dog Publishing. P. 270, 2005.

**Additional reading**

1. Anthony, M., Graziano, A.M. and Raulin, M.L. Research Methods: A Process of Inquiry, Allyn and Bacon. 2009
2. Coley, S.M. and Scheinberg, C. A., "Proposal Writing", Sage Publications. 1990
3. Day, R.A. How to Write and Publish a Scientific Paper, Cambridge University Press. 1992.
4. Fink, A. Conducting Research Literature Reviews: From the Internet to Paper. Sage Publications, 2009.
5. Leedy, P.D. and Ormrod, J.E., Practical Research: Planning and Design, Prentice Hall, 2004.

**Elective Course**

Course Code - SCS CH 3102 E 5016

*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 5016

*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 5016

*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 5016

*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 5016

*Spectroscopic Techniques for Chemists*

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

### UNIT I: Ultraviolet and Visible Spectroscopy and Mass Spectrometry

**UV-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.

**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).

**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, theory of NMR, chemical shift, shielding and deshielding mechanism, magnetic anisotropy, 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), spin-spin interaction, Spin systems, Pople notation, complex spin-spin interaction between two, three and four nuclei (first order spectra), virtual coupling. chemical exchange, effect of deuteration, 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), COSY.

**UNIT IV: Carbon-13 NMR Spectroscopy and combined applications**

**Carbon-13 NMR Spectroscopy:** General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroarmatic and carbonyl carbon), coupling constants and DEPT 13C NMR spectra. General introduction to two-dimensional NMR spectroscopy- HETCOR and NOESY. Resonance of other nuclei-F, P. **Combined problems:** Combined problems relating to structure elucidation by UV, IR, NMR Spectroscopy and Mass Spectrometry.

**Books Suggested**

1. Spectrometric Identification of Organic Compounds, Silverstein, Bassler and TMorrill, John Wiley.
2. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
3. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
4. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
5. Organic Spectroscopy, William Kemp, 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. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4th ed. Tata McGraw Hill, 1994.
9. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.

**CENTRAL UNIVERSITY OF HARYANA**

**** [Established under the Central Universities Act 2009]

www.cuh.ac.in

 **Course Code: SCS CH 3 107 E 5016**

**Course Name: Chemistry of Toxicity and Detoxification**

**Credit Equivalent**: 6 credits

**Course Objectives:** The course is designed to:

* 1. introduce students to the fundamental concepts of toxic and hazardous substances ;
	2. Inter-disciplinary research approach development .

 **Attendance Requirement:**

Students are expected to attend all lectures in order to be able to fully benefit from the course. A minimum of 75 per cent attendance is a must failing which a student may not be permitted to appear in examination**.**

 ( Depending upon the nature of the course , a teacher shall specify the breakup of each criterion into different components like written examination , assignment , case study , quiz , presentation , class participation , panel discussion , group discussion, problem solving exercise s, practical , etc.)

**Unit 1**

**Toxic Properties of Chemical Substances including ignitable,** **corrosive, reactive, incompatible under the following heading:**

Pathway of entry;

detoxication

bioactivation.

Degradation

Addition or conjugation reactions

**Unit 2**

**Physical properties of toxic and hazardous waste**

Chemical pollutant, its oxidation, hydrolysis, biodegradation, groundwater contamination, and overall persistence in the environment related to the following studies:

Vapour pressure,

Vapour density

 Solubility.

**Unit 3**

**Toxic and hazardous characteristic various organic chemicals**

Acids,

Aldehydes,

Amines,

Dioxins,

Ethers,

Cyanides.

**Unit 4**

**Cancer-Causing Chemicals**

Concept of carcinogenesis

Mechanism of chemical carcinogens

Human carcinogens

**Unit 5**

**Common Toxic, and Flammable Gases including**:

Hydrogen

Carbon mono and dioxide

Nitrogen Oxide

**Unit 6**

Biochemical aspects of

 Arsenic,

Cadmium,

Lead,

Mercury,

 Carbon monoxide

**Unit 7**

**Hazardous Properties of Some**

Insecticides

Asbestos,

Flyash,

Ozone and PAN pesticides,

Chemical and Biological agents including warfare Agents

**Unit 8**

Management techniques for toxic and hazardous waste. Model assignments and practical validation

**Unit 9**

Drug toxicity: Mechanism to reduce a drug toxicity; Drug-Chemical; Drug-Drug , Drug –Microbe/enzyme interaction

**Prescribed Text Books:**

1. Patnaik P., A Comprehensive Guide to the Hazardous Properties of Chemical Substances ( III Ed.) John Wiley & Sons, Inc., Hoboken, New Jersey
2. Moffatt H K and Shuckburgh, Environmental Hazards, Imperial College Press.( ISBN 978-981-4313-28-5)

**Suggested Additional Readings:**

1. Batty LC and Hallberg K B, Ecology of Industrial Pollution , Cambridge University press, New Delhi.
2. Oloman C, Material and Energy Balance for Engineers and Environmentalist, Imperial College Press.( ISBN 978-1-84816-368-3).
3. Yen T F, Chemical Processes for Environmental Engineering, Imperial College Press.( ISBN 978-1-86094-759-9).
4. Madu C N, Environmental Planning and management, Imperial College Press.( ISBN 978-1-86094-671-4).
5. Healtth Hazards of Environmental Arsenic Poisoning, Imperial College Press.( ISBN 978-981-4291-81-1).