UNIVERSITY OF DELHI

Syllabus for Semester III and IV for Two-Year Master of Science (M.Sc.) in Chemistry

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Syllabus for Semester I and II for One-Year Master of Science (M.Sc.) in Chemistry

(Effective from Academic Year 2026-27)

Structure-1 DISCIPLINE SPECIFIC CORE COURSES (DSC) FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Course Code**	**Credits**
III	Inorganic Reaction mechanism, Organic photochemistry and Molecular spectroscopy	**CH-DSC-301**	**L=3** **P=1**
	Electron Transfer, Molecular Rearrangements, Pericyclic reactions and Electronic spectroscopy	**CH-DSC-302**	**L=3** **P=1**
IV	Frontiers in Bioinorganic(I), Medicinal Chemistry (I), Irreversible Thermodynamics and Transport Phenomena	**CH-DSC-401**	**L=3** **P=1**
	Frontiers in Bioinorganic(II), Medicinal Chemistry (II),Fast Chemical Processes	**CH-DSC-402**	**L=3** **P=1**

POOL OF DISCIPLINE SPECIFIC ELECTIVES COURSES (DSE) FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	**DSE Pool I**		
	Spectral Techniques in Inorganic Chemistry	**CH-DSE-301**	**L=3** **P=1**
	Chemistry of Nanomaterials	**CH-DSE-302**	**L=3** **P=1**
	Advanced Chemistry of Main Group elements	**CH-DSE-303**	**L=3** **P=1**

	Chemistry of transition metal clusters	CH-DSE-304	L=3 T=1
	Single crystal X-ray diffraction	CH-DSE-306	L=3 P=1
	DSE Pool O		
	Advanced Organic Synthesis and Reagents	CH-DSE-307	L=3 P=1
	Carbocyclic and Heterocyclic Compounds	CH-DSE-308	L=3 P=1
	Chemistry of Biomolecules	CH-DSE-309	L=3 P=1
	Drug Delivery and Pharmaceutical Technologies	CH-DSE-310	L=3 P=1
	DSE Pool P		
	Advanced Polymer Science: Structure, Kinetics and Smart Materials	CH-DSE-311	L=3 P=1
	Advanced Electrochemistry	CH-DSE-312	L=3 P=1
	Advanced Statistical Mechanics	CH-DSE-313	L=3 P=1
	Radiation and Photochemistry with Applications	CH-DSE-314	L=3 P=1
	Physical Chemistry of Materials	CH-DSE-315	L=3 P=1

	Structure, Dynamics and Spectroscopy of Biomolecules	**CH-DSE-316**	**L=3** **P=1**
	DSE Pool Common		
	Research Methodology for Chemists (Only for Structure 1 & 2)	**CH-DSE-305**	**L=3** **P=1**
IV	**DSE Pool I**		
	Organotransition Metal Chemistry and Catalysis	**CH-DSE-401**	**L=3** **P=1**
	Chemistry of Inorganic Materials	**CH-DSE-402**	**L=3** **P=1**
	Advanced Analytical Techniques	**CH-DSE-403**	**L=3** **P=1**
	Nuclear and Radiochemistry	**CH-DSE-404**	**L=3** **T=1**
	Electrochemistry of Energy Storage Systems	**CH-DSE-405**	**L=3** **P=1**
	DSE Pool O		
	Chemistry of Life Processes	**CH-DSE-406**	**L=3** **P=1**
	Chemistry of Supramolecules, Terpenes and Steroids	**CH-DSE-407**	**L=3** **P=1**
	Alkaloids, Polyphenols, and Active Pharmaceutical Ingredients	**CH-DSE-408**	**L=3** **P=1**

	Polymer Chemistry and Role of Catalysis in Chemical Synthesis	CH-DSE-409	L=3 P=1
	DSE Pool P		
	Advanced Quantum Chemistry	CH-DSE-410	L=3 P=1
	Advanced Fluorescence Methods for Chemical and Biomedical Research	CH-DSE-411	L=3 P=1
	Advanced Chemical Kinetics	CH-DSE-412	L=3 P=1
	Advanced Molecular Spectra	CH-DSE-413	L=3 P=1
	Computational Methods in Chemistry	CH-DSE-414	L=3 P=1
	Solid State Chemistry	CH-DSE-415	L=3 P=1
POOL OF SKILL BASED COURSES (SBC) FOR SEMESTERS-III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	Instrumental Analysis-I	CH-SBC-301	L=0 P=2
	Electrochemical Techniques	CH-SBC-302	L=0 P=2
	Qualitative analysis of organic compounds	CH-SBC-303	L=0 P=2

	Modern Instrumental Analysis: Principles and Practice	**CH-SBC-304**	**L=0** **P=2**
	Numerical Methods for AI/ML and Quantum Computing	**CH-SBC-305**	**L=0** **P=2**
IV	Quantitative Analyses of Alloys	**CH-SBC-401**	**L=0** **P=2**
	Instrumental Analysis-II	**CH-SBC-402**	**L=0** **P=2**
	Qualitative analysis of binary mixture of organic compounds	**CH-SBC-403**	**L=0** **P=2**
	Hands on Modelling and Designing Drugs	**CH-SBC-404**	**L=0** **P=2**
POOL OF GENERIC ELECTIVE COURSES (GE) FOR SEMESTERS-III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	Green Chemistry and sustainable development	**CH-GE-301**	**L=3** **P=1**
	Biomolecules, structure and functions-I	**CH-GE-302**	**L=3** **P=1**
	Fundamentals of Spectroscopy	**CH-GE-303**	**L=3** **P=1**
IV	Metals in Medicines	**CH-GE-401**	**L=3** **P=1**
	Chemistry for Mitigation of Environmental Challenges	**CH-GE-402**	**L=3** **P=1**

	Biomolecules, structure and functions-II	**CH-GE-403**	**L=3** **P=1**
	Computational and AI/ML Methods in Chemistry	**CH-GE-404**	**L=3** **P=1**

Structure-2 DISCIPLINE SPECIFIC CORE COURSES (DSC) FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Course Code**	**Credits**
III	Inorganic Reaction mechanism, Organic photochemistry and Molecular spectroscopy	**CH-DSC-301**	**L=3** **P=1**
	Electron Transfer, Molecular Rearrangements, Pericyclic reactions and Electronic spectroscopy	**CH-DSC-302**	**L=3** **P=1**
IV	Frontiers in Bioinorganic(I), Medicinal Chemistry (I), Irreversible Thermodynamics and Transport Phenomena	**CH-DSC-401**	**L=3** **P=1**
	Frontiers in Bioinorganic(II), Medicinal Chemistry (II),Fast Chemical Processes	**CH-DSC-402**	**L=3** **P=1**

POOL OF DISCIPLINE SPECIFIC ELECTIVES COURSES (DSE) FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	**DSE Pool I**		
	Spectral Techniques in Inorganic Chemistry	**CH-DSE-301**	**L=3** **P=1**
	Chemistry of Nanomaterials	**CH-DSE-302**	**L=3** **P=1**
	Advanced Chemistry of Main Group elements	**CH-DSE-303**	**L=3** **P=1**
	Chemistry of transition metal clusters	**CH-DSE-304**	**L=3** **T=1**

	Single Crystal X-ray diffraction	**CH-DSE-306**	**L=3** **P=1**
	DSE Pool O		
	Advanced Organic Synthesis and Reagents	**CH-DSE-307**	**L=3** **P=1**
	Carbocyclic and Heterocyclic Compounds	**CH-DSE-308**	**L=3** **P=1**
	Chemistry of Biomolecules	**CH-DSE-309**	**L=3** **P=1**
	Drug Delivery and Pharmaceutical Technologies	**CH-DSE-310**	**L=3** **P=1**
	DSE Pool P		
	Advanced Polymer Science: Structure, Kinetics and Smart Materials	**CH-DSE-311**	**L=3** **P=1**
	Advanced Electrochemistry	**CH-DSE-312**	**L=3** **P=1**
	Advanced Statistical Mechanics	**CH-DSE-313**	**L=3** **P=1**
	Radiation and Photochemistry with Applications	**CH-DSE-314**	**L=3** **P=1**
	Physical Chemistry of Materials	**CH-DSE-315**	**L=3** **P=1**
	Structure, Dynamics and Spectroscopy of Biomolecules	**CH-DSE-316**	**L=3** **P=1**
	DSE Pool Common		

	Research Methodology for Chemists (Only for Structure 1 & 2)	**CH-DSE-305**	**L=3 P=1**
IV	**DSE Pool I**		
	Organotransition Metal Chemistry and Catalysis	**CH-DSE-401**	**L=3 P=1**
	Chemistry of Inorganic Materials	**CH-DSE-402**	**L=3 P=1**
	Advanced Analytical Techniques	**CH-DSE-403**	**L=3 P=1**
	Nuclear and Radiochemistry	**CH-DSE-404**	**L=3 T=1**
	Electrochemistry of Energy Storage Systems	**CH-DSE-405**	**L=3 P=1**
	DSE Pool O		
	Chemistry of Life Processes	**CH-DSE-406**	**L=3 P=1**
	Chemistry of Supramolecules, Terpenes and Steroids	**CH-DSE-407**	**L=3 P=1**
	Alkaloids, Polyphenols, and Active Pharmaceutical Ingredients	**CH-DSE-408**	**L=3 P=1**
	Polymer Chemistry and Role of Catalysis in Chemical Synthesis	**CH-DSE-409**	**L=3 P=1**
	DSE Pool P		
	Advanced Quantum Chemistry	**CH-DSE-410**	**L=3 P=1**

	Advanced Fluorescence Methods for Chemical and Biomedical Research	**CH-DSE-411**	**L=3** **P=1**
	Advanced Chemical Kinetics	**CH-DSE-412**	**L=3** **P=1**
	Advanced Molecular Spectra	**CH-DSE-413**	**L=3** **P=1**
	Computational Methods in Chemistry	**CH-DSE-414**	**L=3** **P=1**
	Solid State Chemistry	**CH-DSE-415**	**L=3** **P=1**
DISERTATION/ACADEMIC PROJECT/ENTREPRENEURSHIP FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	Dissertation	**CH-D-3201**	**6**
	Academic Project	**CH-AP-3202**	**6**
	Entrepreneurship	**CH-ENT-3203**	**6**
IV	Dissertation	**CH-D-3201**	**6**
	Academic Project	**CH-AP-3202**	**6**
	Entrepreneurship	**CH-ENT-3203**	**6**
POOL OF GENERIC ELECTIVE COURSES (GE) FOR SEMESTERS- III & IV			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	Green Chemistry and sustainable development	**CH-GE-301**	**L=3** **P=1**
	Biomolecules, structure and functions-I	**CH-GE-302**	**L=3** **P=1**

	Fundamentals of Spectroscopy	**CH-GE-303**	**L=3** **P=1**
IV	Metals in Medicines	**CH-GE-401**	**L=3** **P=1**
	Chemistry for Mitigation of Environmental Challenges	**CH-GE-402**	**L=3** **P=1**
	Biomolecules, structure and functions-II	**CH-GE-403**	**L=3** **P=1**
	Computational and AI/ML Methods in Chemistry	**CH-GE-404**	**L=3** **P=1**

Structure-3 DISCIPLINE SPECIFIC CORE COURSES (DSC) FOR SEMESTER- III			
Semester	**Name of the Course**	**Course Code**	**Credits**
III	Advanced Characterization Techniques of Molecules and Materials	**CH-DSC-3301**	**L=3** **P=1**
POOL OF DISCIPLINE SPECIFIC ELECTIVES COURSES (DSE) **FOR SEMESTERS- III & IV**			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
III	**DSE Pool I**		
	Spectral Techniques in Inorganic Chemistry	**CH-DSE-301**	**L=3** **P=1**
	Chemistry of Nanomaterials	**CH-DSE-302**	**L=3** **P=1**
	Advanced Chemistry of Main Group elements	**CH-DSE-303**	**L=3** **P=1**
	Chemistry of transition metal clusters	**CH-DSE-304**	**L=3** **T=1**
	Single Crystal X-ray Diffraction	**CH-DSE-306**	**L=3** **P=1**
	DSE Pool O		
	Advanced Organic Synthesis and Reagents	**CH-DSE-307**	**L=3** **P=1**
	Carbocyclic and Heterocyclic Compounds	**CH-DSE-308**	**L=3** **P=1**
	Chemistry of Biomolecules	**CH-DSE-309**	**L=3** **P=1**
	Drug Delivery and Pharmaceutical Technologies	**CH-DSE-310**	**L=3** **P=1**
	DSE Pool P		

	Advanced Polymer Science: Structure, Kinetics and Smart Materials	CH-DSE-311	L=3 P=1
	Advanced Electrochemistry	CH-DSE-312	L=3 P=1
	Advanced Statistical Mechanics	CH-DSE-313	L=3 P=1
	Radiation and Photochemistry with Applications	CH-DSE-314	L=3 P=1
	Physical Chemistry of Materials	CH-DSE-315	L=3 P=1
	Structure, Dynamics and Spectroscopy of Biomolecules	CH-DSE-316	L=3 P=1
IV	**DSE Pool I**		
	Organotransition Metal Chemistry and Catalysis	CH-DSE-401	L=3 P=1
	Chemistry of Inorganic Materials	CH-DSE-402	L=3 P=1
	Advanced Analytical Techniques	CH-DSE-403	L=3 P=1
	Nuclear and Radiochemistry	CH-DSE-404	L=3 T=1
	Electrochemistry of Energy Storage Systems	CH-DSE-405	L=3 P=1
	DSE Pool O		

	Chemistry of Life Processes	**CH-DSE-406**	**L=3 P=1**
	Chemistry of Supramolecules, Terpenes and Steroids	**CH-DSE-407**	**L=3 P=1**
	Alkaloids, Polyphenols, and Active Pharmaceutical Ingredients	**CH-DSE-408**	**L=3 P=1**
	Polymer Chemistry and Role of Catalysis in Chemical Synthesis	**CH-DSE-409**	**L=3 P=1**
	DSE Pool P		
	Advanced Quantum Chemistry	**CH-DSE-410**	**L=3 P=1**
	Advanced Fluorescence Methods for Chemical and Biomedical Research	**CH-DSE-411**	**L=3 P=1**
	Advanced Chemical Kinetics	**CH-DSE-412**	**L=3 P=1**
	Advanced Molecular Spectra	**CH-DSE-413**	**L=3 P=1**
	Computational Methods in Chemistry	**CH-DSE-414**	**L=3 P=1**
	Solid State Chemistry	**CH-DSE-415**	**L=3 P=1**
Courses on Research Methods/Tools/Writing FOR SEMESTERS- III & IV			
III	Advanced Research Methodology in Chemistry	**CH-SBC-3301**	**L=1 P=1**

	Tools for Research	**CH-SBC-3302**	**L=1** **P=1**
IV	Techniques of Research Writing	**CH-SBC-4301**	**L=1** **P=1**

Structures – 1, 2 and 3 (Level 6.5) Coursework / Research

SEMESTER-III

DSC

DISCIPLINE SPECIFIC CORE COURSE (DSC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Inorganic Reaction mechanism, Organic photochemistry and Molecular spectroscopy CH-DSC-301	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To equip students to understand the various mechanisms operative in inorganic complexes during substitution reactions.
- To provide fundamental understanding of photophysical and photochemical processes including the excited-state reactions of alkenes, aromatics, and carbonyl compounds towards applications of photochemistry in organic synthesis.
- To introduce quantum principles and theoretical models underlying rotational, vibrational, and Raman spectroscopy.
- To enable interpretation of spectra using symmetry, group theory, and analysis of molecular structure and parameters.

Learning outcomes: At the completion of this course, the students should be able to:

- obtain a fundamental understanding of inorganic synthetic chemistry through substitution reactions.
- explain excited-state behaviour, energy transfer, fluorescence, and quenching.

- describe photochemical reactions of alkenes, aromatics, and carbonyl compounds.
- relate photochemical principles to DSSCs, photocatalysis, and OLEDs.

- explain the principles of quantum mechanics, electromagnetic radiation, and spectroscopic laws, and interpret rotational, vibrational, and Raman spectra to determine molecular constants and properties.
- apply symmetry and group theory to assign normal modes and analyse spectral features, including selection rules, polarization, and Stokes/anti-Stokes lines.

THEORY COMPONENT (3 Credits: 45 Hours)

Unit-1: Inorganic Reaction Mechanism (15 Hours)

Substitution Reactions in Metal Complexes: Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.

Unit-2: Organic Photochemistry (15 Hours)

Photophysical Processes: General Introduction, Jablonski diagram, fluorescence, phosphorescence, Effect of solvents, delayed fluorescence, thermally activated delayed fluorescence (TADF) in organic systems, Kasha's rule, energy pooling, exciplexes, excimers, photosensitization, fluorescence quenching mechanisms (static and dynamic), Stern–Volmer plot, The intermolecular processes: resonance energy transfer, energy transfer mechanisms (Förster and Dexter), Photo-induced electron transfer (PET) reactions and the Marcus equation, multiphoton excitation.
Photochemistry of Alkenes, alkynes and aromatic compounds: Cis-Trans isomerization, non-vertical energy transfer; photochemical reactions of olefins. Di-pi-methane rearrangement, Oxa-di-pi-methane rearrangement. Photochemistry of aromatic compound, Excited state transformation of benzene, 1, 2; 1, 3 and 1, 4-photocycloaddition reactions of benzene. Dimerization of aromatic compounds, Nucleophilic photo substitution reactions in aromatic compounds. Photo-Fries rearrangement of ethers and anilides; Singlet molecular oxygen reactions, Barton reaction, Photocyclization (Mallory reaction), Photo-Bergman cyclisation. Nazarov cyclization, Photo-Favorskii rearrangement, Bicyclic rearrangement, Photochemical Wolff rearrangement.
Photochemistry of carbonyl compounds: Photochemistry of enones, α,β-unsaturated ketones); β,γ-unsaturated ketones; Epoxy ketone system, cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); photoreductions. cycloaddition reactions of carbonyl compounds to alkenes (intra and intermolecular), oxetane formation, and the stereochemistry of the product.

Modern Applications of Photochemistry: Applications in C–C, C–N, C–O bond formation, SET (Single Electron Transfer) pathways, Dye-Sensitized Solar Cells (DSSCs), Organic Light-Emitting Diodes OLED)

Unit-3: Molecular Spectroscopy: Rotational, Vibrational and Raman Methods (15 Hours)

Characterization of electromagnetic radiation. Born-Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation (Qualitative Discussion). Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Rotational Spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First and second order Stark effect.

Vibrational Spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect. Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules. Overtones and combination bands.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and vibrational Raman spectroscopy. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

References (Theory)

1. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Cengage Learning India Private Limited, New Delhi, 2010.
2. S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms*, Springer-US, New York, 2003.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong and M. Hagerman, *Shriver and Atkins' Inorganic Chemistry*, Oxford University Press, Delhi, 2010.
4. M. L. Tobe, *Inorganic Reaction Mechanisms*, Thomas Nelson & Sons Ltd., London, 1972.
5. A. Gilbert and J. Baggott, *Essentials of Molecular Photochemistry*, CRC Press, London, UK, 1991.
6. J. Mattay and A. G. Griesbeck, *Photochemical Key Steps in Organic Synthesis*, VCH, New York, 1994.
7. N. J. Turro, *Modern Molecular Photochemistry*, University Press, Menlo Park, CA, 1978.
8. W. M. Horspool, *Aspects of Organic Photochemistry*, Academic Press, 1976.
9. V. K. Ahluwalia and R. K. Parashar, *Organic Reactions Mechanisms*, Narosa Pub. Delhi 5th Edn., 2024.

10. J. D. Coyle, *Photochemistry in Organic Synthesis*, Royal Society of Chemistry, London, 1986.
11. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, Springer New York, NY, 3rd Edn., 2006.
12. C. J. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 6th edn, Tata McGraw-Hill, 2025.
13. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill, 2017.
14. J. M. Hollas, *Modern Spectroscopy*, 4th edn, John Wiley & Sons, 2004.
15. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy: From Radio Waves to Gamma Rays*, I. K. International Publishing House, New Delhi, 2015.
16. R. Kakkar, *Atomic & Molecular Spectroscopy*, Cambridge University Press, 2015.
17. J. C. D. Brand and J. C. Speakman, *Molecular Structure: The Physical Approach*, 2nd edn, Edward Arnold, London, 1975.
18. R. Chang, *Basic Principles of Spectroscopy*, McGraw-Hill, New York, 1970.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR spectroscopy, magnetic susceptibility etc. Selection can be made from the following or any other from the existing literature:

i. Synthesis and characterization of $[Co(NH_3)_6]Cl_3$

ii. Synthesis and characterization of $[Co(NH_3)_5Cl]Cl_2$

iii. Synthesis and characterization of $[Co(NH_3)_5(NO_2)]Cl_2$

iv. Synthesis and characterization of $[Co(NH_3)_5(H_2O)]Cl_3$

v. Synthesis and characterization of Schiff Base ligands and their metal complexes.

Other new novel synthesis reported in literature from time to time

2. Determination of quantum yield of a photochemical reaction e.g., photoreduction of ferrioxalate (actinometry)
3. Photochemical isomerization of trans-stilbene to *cis*-stilbene, to observe the change in absorption peak
4. Study of photochemical decomposition of hydrogen peroxide by titration of remaining H_2O_2 with $KMnO_4$.
5. Photocatalytic degradation of dye e.g. methylene blue using TiO_2 by measuring absorbance with time as dye is degraded
6. Solid state synthesis of cyclobutane dimer of cinnamic acid via [2+2] photocyclization of cinnamic acid (topochemical effects)
7. Synthesis of oxetane derivatives by Paternò–Büchi reaction of carbonyl compound e.g. benzaldehyde or benzophenone and an alkene e.g., isobutene derivative.
8. Endoperoxide formation of furans by photooxygenation through singlet oxygen addition to furans
9. Paternò–Büchi Reaction by cycloaddition of carbonyl compound e.g. benzaldehyde or benzophenone and an alkene e.g., isobutene derivative to form oxetane derivative.

10. Verify Lambert-Beer's law, and determine the concentration of CuSO4/KMnO4/$K_2Cr_2O_7$ in a solution of unknown concentration colourimetrically.
11. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture colourimetrically.
12. Study the influence of pH on the spectrum of potassium dichromate solution.
13. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture by the MLRA method.
14. Study the kinetics of the reaction of phenolphthalein with sodium hydroxide.
15. Analyse the IR/FTIR spectra of given compounds.
16. Analyse the Raman spectra of given compounds and materials.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. F. Basolo and R. K. Murmann, *Inorg. Synth.*, 1953, **4**, 171.
2. J. Bjerrum and J. P. McReynolds, *Inorg. Synth*., 1946, **2**, 216-221.
3. N. J. Turro, V. Ramamurthy and J. C. Scaiano, *Principles of Molecular Photochemistry: An Introduction*, University Science Books, 2009.
4. A. I. Vogel, *Vogel's Textbook of Practical Organic Chemistry*, Longmans, 1956.
5. J. M. Coxan and B. Halton, *Organic Photochemistry*, Cambridge University Press, 2nd edition, 2011.
6. A. Cox and T. J. Camp, *Introductory Photochemistry*, McGraw-Hill Inc., US, 1971.
7. B. Wardle, *Principles and Applications of Photochemistry*, John Wiley & Sons, 2009.
8. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2015.
9. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th edn, Brooks/Cole, 2017.
10. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 2nd revised edn, Holt, Rinehart & Winston of Canada Ltd., 1988.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE (DSC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		

Electron Transfer, Molecular Rearrangements, Pericyclic reactions and Electronic spectroscopy CH-DSC-302	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To provide the knowledge of the various types of electron transfer reactions, their mechanistic aspects, and their link to water splitting and mixed valence complexes. Further, the study of molecular rearrangements would shed light on the magnetism of labile complexes and their catalytic applications.
- To introduce concepts of orbital symmetry and explain types pericyclic reaction – electrocyclic, cycloaddition, and sigmatropic rearrangements where students will apply FMO/PMO approaches to reaction prediction.
- To introduce the principles of atomic and molecular electronic spectra, including electronic states, transitions, and their analysis using key concepts and theoretical models.
- To understand excited-state processes and interpret spectroscopic behaviour such as fluorescence, phosphorescence, and quenching.

Learning outcomes: At the completion of this course, the students should be able to:

- obtain a fundamental understanding of electron transfer reactions and the molecular rearrangements of inorganic complexes.
- predict outcomes of pericyclic reactions using orbital symmetry rules.
- explain mechanisms of Diels–Alder, electrocyclic, and sigmatropic processes.
- apply pericyclic concepts in synthetic design and natural product chemistry
- describe atomic states and selection rules, interpret electronic and photoelectron spectra, and apply theoretical models and group theory to predict transitions and explain excited-state processes and quenching.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Electron Transfer and Molecular Rearrangements **(15 Hours)**

Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reluctant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

Unit-2: Pericyclic Reactions **(15 Hours)**

A general comparison of pericyclic reaction with reactive intermediate involving reactions. Orbital Symmetry and correlation diagrams for electrocyclic and cycloaddition reactions.

Comparative study of Frontier Molecular Orbital (FMO), Perturbation Molecular Orbital (PMO) and Hückel–Mobius approach to discuss the mode of reaction in pericyclic reactions (electrocyclic, cycloaddition reactions and sigmatropic reactions).

Electrocyclic reactions: Stereochemical aspects of electrocyclic reactions of [4]n, [4+2]n and examples of electrocyclic reactions involved in natural products synthesis.

Cycloadditions Reactions: Diels-Alder reaction, endo/exo control, stereospecificity, asymmetric Diels-Alder reaction using chiral Lewis acid and organocatalysts, 1,3-dipolar cycloadditions, mechanisms (Huisgen, nitrile oxide, azide, nitrones), [3,3], higher-order cycloadditions [4+3], [5+2], [6+4] processes and cheletropic reactions.

Sigmatropic Rearrangements: Principles, suprafacial/antarafacial shifts, migration aptitude & stereochemical consequences. Types [i, j] shifts: hydrogen and carbon migrations, Claisen rearrangements (classical, Ireland, Johnson, Eschenmoser), Cope rearrangements, Stevens rearrangement, Thermal and anionic variants, Oxy-Cope, Claisen–Cope combinations, ene-reactions (thermal & Lewis-acid catalyzed), group transfer.

Unit-3: Electronic Spectroscopy of Atoms and Molecules (15 Hours)

Atomic Spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Electronic Spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde).

Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects-viscosity, polarity, hydrogen bonding.

Excited States: Deactivation. Jablonskii diagram. Fluorescence and phosphorescence and factors affecting these. Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.

References (Theory)

1. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Cengage Learning India Private Limited, New Delhi, 2010.
2. S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms*, Springer-US, New York, 2003.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong and M. Hagerman, *Shriver and Atkins' Inorganic Chemistry*, Oxford University Press, Delhi, 2010.
4. M. L. Tobe, *Inorganic Reaction Mechanisms*, Thomas Nelson & Sons Ltd., London, 1972.
5. I. Fleming, *Pericyclic Reactions*, Oxford Chemistry Primers, 2nd ed, 2015.

6. J. Clayden, N. Greeves and S. Warren, *Organic Chemistry*, Oxford University Press, 2nd ed, 2012.
7. S. M. Mukherji, *Pericyclic reactions: A Mechanistic Study*, The Macmillan Company of India Limited, 1979.
8. V. K. Ahluwalia and R. K. Parashar, *Organic Reactions Mechanisms*, Narosa Pub. Delhi 5th Edition, 2024.
9. A. P. Marchand and R. E. Lehr, *Pericyclic Reactions*, Vols. I and II, Academic Press, New York, 1977.
10. C. J. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 6th edn, Tata McGraw-Hill, 2025.
11. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill, 2017.
12. J. M. Hollas, *Modern Spectroscopy*, 4th edn, John Wiley & Sons, 2004.
13. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy: From Radio Waves to Gamma Rays*, I. K. International Publishing House, New Delhi, 2015.
14. R. Kakkar, *Atomic & Molecular Spectroscopy*, Cambridge University Press, 2015.
15. J. C. D. Brand and J. C. Speakman, *Molecular Structure: The Physical Approach*, 2nd edn, Edward Arnold, London, 1975.
16. R. Chang, *Basic Principles of Spectroscopy*, McGraw-Hill, New York, 1970.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Isolation of Precursor complex [Oxidant; nitriloacetic acid complex of pentaamine cobalt (III) complex] [Reductant; Iron(II) complex)
2. Synthesis and characterization of $[CoX(NH_3)_5]^{2+}$ (where X is Cl^-, NO^{2-} and various carboxylates), followed by study of electron transfer reaction with reductant such as Fe(II), Cr(II) complexes.
3. Preparation, molecular rearrangements and applications (transfer hydrogenation and Suzuki-Miyaura coupling) of $[NiCl_2(PPh_3)_2]$.
4. New electron transfer reactions will be added time to time as per the requirement.
5. Photo-Fries rearrangement of aryl esters e.g., phenyl acetate and phenyl benzoate to 2/4-hydroxy acetophenones and 2/4- hydroxyl benzophenones, respectively
6. Effect of solvent polarity on o/p-ratio in Photo-Fries rearrangement reaction by taking different solvents e.g., n-hexane, acetonitrile and isopropanol
7. Diels-Alder reaction ([4+2] cycloaddition) between dienes e.g., anthracene, furan, cyclopentadiene etc., and dienophile e.g., maleic Anhydride
8. 1,3-Dipolar cycloaddition reaction catalysed by Cu(I) e.g., Copper (I) catalysed azide-alkyne cycloaddition (CuAAC, "click") reaction of phenyl azide and phenylacetylene to form 1,4-disubstituted 1,2,3-triazole.
9. Study the effect of structure on the UV spectra of organic compounds.
10. Determine the solvent cut-off wavelengths for the given solvents.
11. Study the effect of solvent on the UV spectra of organic compounds

12. Study the spectra of mesityl oxide/ benzophenone in different solvents and classify the observed transitions in terms of n → π* and π → π* transitions. Discuss the shift in transitions relative to those in acetone.
13. Determine the amount of iron present in a sample using 1,10-phenathroline.
14. Find the stoichiometry of the complex formed between a metal ion (Fe^{3+}) and a ligand (salicylate) by Job's continuous variation method and determine the stability constant of the complex formed.
15. Study the fluorescence spectrum of some common fluorophores, such as rhodamine ad fluorescein.
16. To study the effect of copper ions on fluorescence quenching of rhodamine and/or fluorescein using Stern Volmer's method, and calculate the Stern Volmer's constant.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. M. J. McClellan and M. E. Cass, *J. Chem. Educ.*, 2015, **92**, 1766−1770.
2. A. R. Hilts and J. Cooke, *J. Chem. Edu.*, 2023, **100**, 4119-4121.
3. S. Iyer and J. P. Varghese, *J. Chem. Soc. Chem. Comm.*, 1995, 465-466.
4. V. Percec, G. M. Golding, J. Smidrkal and O. Weichold, *J. Org. Chem.,* 2004, **69**, 3447–3452.
5. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, CRC Press, 3rd edition, 2013.
6. D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, *A Microscale Approach to Organic Laboratory Techniques,* Brooks/Cole Pub Co; 6th edition, 2017.
7. P. B. Cranwell, L. M. Harwood and C. J. Moody, *Experimental Organic Chemistry*, John Wiley & Sons, 3rd Edition, 2017.
8. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2015.
9. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th edn, Brooks/Cole, 2017.
10. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 2nd revised edn, Holt, Rinehart & Winston of Canada Ltd., 1988.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Characterization Techniques of Molecules and Materials CH-DSC-3301 (for Structure III)	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To study the topics such as symmetry in crystallography, crystals systems, Bravais lattices, crystal symmetry, crystallographic point groups and space groups, Miller indices, theory of X-ray diffraction, data collection, data reduction, structure factors and Fourier syntheses, Phase problem, direct methods, Patterson method, crystal structure refinement etc.
- To provide foundational and practical understanding of modern spectroscopic techniques for the structural elucidation, quantification, isomer identification, and mechanistic studies of complex organic structures and reactions.
- Understanding of the principles, instrumentation, and sample preparation methods used in modern analytical and characterization techniques, including microscopy, spectroscopy, diffraction, and magnetic methods for analysing chemical and material systems.
- Interpret experimental data and apply these techniques in research and advanced studies.

Learning outcomes: At the completion of this course, the students should be able to:

- grow crystals of small complexes/compounds.
- analyze the crystallographic data by different statistical method.
- apply multiple spectroscopic techniques to determine the structures of various natural products, biomolecules, synthetic intermediates and industrially important chemicals.
- analyze structural proposals based on comprehensive spectroscopic evidence such as qNMR, isomer identification, and mechanistic analysis.
- understand the principles, instrumentation, and sample preparation techniques used in modern analytical and characterization methods.
- analyze, interpret, and apply spectroscopic, microscopic, diffraction, and magnetic techniques to investigate structural, electronic, optical, and magnetic properties of chemical and material systems.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Crystallography for Inorganic Chemists (15 Hours)

Introduction to Crystallography in respect to Chemistry; Crystal symmetry: 32 point groups and their notations, stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams etc. Miller Indices, crystallographic planes and directions, close pack structures, Miller-Bravais indices for hexagonal systems, various inorganic crystal structure type (Rocksalt, CsCl, Wurtzite, Fluorite, Perovskite, etc.); Brief Introduction to Refinement of Crystal Structure: Refinement by Fourier synthesis, Refinement by least squares method, weighting functions, Goodness Of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms.

Unit-2: Advanced Spectroscopic Techniques for Structural Elucidation of Organic Compounds (15 Hours)

General introduction to 1D and 2D NMR spectroscopy, IR spectroscopy, and mass spectrometry techniques. Application of spectroscopic techniques for the structural elucidation of Natural products: i) Aromatic compounds: for example - Eugenol, Anethole, and Tetrahydrocannabinol; ii) Carbohydrates: for example - Glucosamine, Lactose, and Maltose; iii) Flavonoids: for example - Coumarins, chromones, flavonols (Quercetin, Myricetin, Fisetin), flavan-3-ols (Epicatechin), flavones (Apigenin, Luteolin), flavanones, (Naringenin, Hesperidin), isoflavones (Genistein, Daidzein), Anthocyanins (Cyanidin, Pelargonidin); iv) Alkaloids & Polyphenols: for example - Nicotine, caffeine, Theobromine, Cytisine, Galanthamine, and Curcumin; v) Terpenoids: for example - Limonene, Menthol, Thujones, and Betulinic acid.
Use of NMR techniques for quantification, stereochemistry determination, and mechanistic studies (reaction kinetics, kinetic isotope effects, detection of reaction intermediates, isotope labeling, variable-temperature experiments, variable-pH experiments using case study).

Unit-3: Physical Characterization of Molecules and Materials (15 Hours)

Fundamental principles, general Instrumentation, sample preparation and basic applications of Transmission and scanning Electron Microscopy, UV-visible and Fluorescence Spectroscopy, UV and X-ray Photoelectron spectroscopy, X-ray diffraction, Dynamic Light scattering, Fourier Transform Infra-Red (FTIR) spectroscopy, Nuclear Magnetic Resonance (NMR) spectroscopy, Vibrating Sample Magnetometry (VSM).

References (Theory):

1. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley-Interscience, 3rd Ed., 2009.
2. W. Massa, *Crystal Structure Determination*, Springer, Science & Business Media, 2nd Ed., 2004.
3. P. Mueller, R. Herbst-Irmer, A. L. Spek, T. R. Schneider and M. R. Sawaya, *Crystal structure refinement: A crystallographer's guide to SHELXL*, Oxford University Press, 2006.
4. S. Berger and D. Sicker, *Classics in Spectroscopy: Isolation and Structure Elucidation of Natural Products,* Wiley-VCH, 2009.

5. R. M. Silverstein, F. X. Webster and D. L. Bryce, *Spectrometric Identification of Organic Compounds*, Wiley, 8th ed., 2015.
6. D. L. Pavia, G. M. Lampman, G. A. Kriz and J. R. Vyvyan, *Introduction to Spectroscopy*, Cengage Learning, 5th ed., 2015.
7. W. Kemp, *Organic Spectroscopy*, Macmillan Education, 3rd ed., 1991.
8. Y. Ben-Tal, *et al. Progress in Nuclear Magnetic Resonance Spectroscopy* 2022, **129**, 28–106.
9. S. Laurella, *Applied Magnetic Resonance* 2024, **55**, 1335–1376.
10. C. J. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 6th edn, Tata McGraw-Hill, New Delhi, 2025.
11. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill, New York, 2017.
12. J. M. Hollas, *Modern Spectroscopy*, 4th edn, John Wiley & Sons, Chichester, 2004.
13. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy: From Radio Waves to Gamma Rays*, I.K. International Publishing House, New Delhi, 2015.
14. R. Kakkar, *Atomic and Molecular Spectroscopy*, Cambridge University Press, Cambridge, 2015.
15. J. C. D. Brand and J. C. Speakman, *Molecular Structure: The Physical Approach*, 2nd edn, Edward Arnold, London, 1975.
16. R. Chang, *Basic Principles of Spectroscopy*, McGraw-Hill, New York, 1970.

PRACTICAL COMPONENT **(1 Credit: 15 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis and growth (for single crystals) of inorganic complexes/compounds and their characterization by diffraction methods.
2. Synthesis and growth (for single crystals) of inorganic metal clusters/cages and their characterization by diffraction methods.
3. Isolation and structural elucidation of Eugenol using IR, ^{1}H NMR, and ^{13}C NMR.
4. Identification of a flavonoid, i.e., Quercetin, using 1D and 2D NMR (HSQC/HMBC, etc.).
5. Structural analysis of a carbohydrate molecule, i.e., Lactose, using different NMR techniques.
6. Isolation and spectroscopic identification of Alkaloids, for e.g. Caffeine.
7. Quantification of natural products using NMR (qNMR), for e.g. Curcumin.
8. To prepare nanoparticles of gold, silver and iron oxide via reduction of respective salts in aqueous media
9. To drop-cast nanoparticles of gold, silver and iron oxide on carbon-coated copper grids and analyse the size and shape of the nanoparticles using transmission electron microscopy.
10. To prepare nanoparticles of fluorophore-encapsulated organically modified silica in oil-in-water microemulsion medium.
11. To characterize nanoparticles of gold, silver and fluorophore-encapsulated organically modified silica using UV-visible spectroscopy.

12. To characterize nanoparticles of fluorophore-encapsulated organically modified silica using fluorescence spectroscopy.
13. To determine the hydrodynamic diameters of nanoparticles of gold, silver and iron-oxide using dynamic light scattering.
14. To determine the hydrodynamic diameters of nanoparticles of gold, silver and iron-oxide using dynamic light scattering.
15. To determine the amorphous/crystalline phase of nanoparticles of gold, silver and iron-oxide using powder X-ray diffraction.
16. To prepare samples and study the surface properties of nanoparticles of fluorophore-encapsulated organically modified silica using FTIR and NMR spectroscopies.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. G. H. Stout and L. H Jensen, *X-ray structure determination: A Practical Guide*, Wiley-Interscience, New York, 2nd Ed., 1989.
2. S. Berger and D. Sicker, *Classics in Spectroscopy: Isolation and Structure Elucidation of Natural Products,* Wiley-VCH, 2009.
3. I. L. Finar and A. L. Finar, *Organic Chemistry Vol. 2*, Addison-Wesley, 1998.
4. I. L. Finar, *Organic Chemistry Vol. 1*, Longman, 1998.
5. J. Mann, *Secondary Metabolites*, Oxford University Press, Oxford, UK, 1980.
6. Y. Leng, *Materials Characterization: Introduction to Microscopic and Spectroscopic Methods*, Wiley, Hoboken, 2013.
7. R. M. Silverstein, F. X. Webster, D. J. Kiemle and D. L. Bryce, *Spectrometric Identification of Organic Compounds*, 8th edn, Wiley, Hoboken, 2014.
8. C. N. R. Rao, A. Müller and A. K. Cheetham (eds.), *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, vols. 1–2, Wiley-VCH, Weinheim, 2004.
9. G. A. Ozin and A. C. Arsenault, *Nanochemistry: A Chemical Approach to Nanomaterials*, Royal Society of Chemistry, Cambridge, 2005.
10. A. K. Shukla and S. Iravani (eds.), *Green Synthesis, Characterization and Applications of Nanoparticles*, Elsevier, Amsterdam, 2019.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DSE

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Prerequisite of the course (if any)
		Lecture	Tutorial	Practical		
Spectral Techniques in Inorganic Chemistry CH-DSE-301	**04**	**03**	**__**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To introduce the basic principles underlying major spectroscopic methods used in inorganic chemistry and provide a fundamental understanding of the principles of operation and interpretation of spectra of inorganic compounds for their structural characterization and to acquire knowledge of solving structural problems based on the spectroscopic data.

Learning outcomes: At the completion of this course, the students should be able to:

- understand the basics of various spectroscopic techniques and their use in elucidating structural and electronic features of inorganic compounds.
- apply the fundamentals of various types of spectroscopic techniques like UV, IR, NMR, EPR, NQR and Mossbauer spectroscopy and applications of these techniques to analyse and interpret experimental data collected from inorganic compounds.
- learn the applications of various spectroscopic techniques to handle molecular structures during their higher studies or industrial applications.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: (15 Hours)

Vibrational Spectroscopy: Vibrational motion and energies, number of vibrational modes, anharmonicity, absorption in infrared, FT spectrometers, cell systems, effects of phase on spectra, vibrational spectra and symmetry, selection rules, symmetry of an entire set of normal vibrations, F and G matrix. Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, use of symmetry to determine the number of active infrared and Raman lines, Group theoretical approach for predicting vibrational activity using character tables with examples, rotational fine structure in gas phase IR. Non-resonance overtones and difference bands. Application of Raman and Infrared selection rules to the determination of inorganic structures, bond-strength frequency-shift relations, changes in spectra of donor molecules on coordination, and changes in symmetry on coordination.

Spectra of Coordination and Organometallic Compounds: Introduction, Effect of Coordination on Ligand Bands: Aquo complex, Ammine Complexes, Nitro and Nitrito Complexes, Thiocyanto complexes, Dimethyl Sulfoxide and related complexes, N, N-Dimethylformamide complexes, Complexes of Urea, Complexes of Thiosemicarbazide, Dithiocarbamate and Related complexes, Complexes of Carboxylic acids, Complexes of Amino acids, Complexes of β-Diketones, Complexes of Dimethylglyoxime, Metal Carbonyls, Carbonyl Hydrides, Nitrosyl complexes, Cyano complexes. Change in symmetry on Coordination: Nitrate and carbonate complexes, Sulphate and perchlorate complexes. Organometallic Compounds: Olefin complexes, Sandwich complexes. Metal-Ligand vibrations: Geometrical isomers, Jahn-Teller Effect.

Mössbauer Spectroscopy: Introduction, Mossbauer Effect, Experimental arrangements, Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mossbauer spectra, applications to metal complexes, metal carbonyls, inter halogen compound $I_2Br_2Cl_4$, Iron in very high oxidation states-Fe(V) and Fe(VI) nitride complexes, Fe-S cluster and tin compounds, etc. Partial quadrupole splitting and geometry of the complexes. Temperature- and time-dependent effects: Basic iron acetates, Spin crossover in the complex $[Fe(phen)_2(NCS)_2]$, Valence fluctuation. Conversion electron Mossbauer spectroscopy (CEMS).

Unit-2: (15 Hours)

Electronic Spectroscopy: Vibrational and electronic energy levels in diatomic molecules, potential energy level diagram. Symmetry requirements and selection rules for electronic transitions and intensity-enhancing effects such as spin-orbit and vibronic coupling contributions, d-p mixing in certain symmetries. Polarized absorption spectra. Survey of the electronic spectra of octahedral and tetragonal complexes, including calculations of *Dq*, β, *D*s, *D*t, effects of σ /π bonding, distortions and nephelauxetic behaviour. Intervalence transitions and structural evidence from electronic spectra.

Nuclear Magnetic Resonance Spectroscopy: Basics of NMR, measuring chemical shifts, signal intensities and splitting, Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like ^{1}H, ^{11}B, ^{15}N, ^{19}F, ^{29}Bi, ^{31}P, ^{183}W, ^{195}Pt, etc. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of $\langle S_z \rangle$, contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density, π delocalization, simplified M.O. diagram for Co(II) and Ni(II). Application to planar tetrahedral equilibrium, Contrast agents.

Unit-3: (15 Hours)

Electron Paramagnetic Resonance Spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Shift operators and the second-order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Magnetism: Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where S = ½, van Vleck's equation, its derivation and its applications. Spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P., intramolecular effects, antiferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria.

Nuclear Quadrupolar Resonance (NQR) Spectroscopy: Quadrupolar moment, energy levels of a quadrupolar nucleus, and effects of asymmetry parameters and energy levels. Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

References (Theory)

1. S. F. A. Kettle, *Physical Inorganic Chemistry: A Coordination Chemistry Approach*, Springer, Berlin, Heidelberg, 1996.
2. R. S. Drago, *Physical Methods for Chemists*, East West Press Pvt. Ltd., 2nd ed., 2016.
3. D. N. Sathyanarayana, *Vibrational Spectroscopy: Theory and Applications*, New Age International Publishers, 2004.
4. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, *Structural Methods in Inorganic Chemistry*, EBLS Publications, 1987.
5. D. W. H. Rankin, N. W. Mitzel and C. A. Morrison, *Structural Methods in Molecular Inorganic Chemistry*, Wiley, 2013.
6. F. E. Mabbs, and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, 2008.
7. R. L. Dutta and A. Shyamal, *Elements of Magnetochemistry*, East-West Press, 2nd Ed., 1993.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

Demonstration/Discussion of working principle/Hands-on with substantial literature analysis/Laboratory exercise

1. Analysis of given inorganic compounds/sample using various spectroscopic techniques - IR, UV-Visible, NMR, EPR, etc. Measurement and interpretation of the different spectra for the inorganic compounds and molecules.

2. Study UV-Vis spectra of transition metal complexes and assign electronic transitions using experimental techniques. Study the effect of solvent on the UV-Vis spectra of inorganic compounds.
3. Measure and analyze NMR and EPR spectra for the given inorganic compounds.
4. Facility (UV, IR, EPR, and NMR) visits of the students.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. A. I. Vogel, *Vogel's Quantitative Chemical Analysis (revised by G. Svehla)*, Longmans, ISBN 058-221866-7, 7th Ed., 1996.
2. J. M. Hollas, *Modern Spectroscopy*, 4^{th} Ed., Wiley, 2013.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry of Nanomaterials CH-DSE-302	**04**	**03**	__	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:
- To educate the dramatic changes in properties that occurs by reducing the size and shape of materials.
- To impart knowledge on how to perform the synthesis of such small sizes and shapes of materials.

Learning outcomes: At the completion of this course, the students should be able to:
- learn the basic theoretical aspects of the variations in the physical and chemical properties of the materials by changing the size and shape of various type of materials

- learn the different synthetic procedures of achieving the nanomaterials of desired shape and size.
- learn the different characterization techniques of identifying the nano materials.
- learn about the possible applications of the nanomaterials.

THEORY COMPONENT **(3 Credit: 45 Hours)**

UNIT 1: Introduction and Properties of Nanomaterials **(15 Hours)**

Development and classification of nanomaterials, basics (atoms, molecules, clusters and supramolecules, self-assembly), carbon-based materials, various dimensions and shapes of inorganic/organic nano materials (quantum wells, quantum dots, quantum wires), Toxicity of nanomaterials. Role of size and shape in nanomaterials; specific surface energy, surface stress. Electronic Properties: comparison of bulk materials with nanostructured materials (metals, semiconductors, and insulators). Magnetic Properties: Superparamagnetism, blocking. Important properties in relation to nanomagnetism.

Unit-2: Synthesis of Nanomaterials **(15 Hours)**

Chemical Methods: Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Post-synthetic size-selective processing. Sol-gel, Micelles, and microemulsions. Biological Methods of Synthesis: Use of bacteria, fungi, and Actinomycetes for nanoparticles synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Role of plants in nanoparticle synthesis.

Unit-3: Characterization of Nanomaterials **(15 Hours)**

Characterization Techniques: X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-Vis, IR Spectrophotometers. Optical Properties: Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence. Thermal Properties and Mechanical Properties;

References (Theory)

1. C. Dupas, P. Houdy and M. Lahmani, *Nanoscience: Nanotechnology and Nanophysics*, Springer, 2004.
2. K. J. Klabunde, *Nanoscale Materials in Chemistry*, Wiley Interscience, 2001.
3. S. K. Kulkarni, *Nanotechnology: Principles and Practices*, Capitol Publishing Company, 2007.
4. M. Wilson, K. Kannangara, G. Smith, M. Simmons and B. Raguse, *Nanotechnology: Basic Science and Emerging Technologies*, Overseas Press, 2005.

5. C. P. Poole, Jr. and F. J. Ovens, *Introduction to Nanotechnology*, Wiley Interscience, 2003.
6. A. S. Edelstein, and R. C. Cammarata, *Nanomaterials: Synthesis, Properties and Applications*, Institute of Physics Publishing, 1996.
7. C. N. R. Rao, Müller and A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
8. A. S. Edelstein and R. C. Cammarata, *Nanomaterials: Synthesis, properties and Applications*, Institute of Physics Publishing, 1996.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis of Ag nanoparticles using reduction method, plasmon resonance studies.
2. Synthesis of Co nanoparticles using reduction method, superparamagnetism study.
3. Synthesis of Cu nanoparticles using reduction method, plasmon resonance studies.
4. Synthesis of TiO_2 nanoparticles and bandgap determination (quantum confinement).
5. Synthesis of Fe_3O_4 nanoparticles, superparamagnetism study (using VSM).
6. Synthesis of graphene oxide and RGO (Raman studies).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. V. Deepa, Parvathi and K. Rajagopal, *A Practical Manual on Synthesis of Nanoparticles and its Applications in Biology*, Digital Age Publishers, 1st Ed., 2017.
2. A. M. Dimiev and S. Eigler, *Graphene Oxide: Fundamentals and Applications*, Wiley, 2016.
3. A. Khataee and G. A. Mansoori, *Nanostructured Titanium Dioxide Materials: Properties, Preparation and Applications*, World Scientific Pub. Co. Inc., 2011.
4. A. Barhoumand A. S. H. Makhlouf, *Fundamentals of Nanoparticles: Classifications, Synthetic Methods, Properties and Characterization*, 1st Ed., Elsevier, 2018.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Prerequisite of the course (if any)
		Lecture	Tutorial	Practical		

Advanced Chemistry of Main Group Elements CH-DSE-303	**04**	**03**	**__**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

To acquire the subject knowledge of main group elements (*s, p* block and noble gases) with an emphasis on synthesis, structure, bonding, and reactivities.

Learning outcomes: At the completion of this course, the students should be able to:

- familiar with the main group compounds such as xenon halides, boranes, X-O (X = Si, Cl, S, P), and Z-N (Z = B, P, S), derivatives.
- gaining knowledge for designing a new molecule (ligands) by the proper choice of main group reagents.
- understand the importance and reactivity of organolithium and organomagnesium reagents in organic synthesis.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: **(15 Hours)**

Bonding in main group compounds: VSEPR Theory, Construction of Walsh diagram for triatomic molecules, Hybridization including energetics of hybridization. dπ-pπ bond. Double bond rule and structural discussion of metal-metal multiple bonds between Group 14 elements; some simple reactions of covalently bonded molecules: (i) Atomic inversion (ii) Berry-pseudo rotation. Fluxional behaviour of simple main group five and seven co-ordinated molecules. Frustrated Lewis pairs.
Alkali and alkaline earth metals: Solid- and solution state structures of Organolithium and organomagnesium compounds.

Unit-2: **(15 Hours)**

Noble gases: Physical properties. Preparation, chemical reactions, and structure of noble gas compounds (fluorides, oxides, and oxyfluorides of Xenon, ArF_2, RnF_2).
Boron compounds: Structures of carboranes, metalloboranes, and metallocarboranes.
Compounds of carbon and silicon: Fullerenes and their compounds, Intercalation compounds of graphite, and cyclo[18]carbon. Synthesis and structure of carbides. Classification and structural discussion of silicates and ultramarines.
Compounds of halogen group elements: Oxyacids and oxoanions of halogens.

Unit-3: **(15 Hours)**

Compounds of nitrogen group elements: Synthesis and structure of nitrides. Structural comparison of (i) Oxides and Sulphides of Phosphorus; (ii) cyclodiphosphazene, cyclotriphosphazene and cyclotetraphosphazenes; bonding and nucleophilic substitution reactions of cyclotriphosphazenes; Preparation, structure and bonding of S−N compounds (S_4N_4, S_2N_2, S_4N_2, $(SN)_x$, $[S_3N_3]^-$, $S_3N_3Cl_3$).
Compounds of oxygen group elements: Catenation property; Selenides and tellurides, oxyacids of sulphur.
Reaction in non-aqueous solvents: Characteristic properties of an ionizing solvent, Reaction in liquid ammonia, liquid Sulphur dioxide, dimethyl formamide (DMF), and dimethyl sulphoxide (DMSO). Chemistry of fused salt systems.

References (Theory)

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Prentice Hall, 4th Ed., 1997.
2. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Pearson, 5th Ed., 2018.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong and M. Hagerman, *Shriver & Atkins' Inorganic Chemistry*, W. H. Freeman and Company, New York, 5th Ed., 2010.
4. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, John Wiley, 6th Ed., 2007.
5. N. Wiberg, A. F. Holleman and E. Wiberg, *Holleman-Wiberg's Inorganic Chemistry*, Academic Press Inc., 2001.
6. A. J. Elias, *The Chemistry of the p-Block Elements: Syntheses, Reactions and Applications*, Universities press, Hyderabad, 2018.
7. D. W. Stephan, *Frustrated Lewis Pairs*, American Chemical Society, 2025.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1) Synthesis of triphenylphosphine chalcogenide from PPh_3.
2) Synthesis of phosphazo compounds by Staudinger reaction.
3) Comparative study of IR and ^{31}P NMR for triphenylphosphine oxide, –sulphide and –selenide.
4) Purification of tin powder.
5) Syntheses and characterization of R_2SnCl_2 (R = Benzyl and various substituted benzyl chloride).
6) Reactions of Bn_2SnCl_2 with arene.
7) Estimation of bleaching powder by iodometric titrations.
8) Determination of potassium ion concentration by ion exchange method.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. H. S. Alhasan and N. Alahmadi, *Principles of Qualitative Inorganic Analysis: Precipitation, Separation and Identification of Cations*, Bentham Science Publisher, 2021.
2. G. Svehla, *Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis*, Longman, 5^{th} Ed., 1979.
3. K. Sisido, Y. Takeda and Z. Kinugawa, *J. Am. Chem. Soc.,* 1961, **83**, 538-541.
4. Y. G. Gololobov, I. N. L. F. Zhmurova and Kasukhin, *Tetrahedron*, 1981, **37**, 437-472.
5. T. B. Nguyen, *Clean Technologies*, 2022, **4**, 234-238.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry of Transition Metal Clusters CH-DSE-304	**04**	**03**	**01**	**-**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To gather good understanding of different metal clusters.
- To understand the advanced chemistry and applications of metal clusters and related compounds.

Learning outcomes: At the completion of this course, the students should be able to:

- understand the fundamental principles of metal clusters, electron counting, structural classification and their importance.
- distinguish between different families of clusters, for e.g., carbonyl clusters, halide/sulphide clusters, organometallic clusters, bioinorganic clusters, etc.
- gain good understanding about the type of bonding, preparative methods for different metal cluster compounds and their reactivity.
- explore diverse applications of metal clusters in catalysis, materials science, nanotechnology, and bioinorganic systems.

THEORY COMPONENT **(3 Credits: 45 Hours)**

Unit-1: **(15 Hours)**

Introduction to metal clusters-concept and significance, Classification of clusters-nuclearity based, metal-based, bonding based, based on ligands; types of ligands in metal clusters-classification, structural and electronic role of ligands; structural features of molecular metal clusters-characterization methods, metal cluster geometries: tri-, tetra-, penta, hexanuclear metal clusters, Clusters with Seven or More Metal Atoms; metal carbonyl type clusters, anionic and hydride clusters, halide/sulphide clusters, organometallic clusters; electron counting in medium size cluster (Wade's rule, capping rule), limitations and exceptions, isolobal relationship; Relative Stability of Bridged and Non-bridged Structures.

Unit-2: **(15 Hours)**

Bonding in metal clusters-direct vs. indirect metal-metal bonding, Metal-metal multiple bonds in transition metal clusters, such as double, triple, quadruple, and even quintuple bonds, factors influencing metal-metal bond distances, principal types of compounds having multiple metal-metal bonds-Edge sharing bioctahedra, tetragonal prismatic structures, Trigonal Antiprismatic Structure; specific metal cluster systems- clusters of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt metals, Clusters of V, Mo and W; large metal clusters; main group transition metal mixed clusters-hydride clusters, carbide clusters, bonding; synthesis of metal cluster compounds- Condensation Reactions Induced by Coordinately Unsaturated Species, Condensation Between Coordinately Saturated Species with Different Oxidation States, Generation of Unsaturated Species by Chemical Methods, Displacement Reactions, Ligand-Assisted Condensation Reactions.

Unit-3: **(15 Hours)**

Cluster Reactivity - Reactions with Changes in Cluster Oxidation State, Cluster Reactions Without Changes in the Cluster Oxidation State, Ligand Substitution Reactions in Carbonyl Metal Clusters, Oxidative Additions Involving Ligand Bond Cleavage; catalysis by metal clusters, structure-activity relationship; bioinorganic iron-sulphur clusters-structure and function, Synthetic Analogues of the Active Sites of Iron-Sulfur Proteins, Tetrameric Iron-Sulfur Clusters, Dinuclear 2Fe-2S Analogues; importance and other applications of transition metal clusters. Illustrative examples from recent literature.

TUTORIAL COMPONENT **(1 Credit: 15 Hours)**

1. Tutorial on metal clusters, electron counting and metal-metal bonding with suitable examples.
2. Tutorial to identify the Metals & Ligands, Determine Cluster Type- early/late transition metal cluster, Halides, Carbonyls.
3. Tutorial to Calculate Total Valence Electrons using Wade's rules or related electron counting methods and Visualize the Structure of clusters with suitable examples.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Theory & Tutorial)

1. G. González-Moraga, *Cluster Chemistry: Introduction to Chemistry of Transition Metal and Main Group Element Molecular Clusters*, Springer Berlin, Heidelberg, 1993.
2. N. Greenwood and E. A. Earnshaw, *Chemistry of Elements*, Butterworth-Heinemann, 2nd Ed., 1997.
3. P. Fehlner, J. F. Halet and J.-Y. Saillard, *Molecular Clusters: A Bridge to solid-state Chemistry*, Cambridge University press, 2007.
4. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry: Concepts, Synthesis, and Applications*, Universities Press, India, 2010.
5. C. E. Housecroft, *Metal-Metal Bonded Carbonyl Dimers and Clusters*, Oxford Chemistry Primers, Vol. 44, Oxford, University Press, 1996.
6. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley-Interscience, 6th Ed., 1999.
7. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry*, Pearson, 4th Ed., 2006.
8. R. C. Mehrotra and A. Singh, *Organometallic Chemistry*, New Age International Publishers, 2nd Ed., 2020.
9. M. Weller, F. Armstrong, J. Rourke and T. Overton (Formerly D. F. Shriver, P. W. Atkins and C. H. Langford), *Inorganic Chemistry*, Oxford University Press, India, 6th Ed., 2014.
10. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Cengage Learning India Private Limited, Indian Reprint, 2010.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Research Methodology for Chemists CH-DSE-305	**04**	**03**	**-**	**01**	B.Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- The objective of this course is to make students understand how to formulate chemistry-related research problems, carry out research with safe and ethical practices and connect the research outcomes to society.
- Understand and apply statistical methods for reliable data analysis, including validation through acceptance/rejection criteria and confidence intervals.
- Develop competence in both quantitative and qualitative analysis of various samples.

Learning Outcomes: By the end of the course, students will be able to:

- understand how to identify research problems
- analyze online resources for identifying the gaps in the existing research related to a problem.
- assess potential hazards, minimise the risks, and prepare for emergencies in a chemistry laboratory.
- Understand the importance and process of scientific communication.
- Learn the ecosystem of designing an experiment to publishing the results.
- Develop an understanding of research tools, including their types, sampling techniques, data collection, and evaluation of reliability and validity.
- Apply appropriate statistical and analytical methods to analyze spectroscopic and diffraction data and effectively interpret and present research findings.

THEORY COMPONENT (3 Credits: 45 Hours)

Unit-1: Methods for research (15 Hours)

Concepts: Ways of Reasoning; Brief of Positivism, Interpretivism- Constructivism & Phenomenology and Critical Theory; Qualitative and Mixed-method Research.

Research Planning: Choosing Research Topic; Definitions and Types of Hypotheses; Definition and Formulation of Research Problems utilizing various tools/ databases, especially print resources (like research articles, reviews, monographs, textbooks etc.) and Digital resources (online journals). TOC alerts, E-books; Reviewing Literature, Writing a Review, Merits and demerits of AI tools in research.

Preparing for Publication: Application of Search Engines in literature survey, extensive application of Scifinder for search of topic/substance/reaction in research papers and patents, retrosynthetic analysis to plan conditions, reagents/catalysts and procedures, filtering based on year/publication type/organization/author etc.

Application of chemical structure drawing tools like Chem-draw, Chem sketch, King's Draw (mobile App) for molecular structures with stereo-centers, conformations, metal complexes, polyhedrals, supramolecules, biomolecules. Using the tools to represent multistep reactions, bonding, reactive intermediates and reaction mechanisms.

Application of softwares like Mestrenova/Delta/TopSpin for NMR spectral analyses. Assigning ^{1}H and ^{13}C NMR peaks with integration, peak picking, splitting pattern, coupling constant

determination. Vertical and horizontal expansion for fine analysis. Phase correction, base-line correction. Spectral analysis of 2D NMR – COSY, HSQC, HETCOR, NOESY.
Analyses of journal metrics and criteria to determine appropriate platform for publication.
Safe Handling of Chemicals: Recognising hazards, assessing risks, minimizing risks and preparing for emergencies using Safety Data Sheets and other resources; Understanding Chemical Storage and inventory; Risk Assessment in an experiment.

Unit-2: Tools for research (15 Hours)

Discussion and Design: Best approaches and practices for better research output: Discussion on topics like openness for innovative and constructive design thinking, analysis, and interpretation of data. Concepts of predefined notions, biases; Search and verification of facts and the source of information, the analysis of evidence; truth & causation; Types and authenticity of sources of information- Triangulation.
Data Collection: Exploratory, descriptive, experimental, diagnostic, Sampling techniques- probability & non-probability, Sample size determination, Variables- independent, dependent, controlled
Data Types and Collection Methods: Primary data: questionnaire, interviews, observation, Secondary data: reports, databases- Experimental data collection basics, Validity & reliability of tools, Field studies vs laboratory studies
Data Analysis: Statistical analysis: central tendency, standard deviation, Student's t-test, Q-test, F-test, correlation, regression theory
Utilization of software tools: Excel, SPSS, R (intro level), Graphical representation of data, Interpretation of statistical results.

Unit-3: Techniques of research writing (15 Hours)

Recording, Writing and Presentation Skills of the research findings: Understanding the importance of recording the scientific data, its writing and presentation.
Writing Process & Disseminations and Ethics: Structure, writing while researching, Study the significance, Guide for authors, Revising-Editing-and-Proofing. Ethical principles in research writing. Scientific Misconduct. Consequences of unethical practices. Authorship. Data Management: Ethical data storage.
The Anatomy of a Chemistry Research Paper: IMRaD Structure, Reporting Chemical Data, The Abstract and Title, Preparing supplementary Information for a research paper, Dissertation Writing, Structure of a Review paper.
Technical writing and Style Guidelines: The Style Guide, Grammar for Science, Visual Representation, Numbers and Units.
The Publication Ecosystem: Peer Review, Journal Metrics, Predatory publishing, Copyright.

References (Theory)

1. K. Williamson and G. Johanson, *Research Methods - Information, Systems, and Contexts*, Elsevier, 2nd Ed., 2018.
2. L. R. Gay, G. E. Mills and P. W. Airasian, *Educational Research Competencies for Analysis and Applications, Pearson*, 10th Ed., 2019.
3. C. R. Kothari, *Research Methodology – Methods and Techniques*, New Age International Publishers, 2nd ed., 2004.
4. R. Kumar, *Research Methodology: A Step-by-Step Guide for Beginners*, Pearson Education, 2nd Ed., 2005.
5. N. K. Acharya, *Textbook on Intellectual Property Rights*, Asia Law House, 2001.
6. A. P. Miller and M. D. Davis, *Intellectual Property: Patents, Trademarks and Copyright in a Nutshell*, West Group Publishers, 2000.
7. R. Kumar, *Research Methodology: A Step-by-Step Guide for Beginners*, 2nd edn, Pearson Education, 2005.
8. R. A. Day and A. L. Underwood, *Quantitative Analysis*, Prentice Hall/Pearson, 1991.
9. A. I. Vogel, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education, 2009.
10. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole (Cengage Learning), 2021.
11. C. D. Manning, P. Raghavan and H. Schütze, *Introduction to information retrieval*, Cambridge University Press, 2008.
12. W. C. Booth, G. G. Colomb and J. M. Williams, *The craft of research*, 4th ed., University of Chicago Press, 2016.
13. H. P. Stern, *The scientific publishing handbook: A practical guide to writing and publishing a scientific paper*, Springer, 2019.
14. F. Ecarnot, M.-F. Seronde, R. Chopard, F. Schiele and N. Meneveau, *Writing a scientific article: A step-by-step guide for beginners,* European Geriatric Medicine, 6 (2015) 573–579.
15. S. Gao, *A short comment on how to write research papers for STM journals,* Inorganic Chemistry Frontiers, 1 (2014) 518-520.
16. G. M. Whitesides, *Whitesides' Group: Writing a Paper,* Advanced Materials, 16 (2004) 1375-1377.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

1. Hands-on training for author/structure/CAS/subject/topic search on SciFinder, Scopus, Web of Science, and other search engines.
2. Drawing chemical structures and figures using chemistry software.
3. Analysing ^{1}H and ^{13}C NMR spectra using Mestrenova/Delta/TopSpin software and assign spectral details of all peaks in small organic molecules.
4. Analysing 2D NMR (COSY/HSQC/HETCOR) of small molecules using axis plotting and assigning cross peaks/diagonal peaks to obtain correlations.
5. Analysing safety data sheets for common laboratory chemicals.

6. *N* (*e.g.*, 60) replicate coloured solutions are tabulated with the corresponding absorbance values (*e.g.*, in the range of 0.440-0.470) can be given in a Table. Calculate mean, median, range, average deviation, relative average deviation, standard deviation, variance either by utilizing Excel/ORIGIN/MATLAB/Coding.
7. *N* (*e.g.*, 60) replicate coloured solutions are tabulated with the corresponding absorbance values (*e.g.*, in the range of 0.440-0.470) can be given in a Table. Draw a Histogram with frequency polygon.
8. Analysing UV-VIS data.
9. Analysing Fluorescence data.
10. Analysing FTIR data.
11. Analysing DLS data.
12. Analysing NMR data.
13. Analysing Diffraction data.
14. Draw a Graphical Abstract for a hypothetical paper using drawing software.
15. Write a formal "Experimental Section" for a synthesis performed in the lab, including full spectral characterization data formatting.
16. Prepare a Cover Letter to an Editor and format a manuscript file according to a specific journal's "Guide for Authors."
17. Prepare a supporting information for publication and Review Only.
18. Formatting of references using EndNote software.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. D. C. Finster, M. Gmurczyk, R. Bocwinski and R. H. Hill, *J. Chem. Edu.*, 2026, **103**, 7-9.
2. A. M. Coghill, and L. R. Garson (Eds.), The ACS style guide: Effective communication of scientific information, 3rd ed., American Chemical Society, 2006.
3. National Academies of Sciences, Engineering, and Medicine, Fostering integrity in research, The National Academies Press, 2019.
4. E. Wager and S. Kleinert, Good publication practice for communicating science and technology: An instructional manual, World Association of Medical Editors (WAME), 2011.
5. C. D. Manning, P. Raghavan and H. Schütze, Introduction to information retrieval, Cambridge University Press, 2008.
6. R. A. Day and A. L. Underwood, *Quantitative Analysis*, Prentice Hall/Pearson, 1991.
7. A. I. Vogel, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education, 2009.
8. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole (Cengage Learning), 2021.
9. I. Teraoka, *Polymer Solutions: An Introduction to Physical Properties*, John Wiley & Sons, 2002.

10. J. Torres and S. Bobst, *Toxicological Risk Assessment for Beginners*, Springer, 2015th Ed., 2015.
11. J. N. Miller and J. C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Publishers, 2018.
12. W. McKinney, *Python for Data Analysis,* O'Reilley Publishers, 2022.
13. W. C. Booth, G. G. Colomb and J. M. Williams, *The Craft of Research*, University of Chicago Press, 4th Ed., 2016.
14. H. P. Stern, *The Scientific Publishing Handbook: A Practical Guide to Writing and Publishing a Scientific Paper*, Springer, 2019.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Single Crystal X-Ray Diffraction CH-DSE-306	**04**	**03**	__	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To utilize the application of single crystal X-ray diffraction techniques in identifying the molecular and crystal structures of small molecules.
- To study the intermolecular interaction in the crystal lattice thereby covering some aspects of supramolecular chemistry.
- To learn hands on training on crystal structure solution and refinement.

Learning outcomes: At the completion of this course, the students should be able to:

- understand symmetry in crystallography, crystals systems, Bravais lattices, crystal symmetry, crystallographic point groups and space groups and Miller indices.
- learning about the data collection, data reduction, structure factors and Fourier syntheses, Phase problem, direct methods, Patterson method, crystal structure refinement.

THEORY COMPONENT **(3 Credits: 45 Hours)**

Unit-1: **(15 Hours)**

Introduction, 1D symmetry, Concept of 2D symmetry and lattices, notations of symmetry elements, space groups in 2D, 3D lattices, 32-point groups and their notations, stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams. Miller Indices, crystallographic planes and directions, close pack structures, linear density, planar density, Miller-Bravais indices for hexagonal systems, various ceramic structures (NaCl, ZnS, CaF_2, CsCl etc.)

Unit-2: **(15 Hours)**

Generation and classification of X-ray, X-ray sources, diffraction of X-rays, Bragg's law, the reciprocal lattice, reciprocal relationship, Bragg's law in reciprocal space, Ewald's sphere, Laue Method, Oscillation, rotation and precession methods.
L-P corrections, structure factor, scaling, interpretation of intensity data, temperature factor, symmetry from intensity statistics, structure factor and Fourier synthesis, Friedel's law; exponential, vector and general forms of structure factor, determination of systematic absences for various symmetry or lattice centering, FFT, Anomalous scattering.

Unit-3: **(15 Hours)**

Definition, Direct Methods, structure invariants and semi-invariants, probability methods, Phase determination in practice, Patterson Methods, Patterson Symmetry, completion of structure solution, ΔF synthesis.
Refinement by Fourier synthesis, refinement by ΔF synthesis, Refinement by least squares method, weighting functions, Goodness-Of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms.

References (Theory)

1. G. H. Stout and L. H. Jensen, *X-ray structure determination: A Practical Guide*, Wiley-Interscience, 2nd Ed., 1989.
2. C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti, *Fundamentals of Crystallography*, Oxford University Press, 2nd Ed., 2002.
3. J. D. Dunitz, *X-ray analysis and The Structure of Organic Molecules*, Wiley-VCH, New York, 2nd Ed., 1996.
4. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley-India Edition, 3rd Ed., 2009.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:
Techniques of growing crystals, crystal selection, indexing of crystals, data collection, data reduction, space group determination, structure solution and refinement using SHELXS97 and

SHELXL97, introduction to crystallographic packages (APEX II suite, OLEX2, WinGx, PLATON), Mercury 4.0 for visualization and IUCr validation of the data.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.,* 2009, **42**, 339–341.
2. C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, *J. Appl. Cryst.,* 2020, **53**, 226.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Organic Synthesis and Reagents CH-DSE-307	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To provide understanding of contemporary reaction strategies and reagents including greener approaches, such as reactions using microwave, ultrasonic and electrochemical assisted synthesis of compounds.
- To elaborate disconnection approach for the development of synthetic routes towards various simple and complex natural products and bioactive compounds.
- To strengthen the concepts of synthetic organic chemistry for the generation of complex organic structures that would promote job prospects in the pharmaceutical industry.

Learning outcomes: At the completion of this course, the students should be able to:

- apply modern synthetic reactions and reagents in organic synthesis.

- analyse mechanistic pathways of modern organic reactions.
- explain organic reactions involving sustainable Chemistry.
- design retrosynthetic approach for organic syntheses.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Modern Synthetic Reactions and Reagents **(15 Hours)**

Thermodynamic versus Kinetic enolates, enonate equivalents and enamines: Applications in carbon-carbon bond formation and related reactions.
Phosphorus, Sulphur and nitrogen ylides: Preparation, applications in organic synthesis and mechanism. Umpolung reactions (sulphur compounds, nitro compounds, lithiated ethers and related compounds). Principles and applications of phase transfer catalysis, crown ethers and polymer- supported reagents in organic synthesis. Reactions in ionic liquids, deep eutectic solvents, and aqueous medium, and electrochemical organic transformations.

Unit-2: Philosophy of organic synthesis **(15 Hours)**

Disconnection approach, one group and two group disconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional, 1,4-difunctional and 1,5-difunctional compounds. Tandem reactions, domino reactions and multi- component reactions. Principles of ultrasound and microwave-assisted organic synthesis.

Unit-3: Synthesis of Natural Products **(15 Hours)**

Retrosynthetic analysis and total synthesis natural products such as Gingerol, (z)-jasmone, prostaglandins E2, F2α, (L)-menthol, taxol, gandrisol, and (−)-epicatechin including their industrial methodology (wherever applicable).

References (Theory)

1. F.A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S., 2004.
2. W. Carruthers, *Modern Methods of Organic Synthesis*, Cambridge University Press, 1971.
3. K. C. Nicolaou and E. J. Sorensen, *Classics in Total Synthesis: Targets, Strategies and Methods*, Vol. I – IV, VCH Publishers.
4. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis- - An Introduction*, W. H. Freeman, 1st Edn., 2007.
5. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons, 1984.
6. T. Fuchigami, S. Inagi and M. Atobe, *Fundamentals and Applications of Organic Electrochemistry*, John Wiley & Sons Ltd., 2014
7. P. Wasserscheid, and T. Welton, *Ionic Liquids in Synthesis*, Wiley-VCH Verlag GmbH & Co. KGaA, 2007.

8. J. Fohrhop and G. Penzlin, *Organic Synthesis, Concepts, methods and starting materials*, Wiley-VCH Verlag GmbH, 1986.
9. R. K. Mackie, D. M. Smith and R. A. Aitken, *Guidebook to Organic Synthesis,* Pearson Education Ltd., 3rd Edn., 1999.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis and Characterisation of 5-acetyl-6-hydroxy-4-methyl-2H-chromen-2-one
2. Synthesis of organic compounds using eco-friendly tandem reactions
3. Synthesis of organic compounds using phase transfer catalysts
4. Synthesis of organic compounds using polymer supported reagents/catalysts.
5. Multicomponent Synthesis under Microwave and ultrasonic irradiations.
6. Electrochemical Assisted Synthesis of organic compounds
7. Organic reactions in ionic liquids and deep eutectic solvents.
8. Resolution of DL-Menthol

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. V. K. Ahluwalia and R. Aggarwal, *Comprehensive Practical Organic Chemistry*, University Press, 2000.
2. A. I. Vogel, *Elementary Practical Organic Chemistry Small Scale Preparations*, Pearson, 2nd Edn., 2010.
3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, CRC Press, 3rd edition, 2013.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		

Carbocyclic and Heterocyclic Compounds CH-DSE-308	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To provide understanding of structural features and chemical synthesis of various carbocyclic ring systems including small, medium and large sized rings.
- To elaborate important topics in chemistry as heterocyclic compounds that are widely present in clinical drugs.
- To describe modern methods of synthesis and characterization of heterocycles that will enhance the job opportunities in the pharmaceutical and fine-chemical industries.

Learning outcomes: At the completion of this course, the students should be able to:

- determine synthetic routes for various carbocyclic rings
- illustrate structure and reactions of different 3-5 membered heterocycles
- identify reaction methods for 6-membered and large heterocyclic rings
- evaluate synthetic methods for industrially important carbocycles and heterocycles

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Chemistry of carbocyclic compounds (15 Hours)

Introduction to Carbocycles: Definition, classification (monocyclic, fused, bridged, spiro), IUPAC nomenclature; overview of aromaticity and antiaromaticity.
Aromatic and Non-Aromatic Carbocycles: Aromatic stabilization energy; cyclopropenium, cyclopentadienyl, and tropylium ions; annulenes and their aromatic/antiaromatic nature.
Chemistry of non-benzenoid aromatics: Tropones. tropolones, azulenes.
Small Ring Compounds (3–4 Membered): Cyclopropane and cyclobutane – preparation, structure, ring strain, bond angles, and reactivity.
Medium and Large Rings (8–12 Membered): Synthesis, conformational flexibility, transannular interactions; Baldwin's rules; macrocyclic effects.
Cyclization reactions, ring expansion, and contraction reactions for the synthesis of carbocyclic compounds
Fused and bridged ring systems: Structure and stereochemistry of bicyclic systems (norbornane, adamantane, hydrindane); reactivity and rearrangements.
Caged molecules: Structure, synthesis and reactivity.
Cyclophanes and annulenes: Structure, synthesis, aromaticity, and reactivity of cyclophanes; concept of through-space conjugation.
Catenanes and rotaxanes: Structure, synthesis and reactivity.
Modern synthetic approaches: Transition-metal catalyzed cyclizations; pericyclic reactions (electrocyclic ring closures, Diels–Alder cycloadditions); current applications.

Unit-2: Chemistry of Three to Five-Membered Heterocyclic Compounds (15 Hours)

Nomenclature, spectral characteristics, reactivity and aromaticity
Synthesis and reactions of three and four-membered heterocycles: *e.g.* aziridine, azirine, azetidine, oxiranes, thiarines, oxetenes and thietanes.
Five-membered rings with two and three heteroatoms: pyrazole, imidazole, oxazole, isooxazole, thiazole, isothiazole, triazole, oxadiazole, and thiadiazole.
Benzofused five-membered heterocycles with one heteroatom: indole, benzofuran, benzothiophene.
Chemistry of bicyclic compounds containing one or more heteroatoms.

Unit-3: Chemistry of six-membered and large-membered Heterocyclic Compounds (15 Hours)

Benzofused six-membered rings with one, two and three heteroatoms: benzopyrans, quinolines, isoquinolines, quinoxazalines, acridines, phenoxazines, phenothiazines, benzotriazines, and pteridines.

Seven and large membered heterocycles: azepines, oxepines, thiepines, diazepines, benzodiazepine, benzooxepines, azocane, oxacane, thiocane, azocine, diazocine, benzodiazocine, dioxocine and dithiocine.

References (Theory)

1. F. J. McQuillin and M. S. Baird, *Alicyclic Chemistry*, Cambridge University Press, 2nd Edn., 1983.
2. J. March, *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, Wiley, New York, 1992.
3. A. Goel, R. Pratap and V. J. Ram, *Isolated Pyranones: Multifaceted Building Blocks for Molecular Diversity*, Elsevier, 2022.
4. V. J. Ram, R. Pratap and P. Yadav, *Fused Pyranones: Multifaceted Building Blocks for Molecular Diversity*, Elsevier, 2024.
5. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, Springer, 2007.
6. R. T. Morrison and R.N. Boyd, *Organic Chemistry*, Prentice Hall, 2018.
7. J. Clayden, N. Greeves and S. Warren, "Organic Chemistry", Oxford University Press, 2nd edn., 2012.
8. V. J. Ram, A. Sethi, M. Nath and R. Pratap, *The Chemistry of Heterocycles (Nomenclature and Chemistry of three to five-membered Heterocycles)*, Elsevier, 2019.
9. V. J. Ram, A. Sethi, M. Nath and R. Pratap, *The Chemistry of Heterocycles (Chemistry of six to eight membered N, O, S, P and Se heterocycles)*, Elsevier, 2019.
10. R. M. Acheson, *Introduction to the Chemistry of Heterocyclic Compounds*, John Wiley & Sons, 1976.
11. R. K. Parashar and B. Negi, *Chemistry of Heterocyclic Compounds,* Ane books Private Ltd., 2016.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Synthesis and Characterisation of following Heterocyclic compounds:
Benzimidazole, Benzotriazole, Benzofuran, Benzopyrone, Benzothiophene, 7-Hydroxy-4-methyl-coumarin, [2H]-Chromene, 3,5-Dimethylpyrazole, 2,5-Dimethylfurane, 2,3-diphenylquinoxaline, Indole, 1,2,3,4-Tetrahydrocarbazole.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. V. K. Ahluwalia and R. Aggarwal, *Comprehensive Practical Organic Chemistry*, University Press, 2000.
2. A. I. Vogel, *Elementary Practical Organic Chemistry Small Scale Preparations*, Pearson, 2nd Edn., 2010.
3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, CRC Press, 3rd edition, 2013.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry of Biomolecules **CH-DSE-309**	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To provide the knowledge of the structure, function, and physicochemical properties of biomolecules that will enable the students to understand the physiological significance of these organic molecules in biosystems.

- To elaborate the synthesis of oligosaccharides, peptides and oligonucleotides as contemporary therapeutics and the structure characterization of these complex organic skeletons that would enhance job opportunity of students in pharmaceutical industries and forensic science laboratories.

Learning outcomes: At the completion of this course, the students should be able to:

- understand the structure and function relationship of biomolecules
- explain the chemistry of carbohydrates, lipids, peptides and nucleic acids
- apply concepts of organic chemistry for the chemical synthesis of the biomolecules
- analyse biomolecules using qualitative and quantitative methods

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Chemistry of Carbohydrates and Lipids (15 Hours)

Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, sugar methyl ethers and acid derivatives of sugars, chemical glycosylation methods with concepts of stereocontrolled and regiocontrolled synthesis, application of oligosaccharide synthesis for the development of drugs and vaccines, polysaccharides of industrial and biological importance, dextran, chemistry of sialic acids, heparin, chondroitin sulfate, cell-cell recognition, blood group substances, peptidoglycans, applications in therapeutics.
Classification of lipids, even chain and odd chain (saturated and unsaturated) fatty acids, structural notation, essential fatty acids, phospholipids, glycerophospholipids, sphingolipids, chemical composition and structure of biological membranes, lipid aggregates, Fluid Mosaic model.

Unit-2: Chemistry of Proteins (15 Hours)

Quaternary structure, Ramachandran Plot, composition and structure of collagen, protein stability, Posttranslational modifications, Protein folding and misfolding, chaperons, Classification of naturally occurring peptides, depsipeptide, cyclic and stapled peptides, peptide alkaloids with examples, Sequence determination by mass spectral methods, Modern methods of peptide synthesis with protection and deprotection, Automated solid phase peptide synthesis, problem of racemisation, combinatorial synthesis of peptides, Chemistry of oxytocin, valinomycin, enkephalins, self-assembly and aggregation of peptides.

Unit-3: Chemistry of Nucleic Acids (15 Hours)

Polymorphic nature of DNA and RNA, post-transcriptional modifications (5′-capping, splicing, 3′-polyadenylation), stabilising forces, denaturation, multiple hydrogen-bonding patterns, multistranded DNA structures, sequence determination by chemical and enzymatic methods, genome sequencing, chemical synthesis of DNA, solid phase synthesis, phosphodiester-triester and phosphite methods, phosphoramdite approach, automated DNA synthesizers, purification of oligonucleotides, HPLC and gel electrophoresis. Introduction to PNA, LNA, UNA.

References (Theory)

1. M. Bodanszky, *Peptide Chemistry: A Practical Textbook*, Springer-Verlag, 2nd Ed., (1993).

2. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer-Verlag, 2012.
3. D. L. Nelson and M. M. Cox, *Lehninger Principles of Biochemistry*, W. H. Freeman & Co; 8th ed., 2021.
4. J. M. Berg, G. Gatto Jr., J. Hines, L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman & Co., 10th Ed., 2023.
5. D. Voet and J. G. Voet., *Biochemistry*, Wiley, 4th Ed., 2010
6. R. P. Sinden, *DNA Structure and Function*, Academic Press, 1994.
7. W. Saenger, *Principles of Nucleic Acid Structure*, Springer-Verlag, 1984.
8. S. Neidle and M. Sanderson, *Principles of Nucleic Acid Structure*, Elsevier, 2nd Ed., 2021.
9. M. J. Gait, *Oligonucleotide Synthesis: A Practical Approach*, IRL Press, 1984.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Qualitative tests for disaccharides (Barfoed's Test) and polysaccharides (starch and glycogen)
2. Quantitative Estimation of Reducing Sugars.
3. Isolation of lipids using acetone or a chloroform: methanol mixture (Folch method). Acetone.
4. Qualitative identification of lipids using edible oils or ghee (solubility (Emulsion test), saponification, and acrolein tests).
5. Unsaturation testing of phospholipids from edible oils and their ^{31}P NMR analysis.
6. Acid value/peroxide value of oil
7. Separation of Phospholipids by TLC
8. Determination of phospholipid/ cholesterol ratio from egg yolk.
9. Isolation and spectroscopic characterization of DNA.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. D. T. Plummer, *An Introduction to Practical Biochemistry*, Tata McGraw-Hill, 3rd ed.,1990.
2. W. W. Christie, and X. Han, *Lipid Analysis: Isolation, Separation, Identification and Lipidomic Analysis*, Elsevier, 2016.
3. M. I. Gurr, J. L. Harwood, K. N. Frayn, D. J. Murphy and R. H. Michell, *Lipids: Biochemistry, Biotechnology and Health*, Wiley-Blackwell, 6th ed., 2016.
4. J. Jayaraman, *Laboratory Manual of Biochemistry,* New Age International Publishers, 2011.
5. G. Sattanathan, S.S. Padmapriya and B. Balamuralikrishnan, *Practical Manual of Biochemistry*, Skyfox Publishing Group, 2020.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Drug Delivery and Pharmaceutical Technologies **CH-DSE-310**	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To provide the knowledge of drug delivery technology including polymers and nanomaterial used in encapsulations, various drug formulation methods and drug load determination.
- To elaborate the process of lead identification, further lead optimisation for development of drugs through Clinical trial steps.
- To provide detailed understanding of scale up processes for the commercially available drugs currently employed in pilot plants that will enhance job opportunities in the pharmaceutical industries.

Learning outcomes: At the completion of this course, the students should be able to:

- drug designing and development, their SAR and QSAR.
- mode of action of different drugs.
- role of drugs to inhibit the particular enzymes and treatment of disease.
- drug delivery and pharmaceutical technologies development

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Drug Delivery Technologies (15 Hours)

Importance of Targeted Drug Delivery, Efficacy, Safety and Toxicity Issues. Molecular basis of targeted drug delivery. Drug Release and Uptake Phenomenon. Drug Encapsulation Technologies. Different Carriers for Drug Encapsulation. Nanomaterials (metal-based, metal oxide based and polymeric) in drug encapsulation and drug delivery - characterization, generation, efficacy, toxicity and release profile. Factors affecting drug loading and drug release. Techniques to measure degree of loading and release efficiency. Metabolism and excretion of drug delivery carriers.

Unit-2: Lead identification, optimization and clinical technology (15 Hours)

General considerations, Methods of preparations, characterization and applications of liposomes, ionosomers, resealed erythrocytes, nanoparticulate systems, solid-liquid nanoparticles, dendrimers, organogels, multiple emulsions and nanoemulsions. Overview and application of aquasomes, pharmacosomes, liquid crystalline systems, protein and peptide-based drug delivery systems. Polymers in drug encapsulation and drug delivery: Classification, synthesis and applications of biodegradable and natural polymers in formulation of controlled drug delivery systems. Drug discovery, lead identification and lead optimization, chemical, pharmaceutical and clinical technology development.

Unit-3: Pharmaceutical Technologies Development (15 Hours)

Investigational New Drug (IND) and its applications - criteria, contents, categories, submission, regulation, noteworthy examples. Clinical trials - Phase I, II and III clinical trials. Pilot Plant Scale-Up Techniques- Primary function of the pharmaceutical pilot plant, factors to be considered during development, reporting responsibilities, personnel requirements, space requirements, review of the formula, raw materials, relevant processing equipment, production rates, process evaluation, master manufacturing procedures, GMP consideration, pilot plant design for tablet development.

References (Theory)

1. E. Mathiowitz, Encyclopaedia of controlled delivery 1999.
2. R. Joseph and V. H. L. Lee, *Controlled Drug Delivery – Fundamentals and Applications*, 2nd Ed. 1987.
3. W. M. Saltzman, *Drug Delivery: Engineering Principles and Drug Therapy*, Oxford Press.
4. L. V. Allen Jr., N. G. Popovich and H. C. Arsel, *Ansel's Pharmaceutical Dosage Forms and Drug Delivery Systems*, Lippincott Williams & Wilkins, 2013.
5. L. V. Allen, *The Art, Science and Technology of Pharmaceutical Compounding*, McGraw-Hill Medical, 2002
6. R. K. Khar, *Lachman Liebermans' The Theory and Practice of Industrial Pharmacy*, CBS Publishers and Distributors Pvt. Ltd., 4th Ed., 2020

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Formulation of Polymeric Nanoparticles
2. Preparation of Microparticles / Microspheres
3. Preparation of Hydrogels
4. Formulation of Transdermal Drug Delivery Systems
5. Mucoadhesive Drug Delivery System

6. Solid Lipid Nanoparticles (SLNs)
7. Controlled-Release Tablet Formulation
8. Characterization Techniques; FTIR for drug–excipient compatibility, UV–Vis spectroscopy for concentration analysis, DSC / TGA for thermal analysis, SEM for surface morphology

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. P. Khirwadkar, S. S. Babu, I. M. Kumaar, P. Jahnavi and R. V. *Khandeshi Textbook of Novel Drug Delivery Systems*, Shashwat Publication, 2024.
2. M. Chhikara and S. Narwal, *Drug Delivery System: Design, Development & Evaluation Technologies*, Jec publication, 2025.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Polymer Science: Structure, Kinetics and Smart Materials CH-DSE-311	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:
- Understand the structural and conformational behavior of polymer chains in ideal and real systems.
- Analyse thermodynamic, morphological, and phase properties of polymer solutions, melts, blends, and copolymers.
- Apply theoretical models to describe molecular motion, dynamics, and crystallization, including thermal transitions (Tg and melting).

- Understand polymerization kinetics and the applications of stimuli-responsive (smart) polymers.

Learning outcomes: At the completion of this course, the students should be able to:

- explain polymer chain models (ideal and real), scaling laws, excluded volume effects, and analyse polymer motion in solutions using theoretical and experimental approaches.
- interpret thermodynamic properties, phase behavior, and structural features of polymer systems, including solutions, melts, blends, copolymers, gels, and elastomers.
- evaluate microstructure, crystallization, polymerization kinetics, and the functional behavior of smart polymers for advanced applications.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Polymer Physics and Thermodynamics (15 Hours)

Overview and classification of polymers, Properties of an isolated polymer molecule: Ideal chain, Freely-jointed Gaussian chain, Distribution of segments in polymer chain, non-ideal chain, excluded volume, Dimension of real chains and scaling laws, Self-avoiding walk.
Concentrated solution and melts: Thermodynamic properties of polymer solutions, concentration fluctuation in polymer solutions, polymer blends, block copolymer.
Polymer gels: Elasticity of rubber, Stress optical law, interaction between partial chains, swelling of gels.

Unit-2: Polymer Dynamics and Microstructure (15 Hours)

Molecular motion of polymers in dilute solution: General theory of Brownian motion, Rouse and Zimm Bead Spring models, hydrodynamics interactions, dynamic light scattering.
Polymer microstructure: Microstructure based on chemical structure and geometrical structure. Meaning of glass transition temperature (Tg), factors influencing the glass transition temperature, importance of glass transition temperature Tg and molecular weight, Tg and melting point.

Unit-3: Liquid Crystals and Optical Materials (including Non Linear) (15 Hours)

Structure of macromolecules: Polymer crystals: crystallization in polymers, factors determining crystal structure. Morphology of solution grown single crystal and bulk grown crystal. Semicrystalline polymers: spherulites, degree of crystallinity, crystallization and melting. Kinetics of crystallization. Molecular mechanism of crystallization, factors affecting melting.
Kinetics of polymerization: Kinetics and statistics of step growth polymerization, size distribution in linear polymers, nonlinear polymerization and prediction of gel point. Kinetics of free radical chain polymerization, cationic polymerization, anionic polymerization and polycondensation.
*Stimuli-sensitive (smart) polymers: light, p*H- and temperature-sensitive smart polymers and their applications.

References (Theory)

1. I. Teraoka, *Polymer Solutions*, Wiley-Interscience, John Wiley & Sons Inc., 2002.
2. R. J. Young and P. A. Lovell, *Introduction to Polymers*, 2nd edn, Chapman & Hall, 1991.
3. S. R. Sandler, W. Karo, J. Bonesteel and E. M. Pierce, *Polymer Synthesis and Characterization: A Laboratory Manual*, Academic Press, New York, 1998.
4. P. A. Lovell and M. S. El-Aasser, *Emulsion Polymerization and Emulsion Polymers*, Wiley, 1997.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis of polymer colloidal particles via emulsion polymerization.
2. Examination of the Tyndall effect in the prepared colloidal polymer dispersions.
3. Execution of addition and condensation polymerization reactions.
4. Structural characterization of synthesized or supplied polymers.
5. Determination of polymer molecular weight using the viscosity method.
6. Study of radical polymerization under varying concentrations of chain-transfer agents and initiators.
7. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and assessment of head-to-head monomer linkages.
8. Thermal analysis of the given polymer using DSC, including determination of its glass transition temperature (Tg).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. I. Teraoka, *Polymer Solutions*, Wiley-Interscience, John Wiley & Sons Inc., 2002.
2. R. J. Young and P. A. Lovell, *Introduction to Polymers*, 2nd edn, Chapman & Hall, 1991.
3. S. R. Sandler, W. Karo, J. Bonesteel and E. M. Pierce, *Polymer Synthesis and Characterization: A Laboratory Manual*, Academic Press, New York, 1998.
4. P. A. Lovell and M. S. El-Aasser, *Emulsion Polymerization and Emulsion Polymers*, Wiley, 1997.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Electrochemistry CH-DSE-312	**04**	**03**	**__**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- Develop understanding of the electrode–solution interface, electric double layer models, and thermodynamics of electrified interfaces.
- Introduce equivalent circuit models and mathematical tools for analyzing electrochemical systems and transient responses.
- Explain electrode kinetics, electron transfer, adsorption phenomena, and mass transport mechanisms.
- Apply experimental and transient techniques (e.g., voltammetry, chrono-methods, impedance spectroscopy) to study electrochemical reactions and mechanisms.

Learning outcomes: At the completion of this course, the students should be able to:

- analyse the electrode–solution interface using electric double layer models and equivalent circuit/Laplace methods.
- apply electrode kinetics concepts (Butler–Volmer, Tafel, Marcus) and evaluate adsorption and mass transport processes.
- interpret electrochemical data using techniques such as chronoamperometry, chronopotentiometry, cyclic voltammetry, and impedance spectroscopy.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Fundamentals & Electric Double Layer (15 Hours)

Nature of Electrode Solution Interface, Faradaic and Non-faradic Processes, Ideal Polarizable Electrode, Potentials, Fermi Energy, and Absolute Potential, Equivalent Circuit Models-Series and Parallel RC Circuits, Potential Step, Current Step, Potential Ramp and Sinusoid, Method of Laplace transform and its application in Electrochemistry.

Adsorption and Electric Double Layer: Thermodynamics of the double layer, Electrocapillary phenomena; Structure of electrified interfaces - Helmholtz, Gouy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models.

Unit-2: Electrode Kinetics & Heterogeneous Electron Transfer (15 Hours)

Electrode Kinetics: Overpotentials, Exchange current density and transfer coefficient, Derivation of Butler-Volmer equation and its physical implications, Tafel plot, Multistep electrode reactions; Marcus microscopic model of electron transfer. Inner-Sphere Electrode Reactions and Electrocatalysis.

Mass transfer by diffusion, Migration, Convection, and electrode surface constraints. Adsorption – Ionic and organic molecules, Adsorption isotherms-Langmuir, Frumkin, Temkin; Experimental evaluation of surface excesses and electrical parameters.

Unit-3: Relaxation Methods and Transient Techniques (15 Hours)

Constant Potential Chronoamperometry: Reversible and quasi-reversible charge transfer, Cottrell equation, Influence of uncompensated solution resistance, Reversible charge transfer, Application of cyclic voltammetry for characterization of various electrochemical processes.
Constant Current Chronopotentiometry: Reversible and quasi-reversible charge transfer, Sand equation.
Impedance Methods: Reversible and quasi-reversible charge transfer, Warburg equation, Influence of uncompensated solution resistance.

References (Theory)

1. A. J. Bard, L. R. Faulkner and H. S. White, *Electrochemical Methods: Fundamentals and Applications*, 3rd edn, John Wiley & Sons, New York, 2022.
2. K. B. Oldham, J. C. Myland and A. M. Bond, *Electrochemical Science and Technology: Fundamentals and Applications*, John Wiley & Sons Ltd., 2012.
3. J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry 1: Ionics*, 2nd edn, Springer, 1998.
4. J. O'M. Bockris, A. K. N. Reddy and M. E. Gamboa-Aldeco, *Modern Electrochemistry 2A: Fundamentals of Electrodics*, 2nd edn, Springer, 2001.
5. V. S. Bagotsky, Fundamentals of Electrochemistry, Wiley, Hoboken, 2nd edn., 2006.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

Cyclic Voltammetry (CV):

1. Verify the Randles-Sevcik equation for cyclic voltammetry. Use a reversible system (10 mM mixture of $K_3[Fe(CN)_6]$ and $K_4[Fe(CN)_6]$ in 2M KCl). Identify the peak current and peak potential at different scan rates.
2. Verify the reversibility of the Fe^{2+}/Fe^{3+} system by using the ratio of cathodic and anodic peak currents.
3. Find the quantities such as:
   i. formal potential (E^0)
   ii. number of electrons transferred
   iii. diffusion coefficient (D)

iv. area (A) and concentration (C) by using CV.

4. Record the effect of supporting electrolyte concentration on CV.
5. Chronocoulometry:
   i. Verify the Anson equation using potential step chronocoulometry.
   ii. The surface area of an electrode is determined via a chronocoulometric measurement.
6. Chronopotentiometry:
   i. Verify Sand equation by measuring transition times under galvanostatic conditions.
7. Impedance:
   i. Verify Waburg equation using electrochemical impedance spectroscopy.
   ii. Determine the exchange current density and double layer capacity of a redox reaction using platinum electrode. (Aqueous solution of 10 mM $Fe(NH_4)_2(SO_4)_2$ + 1 M $HClO_4$)

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. R. Holze, *Experimental Electrochemistry: A Laboratory Textbook*, WILEY-VCH; 2009.
2. A. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, Wiley, New York, 2nd edn., 2001.
3. R. G. Compton and C. E. Banks, Understanding Voltammetry, Imperial College Press, London, 2nd edn., 2011.
4. N. Elgrishi, K. J. Rountree, B. D. McCarthy, E. S. Rountree, T. T. Eisenhart and J. L. Dempsey, J. Chem. Educ., 2018, 95, 197–206.
5. D. K. Gosser Jr., Cyclic Voltammetry: Simulation and Analysis of Reaction Mechanisms, VCH, New York, 1993.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		

Advanced Statistical Mechanics CH-DSE-313	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- Develop understanding of the grand canonical ensemble and partition functions for thermodynamic systems, including translational, rotational, and vibrational motions.
- Analyse imperfect gases using cluster integrals, virial expansion, and related corrections.
- Introduce the Ising model, lattice statistics, and key approximation methods in statistical mechanics.
- Understand distribution and correlation functions in fluids and basic simulation techniques such as Monte Carlo and molecular dynamics.

Learning outcomes: At the completion of this course, the students should be able to:

- derive and apply partition functions in the grand canonical ensemble to evaluate thermodynamic properties of systems, including translational, rotational, and vibrational motions.
- analyse imperfect gases using cluster integrals, virial coefficients, and activity expansions.
- apply statistical models such as the Ising model and mean-field approximations to study interacting systems.
- interpret distribution and correlation functions in fluids and use basic computational methods such as Monte Carlo and molecular dynamics simulations.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Statistical Mechanics of Real Gases (15 Hours)

Grand Canonical Ensemble, Derivation of Partition function and calculation of different thermodynamic properties. Classical and Quantum partition functions for translation, rotation and vibration and their relation. Equation of state of an imperfect gas, Partition functions and cluster integrals, Pressure of gas expressed as a power series in activity, Irreducible cluster integrals, Virial expansion for a gas, and Calculation of Virial coefficients of an imperfect gas.

Unit-2: Statistical Mechanics of Lattice Systems (15 Hours)

One-dimensional Ising Model. Nearest neighbor lattice statistics. Derivation of Partition function and its relation with the relevant thermodynamic properties. Ising model of a ring with periodic boundary conditions. Lattice gas and Binary alloy. Mean field approximation. Bragg Williams approximation.

Unit-3: Statistical Mechanics of Fluids (15 Hours)

Definition of distribution and correlation functions. Thermodynamic properties of a fluid and the radial distribution function, Potential of mean force and the superposition approximation, Basics of computer simulation methods and models of intermolecular potentials. Monte Carlo and Molecular dynamics simulations.

References (Theory)

1. D. A. McQuarrie, *Statistical Mechanics*, Viva Books Pvt. Ltd., New Delhi, 2003.
2. T. L. Hill, *Statistical Mechanics: Principles and Selected Applications*, Dover Publications Inc., New York, 1987.
3. B. Bagchi, *Statistical Mechanics for Chemistry and Materials Science*, CRC Press, 2018.
4. L. D. Landau and E. M. Lifshitz, *Statistical Physics*, vol. 5, part 1, 3rd edn, Pergamon Press, 1980.
5. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford Science Publications, Oxford, 1987.
6. K. Huang, *Statistical Mechanics*, John Wiley & Sons, New York, 1987.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).
2. Elements of the C/C++/FORTRAN/BASIC languages, including strings and graphics.
3. Decimal-binary conversion
4. Numerical differentiation, quadrature and finding roots
5. Intrapolation & interpolation of data
6. Calculate Entropy (*S)* from *Cp* data
7. Calculate Enthalpy (*H*) from *Cp* data
8. Calculate Free Energy (*G*) from *Cp* data
9. Verification of Nernst Heat Theorem
10. Gauss-Siedel method and its use in solving simultaneous equations (e.g. Lambert-Beer's law)

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. D. A. McQuarrie, Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi, 2003.
2. T. L. Hill, Statistical Mechanics: Principles and Selected Applications, Dover Publications Inc., New York, 1987.
3. B. Bagchi, Statistical Mechanics for Chemistry and Materials Science, CRC Press, 2018.

4. L. D. Landau and E. M. Lifshitz, Statistical Physics, vol. 5, part 1, 3rd edn, Pergamon Press, 1980.
5. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford Science Publications, Oxford, 1987.
6. K. Huang, Statistical Mechanics, John Wiley & Sons, New York, 1987.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Radiation and Photochemistry with Applications CH-DSE-314	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives: Students will understand and explain

- Key principles of molecular photochemistry, radiationless transitions
- Radiation dosimetry, and flash photolysis, and will be introduced to theories of multiphoton and reversible energy transfer

Learning outcomes: At the completion of this course, the students should be able to

- learn the principles and applications of advanced molecular photochemistry and radiation chemistry.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Molecular Photochemistry (15 Hours)

Transitions between states (Chemical, classical and quantum dynamics, vibronic states). Potential energy surfaces; transitions between potential energy surfaces, The Franck-Condon Principle and radiative transitions. A classical model of radiative transitions. The absorption and emission of light - state mixing, spin-orbit coupling and spin forbidden radiative transitions, absorption complexes, delayed fluorescence and phosphorescence.

Unit-2: Photophysical radiationless transitions (15 Hours)

Wave mechanical interpretation of radiationless transitions between state factors that influence the rate of vibrational relaxation. Energy transfer: Theory of radiationless energy transfer, energy transfer by electron exchange: An overlap or collision mechanism. The role of energetics in energy transfer mechanism. Diffusion controlled quenching. The Perrin formulation. Triplet-triplet, triplet-singlet, singlet-triplet energy transfer. Multiphoton energy transfer processes, reversible energy transfer.

Unit-3: Radiation Chemistry, Dosimetry and Photolysis (15 Hours)

G-value. The mechanism of interaction of high energy radiation with matter, Photoelectric effect, Compton effect, Pair production, total absorption co-efficient, excitation and ionization, Stopping power and linear energy transfer.

Radiation dosimetry: Radiation dose and its measurement, standard free air chamber method, chemical dosimeter (Frick's Dosimeter). Short lived intermediates (ions, excited molecules, free radicals: Various mechanisms of their formation and energy transfer processes).

Flash photolysis: Principle and its applications. Radiolysis of water and aqueous solutions. Radiolysis of molecules of biological interest (carbohydrates, amino acids, peptides, and nucleic acids).

References (Theory)

1. N. J. Turro, *Modern Molecular Photochemistry*, University Science Books, 1991.
2. A. Gilbert and J. Baggott, *Essentials of Molecular Photochemistry*, Blackwell Scientific, 1990.
3. P. W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edn, Oxford University Press, 2006.
4. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, 3rd edn, University Science Books, 2001.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Recording absorption and emission spectra of different fluorescent dyes (e.g., fluorescein, rhodamine or other dye molecules) and determining Stokes shifts.
2. Measurement of fluorescence quantum yield of dyes using a reference standard.
3. Evaluation of solvent effects on fluorescence emission spectra of a dye in polar vs. non-polar solvents.
4. Evaluation of CMC of surfactant molecules (Cationic, anionic and neutral) using fluorescence spectroscopy.
5. Dynamic and static quenching studies using a suitable dye-quencher pair; calculation of quenching constants.

6. Dynamic and static quenching studies in heterogenous medium and calculation of quenching constants.
7. Determine energy transfer efficiency between donor-acceptor dye pairs.
8. Study intrinsic tryptophan fluorescence to monitor protein folding/unfolding.
9. Effect of pH on the fluorescence properties of pH-sensitive molecules.
10. Record the fluorescence spectra of a weak acid (α-naphthol or others) at different pH and determine the dissociation constant in the excited state.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Edn., Springer, 2006.
2. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, Springer, New York, 3rd edn., 2006.
3. J. N. Demas, *Excited State Lifetime Measurements*, Academic Press, New York, 1983.
4. D. M. Jameson, *Introduction to Fluorescence*, CRC Press, Boca Raton, 2014.
5. B. Valeur and M. N. Berberan-Santos, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH, Weinheim, 2nd edn., 2012.
6. C. A. Parker, *Photoluminescence of Solutions*, Elsevier, Amsterdam, 1968.
7. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, Wiley, Chichester, 2nd edn., 2009.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Physical Chemistry of Materials CH-DSE-315	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- Introduce fundamental concepts of nanomaterials (including quantum confinement) and diffraction techniques.

- Explain superconductivity, types of superconducting materials, and multiphase materials such as ferrous and non-ferrous alloys.
- Provide understanding of liquid crystals and optical materials, including nonlinear properties.
- Develop basic knowledge of materials used in solid-state devices.

Learning outcomes: At the completion of this course, the students should be able to:

- understand nanoscience concepts, including synthesis approaches, exciton Bohr radius, and quantum confinement, and apply diffraction techniques for structural analysis.
- explain superconductivity (BCS theory, high Tc materials) and phase transformations in ferrous and non-ferrous alloys.
- describe liquid crystals, their types and transitions, and the principles of optical materials (semiconducting, lanthanide-doped, organic).
- understand nonlinear optical materials and their applications in solid-state devices.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Nanoparticles and Diffraction Methods (15 Hours)

Introduction to nanomaterials: classification and size-dependent properties, Quantum dots: band gap, excitons, quantum confinement effect, Bohr radius, Optical and electronic properties of low-dimensional systems, Applications of quantum dots in electronics, sensing, and biomedicine.
Synthesis and Stabilization of Nanomaterials: Top-down and bottom-up approaches, Chemical methods for nanoparticle synthesis (reduction, sol–gel, hydrothermal, etc.), Self-assembly processes and supramolecular organization, Role of capping agents, surfactants, and stabilizers, Factors affecting size, shape, and stability of nanoparticles.
Reactivity and Catalysis in Nanomaterials: Surface chemistry and high surface-to-volume ratio effects, Reactivity of nanoparticles and size-dependent catalytic activity, Heterogeneous catalysis using nanomaterials, Applications in environmental and industrial catalysis.
Green Chemistry and Sustainable Materials: Principles of green synthesis and clean technologies, Use of green solvents: supercritical fluids and ionic liquids, Green catalysts and eco-friendly synthetic routes, Applications: auto-exhaust catalysts, pollution control, sustainable materials.
Diffraction Techniques and Materials Characterization (Overview): Basic concepts of diffraction and scattering (no detailed crystallography), Powder X-ray diffraction: principle and applications, Debye–Scherrer equation for crystallite size estimation. Williamson–Hall analysis for lattice strain, Brief comparison with electron and neutron diffraction techniques.
Band theory of solids: conductors, semiconductors, and insulators, Density of states and band gap engineering, Defects in solids and their influence on material properties, Introduction to optical and electronic characterization methods

Unit-2: Superconductivity and Multiphase Materials (15 Hours)

Superconductivity: Conventional Superconductors; Types of Superconductive Materials, Magnetic Properties, BCS Theory; High temperature superconductors, Cuprates- & Iron superconductors; Theory of High Tc superconductors; Uses of high temperature Superconductors; Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials.

Organic solids, fullerenes, molecular devices: Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes - doped fullerenes as superconductors.

Multiphase Materials: Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications

Unit-3: Liquid Crystals and Optical Materials (including Non Linear) (15 Hours)

Liquid crystals: Mesomorphic behavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Types and mechanism of optical materials (semiconducting, lanthanide doped and organic emitting); Transition through various energy levels and understanding through Franck-Condon principle, Jablonsky diagram etc.; radiative and non-radiative emission and life time analysis.

Nonlinear optical materials: nonlinear optical effects, second and third order- molecular hyperpolarizability and second order electric susceptibility- materials for second and third harmonic generation.

Materials for solid-state devices: Rectifiers, transistors, capacitors IV-V compounds, low-dimensional quantum structures; optical properties. artificial photosynthetic devices, optical storage memory and switches- sensors.

References (Theory)

1. C. N. R. Rao, A. Müller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH GmbH & Co., 2007.
2. G. Cao, *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, Imperial College Press, London, 2011.
3. W. D. Callister, *Materials Science and Engineering: An Introduction*, 10th edn, Wiley, 2018.
4. G. W. Gray (ed.), *Thermotropic Liquid Crystals*, John Wiley, 1987.
5. N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Saunders College Publishing, 1976.
6. H. V. Keer, *Principles of the Solid State*, Wiley Eastern, 1993.
7. J. M. G. Cowie, *Physics and Chemistry of Polymers*, 3rd edn, Blackie Academic and Professional, 2007.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Preparation of semiconducting CdSe, ZnSe, In_2S_3 (any of one) nanomaterials by any soft chemical approach (emulsion based, co-precipitation etc.).
2. Determination of crystal phase, calculation of crystallite size and lattice strain using powder diffraction pattern of any prepared or known sample.
3. Preparation of any metallic nanoparticle (for example Ag, Cu, Ni-any of one) using standard reducing and capping agent.
4. Preparation of a liquid crystals using soft chemical route.
5. Determination of band gap of a semiconducting nanoparticle (in solution) using UV visible spectrophotometer.
6. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).
7. Measurement of photoluminescence properties of semiconducting nanomaterials (at least one) using fluorescence spectroscopy.
8. Measurement of photoluminescence properties of lanthanide doped nanomaterials using fluorescence spectroscopy.
9. Studying photocatalytic degradation of environmentally pollutant dye (Crystal Violet, Rhodamine B, methyl orange etc.) by any semiconducting (In2S3, CdSe, ZnO- any of one) or metallic nanoparticles under visible light irradiation and using UV-Visible spectrophotometer.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. C. N. R. Rao, A. Müller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH GmbH & Co., 2007.
2. J. N. Gurtu, *Advanced Physical Chemistry Experiments*, Pragati Publications, 2008.
3. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, 18th edn, R. Chand & Co., New Delhi, 2018.
4. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 2nd edn, 1999.
5. C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, 4th edn, 2017.
6. W. Kemp, *Organic Spectroscopy*, 3rd edn, 2002.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Structure, Dynamics and Spectroscopy of Biomolecules CH-DSE-316	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- Introduce chemical bonding, thermodynamics, and structural principles in biological macromolecules, including amino acids, proteins, and nucleic acids.
- Explain biomolecular structures and their stabilizing interactions.
- Describe separation and characterization techniques such as chromatography, electrophoresis, and spectroscopic/scattering methods.
- Develop understanding of computational modelling of macromolecules using molecular mechanics and dynamics.

Learning outcomes: At the completion of this course, the students should be able to:

- analyse biomolecular structures, including proteins and nucleic acids, and their conformational properties.
- apply separation techniques such as chromatography, electrophoresis, and ultracentrifugation.
- perform basic modelling and simulation of macromolecules using energy minimization and molecular dynamics.
- interpret data from spectroscopic, scattering, and optical methods for biomolecular studies.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1 **(15 Hours)**

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; polypeptide chain geometries and internal rotational angles; Ramachandran plots; Structures of nucleic acids. Protein structure and function. Stabilizing interactions in biomolecules; Properties of nucleosides and nucleotides; composition of nucleic acids.

Unit-2 **(15 Hours)**

Complexities in modelling macromolecular structure; Molecular mechanics; simulating macromolecular structure; energy minimization; Molecular Dynamics.
Physical methods: Ultracentrifugation and other hydrodynamic techniques; Light scattering, fundamental concepts, scattering from a number of small particles: Rayleigh scattering,

scattering from particles that are not small compared to the wavelength of radiation; Dynamic light scattering; Low angle X-Ray scattering; Neutron scattering; Raman scattering

Unit-3: **(15 Hours)**

General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

Optical methods and applications: Optical techniques in biological systems: Absorption spectroscopy, Fluorescence spectroscopy, Linear and Circular Dichroism, Single and multidimensional NMR spectroscopy. Single molecule spectroscopy of biomolecules.

References (Theory)

1. A. L. Lehninger, D. L. Nelson and M. M. Cox, *Principles of Biochemistry*, W. H. Freeman, 4th edn, 2004.
2. C. R. Cantor and P. R. Schimmel, *Biophysical Chemistry*, vols. 1–3, W. H. Freeman, 1980.
3. D. Voet, J. G. Voet and C. W. Pratt, *Biochemistry*, Wiley, 5th edn, 2023.
4. J. M. Berg, J. L. Tymoczko, G. J. Gatto Jr. and L. Stryer, *Biochemistry*, Macmillan Learning, 9th edn, 2019.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

Structural studies of Proteins:

1. To study UV-Vis spectra of lysozyme solutions at varying protein concentrations in order to identify and analyse the characteristic absorption peaks associated with its aromatic amino-acid residues.
2. To study UV-Vis spectra of Human Serum Albumin solutions at varying protein concentrations in order to identify and analyse the characteristic absorption peaks associated with its aromatic amino-acid residues.
3. To record fluorescence spectra of lysozyme solutions at varying protein concentrations in order to observe and analyse changes in fluorescence intensity and emission characteristics of aromatic amino acid residues.
4. To record fluorescence spectra of Human Serum Albumin solutions at varying protein concentrations in order to observe and analyse changes in fluorescence intensity and emission characteristics of aromatic amino acid residues.
5. Circular Dichroism spectroscopy to analyse the secondary structure of lysozyme at varying protein concentrations.
6. Circular Dichroism spectroscopy to analyse the secondary structure of Human Serum Albumin at varying protein concentrations.

Activity analysis of Proteins:

7. To analyse the enzymatic activity of lysozyme at varying protein concentrations.

8. To analyse the enzymatic activity of Human Serum Albumin at varying protein concentrations.
9. To perform a kinetic study of enzymatic activity as a function of protein concentration using the Michaelis–Menten model.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. A. L. Lehninger, D. L. Nelson and M. M. Cox, *Principles of Biochemistry*, 4th edn, W. H. Freeman, 2004.
2. C. R. Cantor and P. R. Schimmel, *Biophysical Chemistry*, vols. 1–3, W. H. Freeman, 1980.
3. D. Voet, J. G. Voet and C. W. Pratt, *Biochemistry*, 5th edn, Wiley, 2023.
4. J. M. Berg, J. L. Tymoczko, G. J. Gatto Jr. and L. Stryer, *Biochemistry*, 9th edn, Macmillan Learning, 2019.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

RESEARCH METHODS/TOOLS / WRITING

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Advanced Research Methodology in Chemistry CH-SBC-3301	**02**	**01**	**-**	**01**	UG	**--**

Course objectives:

- This course will benefit the students to understand and formulate chemistry-related research problems and connect the research outcomes to society.
- The course also aims to provide knowledge about various bibliometric tools, search engines, and software necessary for conducting research in chemistry.
- The course will also help students learn the safe handling of chemicals and assess the risks associated with chemical reactions, as well as methods to minimize these risks while conducting research in a chemistry laboratory including safe chemical storage practices.

Learning Outcomes: By the end of the course, students will be able to:

- identify research problems
- analyze online resources for identifying the gaps in the existing research related to a problem.
- propose workable solutions for a research problem.
- apply chemical drawing tools for drawing structures/mechanisms.
- assess potential hazards, minimise the risks, and prepare for emergencies in a chemistry laboratory.

THEORY COMPONENT **(1 Credit: 15 Hours)**

Unit-1:

Concepts: Ways of Reasoning; Brief of Positivism, Interpretivism- Constructivism & Phenomenology and Critical Theory; Qualitative and Mixed-method Research.

Research Planning: Choosing Research Topic; Definitions and Types of Hypotheses; Definition and Formulation of Research Problems utilizing various tools/ databases, especially print resources (like research articles, reviews, monographs, textbooks etc.) and Digital resources (online journals). TOC alerts, E-books; Reviewing Literature, Writing a Review, Merits and demerits of AI tools in research.

Preparing for Publication: Application of Search Engines in literature survey, extensive application of Scifinder for search of topic/substance/reaction in research papers and patents, retrosynthetic analysis to plan conditions, reagents/catalysts and procedures, filtering based on year/publication type/organization/author etc.

Application of chemical structure drawing tools like Chem-draw, Chem sketch, King's Draw (mobile App) for molecular structures with stereo-centers, conformations, metal complexes, polyhedrals, supramolecules, biomolecules. Using the tools to represent multistep reactions, bonding, reactive intermediates and reaction mechanisms.

Application of softwares like Mestrenova/Delta/TopSpin for NMR spectral analyses. Assigning 1H and 13C NMR peaks with integration, peak picking, splitting pattern, coupling constant determination. Vertical and horizontal expansion for fine analysis. Phase correction, base-line correction. Spectral analysis of 2D NMR – COSY, HSQC, HETCOR, NOESY.

Analyses of journal metrics and criteria to determine appropriate platform for publication.

Safe Handling of Chemicals: Recognising hazards, assessing risks, minimizing risks and preparing for emergencies using Safety Data Sheets and other resources; Understanding Chemical Storage and inventory; Risk Assessment in an experiment.

References (Theory):

1. K. Williamson and G. Johanson, *Research Methods - Information, Systems, and Contexts*, Elsevier, 2nd Ed., 2018.

2. L. R. Gay, G. E. Mills and P. W. Airasian, *Educational Research Competencies for Analysis and Applications, Pearson*, 10th Ed., 2019.
3. C. R. Kothari, *Research Methodology – Methods and Techniques*, New Age International Publishers, 2^{nd} ed., 2004.
4. R. Kumar, *Research Methodology: A Step-by-Step Guide for Beginners*, Pearson Education, 2nd Ed., 2005.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

1. Hands-on training for author/structure/CAS/subject/topic search on SciFinder, Scopus, Web of Science, Google Scholar, and other search engines
2. Hands-on training on learning tools for citation/h-index/i-index of authors/institutions.
3. Summarizing known synthetic strategies for a natural product using SciFinder.
4. Enlisting newly reported molecules for medicinal/material applications.
5. Drawing chemical structures and figures using chemistry software.
6. Analysing ^{1}H and ^{13}C NMR spectra using Mestrenova/Delta/TopSpin software and assign spectral details of all peaks in small organic molecules.
7. Analysing 2D NMR (COSY/HSQC/HETCOR) of small molecules using axis plotting and assigning cross peaks/diagonal peaks to obtain correlations.
8. Analysing safety data sheets for common laboratory chemicals.
9. Analysing chemical storage in a laboratory (incompatibles, flammables, corrosives etc.).
10. Creating an inventory of chemicals in a laboratory.
11. Hands-on training on risk assessment of an experiment.
12. Performing risk assessment on a synthetic protocol.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. D. C. Finster, M. Gmurczyk, R. Bocwinski and R. H. Hill, *J. Chem. Edu.*, 2026, **103**, 7-9.
2. J. Torres and S. Bobst, *Toxicological Risk Assessment for Beginners*, Springer, 2015^{th} Ed., 2015.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

TOOLS FOR RESEARCH

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Tools for Research CH-SBC-3302	**02**	**01**	**-**	**01**	UG	**--**

Course Objectives:

- Understand and apply statistical methods for reliable data analysis, including validation through acceptance/rejection criteria and confidence intervals.
- Develop competence in both quantitative and qualitative analysis of various samples.

Learning Outcomes: After completing this course, learners will be able to:

- develop an understanding of research tools, including their types, sampling techniques, data collection, and evaluation of reliability and validity.
- apply appropriate statistical and analytical methods to analyze spectroscopic and diffraction data and effectively interpret and present research findings.

THEORY COMPONENT (1 Credit, 15 Hours)

Unit-1: Discussion and Design (4 Hours)

Best approaches and practices for better research output: Discussion on topics like openness for innovative and constructive design thinking, analysis, and interpretation of data. Concepts of predefined notions, biases; Search and verification of facts and the source of information, the analysis of evidence; truth & causation; Types and authenticity of sources of information-Triangulation.

Unit-2: Data Collections (4 Hours)

Exploratory, descriptive, experimental, diagnostic, Sampling techniques- probability & non-probability, Sample size determination, Variables- independent, dependent, controlled
Collection Methods- Primary data: questionnaire, interviews, observation, Secondary data: reports, databases- Experimental data collection basics, Validity & reliability of tools, Field studies vs laboratory studies
Types of Data: nominal, ordinal, interval, ratio

Unit-3: Data Analysis (7 Hours)

Statistical analysis: central tendency, standard deviation, Student's t-test, Q-test, F-test, correlation, regression theory

Utilization of software tools: Excel, SPSS, R (intro level), Graphical representation of data, Interpretation of statistical results

References (Theory)

1. K. Williamson and G. Johanson, *Research Methods: Information, Systems, and Contexts*, 2nd edn, Elsevier, 2018.
2. L. R. Gay, G. E. Mills and P. W. Airasian, *Educational Research: Competencies for Analysis and Applications*, 10th edn, Pearson, 2019.
3. C. R. Kothari, *Research Methodology: Methods and Techniques*, 2nd edn, New Age International Publishers, 2004.
4. N. K. Acharya, *Textbook on Intellectual Property Rights*, Asia Law House, 2001.
5. A. P. Miller and M. D. Davis, *Intellectual Property: Patents, Trademarks and Copyright in a Nutshell*, West Group Publishers, 2000.
6. R. Kumar, *Research Methodology: A Step-by-Step Guide for Beginners*, 2nd edn, Pearson Education, 2005.
7. R. A. Day and A. L. Underwood, *Quantitative Analysis*, Prentice Hall/Pearson, 1991.
8. A. I. Vogel, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education, 2009.
9. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole (Cengage Learning), 2021.

PRACTICAL COMPONENTS (Any *ten* practical) (1Credit, 30 Hours)

Suggested/Recommended List of Experiments:

1. N (*e.g.*, 60) replicate coloured solutions are tabulated with the corresponding absorbance values (*e.g.*, in the range of 0.440-0.470) can be given in a Table. Calculate mean, median, range, average deviation, relative average deviation, standard deviation, variance either by utilizing Excel/ORIGIN/MATLAB/Coding.
2. N (*e.g.*, 60) replicate coloured solutions are tabulated with the corresponding absorbance values (*e.g.*, in the range of 0.440-0.470) can be given in a Table. Draw a Histogram with frequency polygon.
3. Analysing UV-VIS data.
4. Analysing Fluorescence data.
5. Analysing FTIR data.
6. Analysing DLS data.
7. Analysing NMR data.
8. Analysing Diffraction data.
9. Calculate the 90% and 99% confidence interval for the determined % of a metal (*e.g.*, Iron) in an ore with $\bar{x}$ (e.g., 15.50), s (e.g., 0.10) and number of observations, n (e.g., 4, 10, 20, 50) etc by utilizing the Table of Student's t.

10. Comparison of two standard deviations (s_1, s_2) with number of individual results (n_1, n_2) respectively by utilizing F-values.
11. Criteria for rejection of an Observation by utilizing Q-test.
12. Draw the Control Charts.
13. Evaluation/Recognition of Significant Figures.
14. Application of Method of Least Squares.
15. Application of Random Walk Model
a) Calculate Mean Displacement and Mean Square Displacement of a 1D Random-Walker with number of steps, N and step-length, b.
b) Calculate Mean Displacement and Mean Square Displacement along x- and y-directions of a 2D Random-Walker with number of steps, N and uniform step-length, b.
c) Calculate Mean Displacement and Mean Square Displacement along x-, y- and z-directions of a 3D Random-Walker with number of steps, N and uniform step-length, b.
16. Calibration Curve Construction and Regression Analysis: Construct calibration curves using absorbance/intensity versus concentration data. Determine slope, intercept, correlation coefficient (R^2), LOD, and LOQ using Excel/ORIGIN/MATLAB/Python.
17. Linear and Non-Linear Curve Fitting: Fit experimental data to linear, polynomial, exponential, Gaussian, Lorentzian, and sigmoid functions. Compare goodness-of-fit parameters.
18. Error Propagation Analysis: Calculate propagated uncertainties in derived quantities using software tools.
19. Analysis of Replicate Measurements: Determine confidence limits, pooled standard deviation, coefficient of variation (%CV), and relative standard deviation (%RSD).
20. Analysis of Variance (ANOVA): Perform one-way ANOVA for comparison of multiple datasets. Interpret F-statistic and significance level.
21. Correlation and Covariance Analysis: Calculate Pearson correlation coefficient and covariance matrices for multivariate datasets.
22. Principal Component Analysis (PCA): Perform PCA on spectroscopic or analytical datasets. Visualize score plots and loading plots.
23. Multivariate Data Analysis: Classification and clustering of analytical data using hierarchical clustering and k-means methods.
24. Baseline Correction and Smoothing of Spectroscopic Data: Apply moving-average, Savitzky–Golay, and Fourier filtering methods to UV-Vis, FTIR, Raman, or fluorescence spectra.
25. Peak Detection and Peak Integration: Identify spectral peaks and calculate peak areas and widths using software.
26. Deconvolution of Overlapping Peaks: Resolve overlapping peaks in UV-Vis, FTIR, fluorescence, diffraction, or chromatography data.
27. Fourier Transform Applications: Perform Fast Fourier Transform (FFT) analysis of experimental signals and interpret frequency-domain information.
28. Machine Learning Applications in Analytical Chemistry: Use regression and classification algorithms for prediction and pattern recognition from experimental data.

29. Numerical Solution of Differential Equations: Solve kinetic and transport equations using Euler and Runge–Kutta methods.
30. Molecular Diffusion Simulation: Simulate 1D, 2D, and 3D diffusion processes and compare with theoretical models.
31. Automated Data Processing Using Python/MATLAB: Import experimental datasets, perform statistical analysis, generate plots, and prepare reports automatically.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. R. A. Day and A. L. Underwood, *Quantitative Analysis*, Prentice Hall/Pearson, 1991.
2. A. I. Vogel, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education, 2009.
3. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole (Cengage Learning), 2021.
4. I. Teraoka, *Polymer Solutions: An Introduction to Physical Properties*, John Wiley & Sons, 2002.
5. J. N. Miller and J. C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Publishers, 2018.
6. W. McKinney, *Python for Data Analysis,* O'Reilley Publishers, 2022.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Instrumental Analysis-I CH-SBC-301	**02**	**00**	**--**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course Objectives:

The objective of the course is to teach instrumental analysis.

Learning Outcomes: At the completion of this course, the students should be able to:

• understand fundamental principles behind modern analytical, spectroscopic, thermal, electrochemical, and separation techniques used in chemistry.

PRACTICAL COMPONENT **(2 Credit: 60 Hours)**

Suggested/Recommended List of Experiments:

Any three/four techniques covered in the semester out of the following syllabus:

1. Instrumental methods of analysis utilizing- pH-meter, potentiometer, turbidity meter, electrochemical methods, Flame photometer, Atomic absorption spectrophotometer, FTIR, Fluorescence, UV-Vis-NIR, CV.
2. Separation Techniques-Solvent Extraction, Cation/Anion Exchange, TLC.
3. Separation of mixtures of metal ions by ion exchange chromatography.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. G. Brauer, *Handbook of Preparative Inorganic Chemistry*, Vol. 1 and 2, Academic Press, New York, 2nd Ed., 1967.
2. G. Marr and B. W. Rockett, *Practical Inorganic Chemistry*, Van Nostrnad Reinhold London, 1972.
3. G. Pass and H. Sutcliffe, *Practical Inorganic Chemistry*, Chapman and Hall, 2nd Ed., 1985.
4. J. D. Woolins, *Inorganic Experiments*, Wiley – VCH Verlag GmbH and Co., 2003.
5. G. D. Christian, P. K. Dasgupta and K. A. Schug, *Analytical Chemistry (An Indian Adaptation)*, Wiley India Pvt. Ltd., 2020.
6. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, Boston (USA): Cengage Learning Publishers, 7th Ed., 2016.
7. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, CBS Publishers & Distributors, 7th Ed., 2004.
8. B. K. Sharma, *Instrumental Methods of Chemical Analysis,* Krishna Prakashan Media; Meerut (India), 25th Ed., 2005.
9. Z. G. Khan, *Practical Instrumental Method of Analysis*, Birla Publications Pvt. Ltd., Delhi, 2022.
10. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Textbook of Quantitative Chemical Analysis*, Longman Group UK Limited, 5th ed., 1989.
11. G. D. Christian, *Analytical Chemistry*, John Wiley & Sons Inc., 6th Ed., 2004.
12. N. G. Graham and J. P. Ingrid, *X-ray Absorption Spectroscopy*, De Gruyter, 2025.
13. M. Z. Jian and C. H. S. John, *Advanced Transmission Electron Microscopy: Imaging and Diffraction in Nanoscience*, Springer; 2016.
14. M. T. Terry, *Thermal Conductivity: Theory, Properties, and Applications*, Springer New York, 2004.

15. E. Barsoukov and J. R. Macdonald, *Impedance Spectroscopy: Theory, Experiment, and Applications*, A John Wiley & Sons, 2005.
16. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Academic Science, 2008.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite of the course (if any)
		Lecture	Tutorial	Practical		
Electrochemical Techniques CH-SBC-302	**02**	**00**	**--**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To understand the fundamental principles of electrochemical processes.
- To utilize electroanalytical techniques for qualitative and quantitative analysis of chemical species.
- To perform and interpret the data of experimental measurements using modern electroanalytical methods.

Learning outcomes: At the completion of this course, the students should be able to:

- gaining skills related to many real-world application energy conversion and storage.
- help them to learn the advantages and limitations of major electroanalytical methods.

PRACTICAL COMPONENT (2 Credit: 60 Hours)

Suggested/Recommended List of Experiments:

1. Cyclic Voltammetric characterization of nanoparticles such as MnO_2, Fe_3O_4, NiO, Co_3O_4.
2. Cyclic Voltammetric characterization of metal complexes such as tetraamminecopper(II) sulfate complex and ferrocene derivatives, etc.
3. Electrodeposition of zinc on a stainless steel metal plate using Chronoamperometric technique
4. Determination of charge transfer resistance in metal oxide nanoparticles using Electrochemical impedance spectroscopy.

5. To determine the corrosion rate of an iron (Fe) and/or Ni electrodes at different pH values using electrochemical techniques.
6. Redox Conductometric Titrations of Fe^{2+} vs Potassium dichromate ($K_2Cr_2O_7$) in acidic medium and any other suitable redox pairs.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. E. Noam and G. Eliezer, *Physical Electrochemistry: Fundamentals, Techniques, and Applications*, WILEY-VCH, 2nd Ed., 2018.
2. C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, WILEY-VCH, 2nd Ed., Completely Revised and Updated Edition, 2007.
3. D. Pletcher, R. Greff, R. Peat, L. M. Peter and J. Robinson, *Instrumental Methods in Electrochemistry*, Horwood Publishing Ltd., 2001.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Qualitative analysis of organic compounds CH-SBC-303	**02**	**0**	—	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To train the students in experimental skills for identification of functional groups in organic compounds and spectroscopic characterization of organic compounds to determine the chemical structures.
- To gain hands-on training in various separation and purification techniques.

Learning outcomes: At the completion of this course, the students should be able to:

- identify one or more functional groups in an organic compound using qualitative chemical methods.
- characterize organic compounds by its chemical modification
- analyse chemicals structures of organic molecules using detailed spectroscopic studies.

PRACTICAL COMPONENT (2 Credits: 60 Hours)

Suggested/Recommended List of experiments:

1. Semi-micro qualitative analysis of single/polyfunctional compounds.
2. Characterization of organic compounds by synthetically derivatizing them.
3. Application of spectral data (IR, UV, NMR and mass) for structural elucidation of the organic compound.
4. Any other relevant experiment added from time to time during the semester.

ESSENTIAL/RECOMMENDED READINGS (Practical)

1. V. K. Ahluwalia and R. Aggarwal, *Comprehensive Practical Organic Chemistry*, Universities Press Pvt. Ltd., 2010.
2. A. I. Vogel, *Elementary Practical Organic Chemistry Small Scale Preparations*, Pearson, 2nd Edn., 2010.
3. F. G. Mann and B. C. Saunders, *Practical Organic Chemistry*, Orient Longmans, 4th Ed. 1990.
4. V. K Ahluwalia., P. Bhagat and R. Aggarwal, *Laboratory Techniques in Organic Chemistry*, I. K. International Publishing House, 2005.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Modern Instrumentations : Principles and Practices CH-SBC-304	**02**	**00**	**__**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- Introduce fundamental principles of analytical and optical instrumentation, including molecular spectroscopy techniques such as UV–Vis, IR, CD, fluorescence, and time-resolved methods.
- Explain separation and electrochemical techniques, including chromatography, electrophoresis, dialysis, cyclic voltammetry, and impedance spectroscopy.
- Explore advanced analytical and characterization methods such as DLS, ITC, flow cytometry, diffraction techniques, and microscopy.

Learning outcomes: On successful completion of the course, students will be able to:

- explain and interpret molecular spectroscopy techniques (UV–Vis, IR, fluorescence, CD, time-resolved) and their application to chemical systems.
- describe and apply separation, electrochemical, and analytical techniques (chromatography, electrophoresis, CV, impedance, DLS, ITC, flow cytometry) to solve practical problems.
- analyse structural and morphological features using diffraction and microscopy techniques and understand their integration in research and quality control.

PRACTICAL COMPONENT (2 Credit: 60 Hours)

Suggested/Recommended List of Experiments:

1. Determine the concentration and purity of calf-thymus DNA using an UV-visible spectrophotometer.
2. Verify Lambert–Beers Law using dilute solutions of fluorescein and rhodamine B using an UV-visible spectrophotometer. Determine the unknown concentration of the chromophore from calibration curve.
3. Study the fluorescence spectra of fluorescein and rhodamine B using a fluorimeter, and compare that with their respective absorption spectra.
4. Observe fluorescence decay curves from fluorescence lifetime measurements of fluorescein and rhodamine B using pulsed excitation.
5. Determine the quenching constant by studying the fluorescence quenching of fluorescein or rhodamine B by copper sulphate as the quencher, using the Stern-Volmer's method.
6. Determine the critical micelle concentration of sodium dodecyl sulphate fluorimetrically using pyrene or fluorescein as the fluorophore.
7. Study the transmigration of calf-thymus and any other given DNA using agarose gel electrophoresis. Analyse size distribution and band visualization.
8. Determine the crystalline phase of as synthesized/given magnetic nanoparticles using powder XRD method. Determine the size of the crystals from the XRD data using the Scherrer's equation.
9. Determine the hydrodynamic size and size distribution of an aqueous dispersion of as synthesized/given magnetic nanoparticles and/or latex beads using dynamic light scattering (DLS) method.
10. Identify common functional groups (hydroxyl, carboxyl, amino, etc.) through analysis of FTIR spectra of simple organic compounds (alcohol, acid, ketone).

11. Observe secondary structure signatures (α-helix, β-sheet) of common proteins such as bovine serum albumin (BSA) using Circular Dichroism (CD) spectral data. Study the change in secondary structure of BSA upon addition of denaturants such as urea and sodium dodecyl sulphate (SDS).
12. Demonstration: Sample preparation, observation and visualization of internal structure of as synthesized/given magnetic nanoparticles using transmission electron microscope (TEM) instrument.
13. Demonstration: Visualization of diffraction rings and identification of hkl planes of as synthesized/given magnetic nanoparticles from selected area electron diffraction (SAED) data using transmission electron microscope (TEM) instrument.
14. Demonstration: Observation of elemental/chemical composition of as synthesized/given magnetic nanoparticles from energy dispersive x-ray spectroscopic (EDX) data using transmission electron microscope (TEM) instrument.
15. Demonstration: Sample preparation, observation and visualization of surface morphology of as synthesized/given magnetic nanoparticles and/or latex beads using scanning electron microscope (SEM) instrument.
16. Demonstration: Sample preparation, observation and analysis of height and surface roughness of as synthesized/given magnetic nanoparticles and/or latex beads using atomic force microscope microscope (AFM) instrument.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2015.
2. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd edn, Springer, New York, 2006.
3. Z. Gryczynski and I. Gryczynski, *Practical Fluorescence Spectroscopy*, 1st edn, Taylor and Francis, New York, 2020.
4. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th edn, Brooks/Cole, 2017.
5. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 2nd revised edn, Holt, Rinehart & Winston of Canada Ltd., 1988.
6. E. V. Hunter, *Practical Electron Microscopy: A Beginner's Illustrated Guide*, Cambridge University Press, Cambridge, 2012.
7. P. Echlin, *Handbook of Sample Preparation for Scanning Electron Microscopy and X-Ray Microanalysis*, Springer, 2009.
8. C. Suryanarayana and M. G. Norton, *X-Ray Diffraction: A Practical Approach*, Springer, 2013.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Numerical Methods for AI/ML and Quantum Computing CH-SBC-305	**02**	**00**	—	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- Understand numerical methods, computational errors, and efficiency in AI/ML and quantum computing.
- Apply numerical techniques to solve chemical problems using computational tools.
- Explore AI/ML methods for chemical data analysis.
- Achieve a foundational understanding of quantum computing and its applications in chemistry.

Learning outcomes: On successful completion of the course, students will be able to:

- identify and mitigate computational errors in chemical calculations.
- implement numerical methods for linear systems, differential equations, optimization, and data analysis.
- apply AI/ML techniques to chemical datasets.
- applications of quantum computations a simulate basic quantum algorithms for chemical problems.

PRACTICAL COMPONENT (2 Credit: 60 Hours)

Suggested/Recommended Suggested/Recommended List of Experiments:

1. Using tools like Jupyter notebooks/Google Colab and libraries like Numpy, SciPy, scikit-learn, PyTorch and others.
2. Solve small chemical-related linear systems using LU and QR decomposition in Python (NumPy) and Fortran.

3. Implement Jacobi and Gauss–Seidel methods for large sparse matrices (e.g., molecular interaction matrices).
4. Implement gradient descent and variants to minimize chemical energy functions or ML loss.
5. Use finite differences and quadrature rules (Simpson, Gaussian) for estimating molecular properties.
6. Solve reaction kinetics or simple molecular dynamics using Euler and Runge–Kutta methods.
7. Apply interpolation, polynomial approximation, and smoothing on noisy chemical datasets.
8. Implement k-means and hierarchical clustering for chemical data (molecular properties, spectra).
9. Use Qiskit or Google Cirq (free) to simulate qubits, quantum gates, and simple VQE circuits for small molecules (H_2, LiH).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. P. Janet and H. J. Kulik, J. Chem. Educ., 2021, *98*, 2892–2898.
2. C. J. Heard, J. Chem. Educ., 2024, *101*, 2957–2959.
3. J. N. Wei, D. Duvenaud and A. Aspuru-Guzik, Chem. Rev., 2021, *121*, 9816–9872.
4. a) https://jupyter.org/, b) https://colab.research.google.com/, c) https://www.python.org/, d) https://numpy.org/, e) https://scikit-learn.org/stable/, f) https://pytorch.org/

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Green Chemistry and Sustainable Development CH-GE-301	**04**	**03**	__	**01**	UG	--

Course objectives:

- To teach Green Chemistry approach towards sustainable development.

Learning outcomes: At the completion of this course, the students should be able to:

- understand Green Chemistry and its principles.
- recognize the applications of Green Chemistry principles in catalysis.
- designing chemical reactions with Green Chemistry approach.
- realize the significance of green chemistry in industries specially to provide cleaner energy.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Introduction to Green Chemistry (15 Hours)

Green Chemistry: An interdisciplinary approach towards sustainable development History of emergence of Green Chemistry through some industrial disasters, environmental movements for public awareness and some important environmental laws, Definition of Green Chemistry, Need for Green Chemistry, goals of Green Chemistry, Green Chemistry advances towards a sustainable future, Green Chemistry v/s Environmental Chemistry, Green Chemistry and its interdisciplinary nature, Twelve Principles of Green Chemistry and their illustrations with examples.

Unit-2: Catalysis for Green Chemistry with Examples (15 Hours)

Catalytic oxidation using H_2O_2, Bio-catalysis, Photocatalysis, Earth abundant metal based catalysis with green chemistry principles. Green reagents, Green solvents including solvent free synthesis of some organic compounds and inorganic complexes, alternative sources of energy, Green energy and sustainability.

Unit-3: Application of Green Chemistry in Real World Cases (15 Hours)

Wealth from waste, Industrial case studies Green Nanotechnology, Greener approaches for nanoparticle synthesis pharmaceutical industries: The largest waste producer problems and solutions through Green Chemistry benefits of greening industries, Need for Academia-Industry collaborations, Innovations stemming from Academia-Industry collaborations Emerging Green Technologies. Green solvents, Next generation catalyst design, Microwave assisted synthesis etc.

References (Theory):

1. P. T. Anastas and J. C. Warner, *Green Chemistry-Theory and Practical*, Oxford University Press, 1998.
2. A. S. Matlack, *Introduction to Green Chemistry*, New York: Marcel Dekker, CRC Press, 2001.
3. M. C. Cann and M. E. Connely, *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000.
4. R. K. Sharma and R. Bandichhor, *Hazardous Reagent Substitution: A Pharmaceutial Perspectives*, Royal Society of Chemistry, Green Chemistry Series, 2017.
5. M. A. Ryan and M. Tinnes, *Introduction to Green Chemistry*, American Chemical Society, Washington, 2002.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Solvent-Free Synthesis: Mechanochemical solvent-free synthesis of an azomethine (Schiff base). This involves grinding solid reactants together, eliminating the need for hazardous organic solvents.
2. Extraction of D-limonene from orange peel (a waste product) using liquid or supercritical CO_2 prepared from dry ice.
3. Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.
4. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
5. Green syntheses of magnetic Fe_3O_4 nanoparticles using potato extract and its characterization.
6. Microwave Assisted One Pot Synthesis of Nickel Porphyrin Complex.
7. Greener Method of Synthesis of substituted Bis(acetylacetanato)copper(II).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. R. K. Sharma, I. T. Sidhwani and M. K. Chaudhari, *Green Chemistry Experiments: A Monograph*, I. K. International Publishing House Pvt. Ltd., New Delhi, Bangalore, 2013.
2. M. Lancaster, *Green Chemistry: An Introductory Text*, RSC publishing, 2nd Ed., 2010.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Biomolecules, structure and functions-I **CH-GE-302**	**4**	**3**	**0**	**1**	UG	NIL

Course Objectives: This course will provide fundamental understanding of enzymes and their application in various biological processes.

Learning Outcomes: At the completion of this course, the students should be able to:
- understand structure and function of enzymes
- explain biological roles of enzymes in biochemical pathways
- design small drug molecules based on receptor interaction studies.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Introduction (15 Hours)

Introduction to Bio-molecules, Amino Acids: Structure, classification and Properties of Amino Acids., Peptide bond, Protein Structure: Primary, Secondary, Tertiary and Quaternary Structure. Protein types: Globular and Fibrous. Protein Functions. Synthesis of α-amino acids and peptides, titration curve of amino acid.

Unit-2: Structure, function of Proteins and Enzymes (15 Hours)

Structure, function and properties of proteins, classification, and characteristics of enzymes. Properties and mechanism of enzyme activity, factors affecting enzyme activity, coenzymes, and cofactors, specificity of enzyme activity. Purification of optically active amino acids using enzyme as a catalyst. Enzyme inhibitors and their importance, Type of enzyme inhibition (competitive, uncompetitive, and non-competitive inhibition). Identification of enzyme active site using inhibitor binding, affinity labelling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Unit-3: Enzymes link to human diseases (15 Hours)

Enzyme as a biological catalyst for cellular metabolism. Specific examples to chymotrypsin, ribonuclease, lysozyme, carbonic anhydrase, serine proteases and carboxypeptidase A. Enzymes link to human diseases such as Arthritis, Cancer, Gout, Perkinson's, Alzheimers. Enzymes such as Monoamine oxidase, Urease, Cyclooxygenase-2, Acetylcholinesterase, thymidylate synthase. Amine based enzyme inhibitors: 2-phenyl ethylamines (dopamine and serotonin), sulfanilamide and its derivatives, Antibiotic, Anti-inflammatory, Anti-cancer drugs.

References (Theory):

J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman and Co., 9th Ed., 2019.
2. D. L. Nelson, M. M. Cox and A. L. Lehninger, *Principles of Biochemistry*, W. H. Freeman and Co., International Edition, 2017.
3. S. Kuashik and A. Singh, *Biomolecules: From Genes to Proteins, Berlin*, Boston: De Gruyter, 1st Ed., 2023.

4. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer-Verlag, 1989.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis of amine compound from alkyl halide
2. Synthesis of sulfanilamide from aniline
3. Preparation of buffers.
4. Qualitative tests for amino acids.
5. Study of the titration curve of alanine.
6. Estimation of glycine by Sorenson Formol Titration
7. Qualitative analysis of proteins- Ninhydrin test, Biuret test, Millon's reagent test, Xanthoproteic test.
8. Estimation of proteins by Lowry's method.
9. Study on the effect of starch, pH, copper sulfate and temperature on the action of salivary amylase.
10 Protein Separation and Purification techniques.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. S. Kukreti, *Manual of Biochemistry Workshop Department of Chemistry*, University of Delhi, 2012.
2. A. I. Vogel, *Vogel's Textbook of Practical Organic Chemistry*, Wiley, 5th Edn., 1989.
3. F. G. Mann and B. C. Saunders, *Practical Organic Chemistry*, Orient Longmans, 4th Ed., 1990.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical/ Practice		

						(if any)
Fundamentals of Spectroscopy CH-GE-303	**4**	**3**	**0**	**1**	UG	NIL

Course Objectives:
- Understand quantum principles underlying atomic and molecular spectroscopy, including rotational, vibrational, Raman, and electronic transitions with selection rules.
- Apply concepts such as Franck–Condon principle and Jablonski diagram to analyse excited-state processes, fluorescence, phosphorescence, and quenching.
- Develop basic understanding of NMR, NQR, and Mössbauer spectroscopy.

Learning Outcomes: At the completion of this course, the students should be able to
- explain quantum principles, atomic states, selection rules, and effects such as Zeeman and Stark splitting.
- interpret rotational, vibrational, Raman, and electronic spectra to determine molecular properties and understand excited-state processes.
- describe the basic principles of NMR, NQR, and Mössbauer spectroscopy.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Fundamentals of Atomic and Molecular Spectroscopy (15 Hours)

Spectroscopic methods: Characterization of electromagnetic radiation. Born-Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation (Qualitative Discussion). Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Molecular Spectroscopy: Basics of molecular spectroscopy. Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and / or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First and second order Stark effect.

Unit-2: Vibrational and Raman Spectroscopy (15 Hours)

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect. Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules. Overtones and combination bands.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and vibrational Raman spectroscopy. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

Unit-3: Electronic and Magnetic Resonance Spectroscopy (15 Hours)

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde).

Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding.

Excited states: Deactivation. Jablonskii diagram. Fluorescence and phosphorescence and factors affecting these. Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.

NMR spectroscopy: Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

NQR spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications.

Principles of Mössbauer spectroscopy: Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination

References (Theory)

1. C. J. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 6th edn, Tata McGraw-Hill, 2025.
2. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill, 2017.
3. J. M. Hollas, *Modern Spectroscopy*, 4th edn, John Wiley & Sons, 2004.
4. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy: From Radio Waves to Gamma Rays*, I.K. International Publishing House, New Delhi, 2015.
5. R. Kakkar, *Atomic & Molecular Spectroscopy*, Cambridge University Press, 2015.
6. J. C. D. Brand and J. C. Speakman, *Molecular Structure: The Physical Approach*, 2nd edn, Edward Arnold, London, 1975.
7. R. Chang, *Basic Principles of Spectroscopy*, McGraw-Hill, New York, 1970.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Verify Lambert-Beer's law, and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration colourimetrically.
2. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture colourimetrically.
3. Study the influence of pH on the spectrum of potassium dichromate solution.
4. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture by the MLRA method.
5. Study the kinetics of the reaction of phenolphthalein with sodium hydroxide
6. Study the effect of structure on the UV spectra of organic compounds.
7. Study the effect of solvent on the UV spectra of organic compounds
8. Study the spectra of mesityl oxide/ benzophenone in different solvents and classify the observed transitions in terms of $n\rightarrow\pi^*$ and $\pi\rightarrow\pi^*$ transitions. Discuss the shift in transitions relative to those in acetone.
9. Determine the amount of iron present in a sample using 1,10-phenathroline.
10. Find the stoichiometry of the complex formed between a metal ion (Fe3+) and a ligand (salicylate) by Job's continuous variation method and determine the stability constant of the complex formed.
11. Study the fluorescence spectrum of some common fluorophores, such as rhodamine ad fluorescein.
12. To study the effect of copper ions on fluorescence quenching of rhodamine and/or fluorescein using Stern Volmer's method, and calculate the Stern Volmer's constant.
13. Analyse the IR/FTIR spectra of given compounds.
14. Analyse the Raman spectra of given compounds and materials.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2015.
2. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th edn, Brooks/Cole, 2017.
3. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 2nd revised edn, Holt, Rinehart & Winston of Canada Ltd., 1988.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SEMESTER-IV

DSC

DISCIPLINE SPECIFIC CORE COURSE (DSC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Frontiers in Bioinorganic(I), Medicinal Chemistry (I), Irreversible Thermodynamics and Transport Phenomena CH-DSC-401	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To learn how metal ions function as essential components in biological processes, as well as their structural roles in proteins.
- To offer students a structured view of evolution of medicinal chemistry highlighting major milestones. They will understand interaction of drugs with targets at a molecular level with mechanistic insights for rational drug design, optimization and development of therapeutics.
- Introduce entropy production and non-equilibrium stationary states, and explain Onsager reciprocal relations, Curie–Prigogine principle, and their thermodynamic significance.
- Discuss coupled transport phenomena and practical applications of irreversible thermodynamics in physical and chemical systems.

Learning outcomes: At the completion of this course, the students should be able to:

- comprehend the diverse physiological, functional and structural roles of metal ions in biological systems.
- analyse how metal–ligand interactions determine the reactivity of metalloproteins.
- relate how new therapeutic agents are identified, along with an appreciation of major milestones in drug discovery
- indicate the principles governing drug discovery, development and mechanisms of drug action.
- apply contemporary strategies, tools, and methodologies used in modern drug discovery research

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Advanced Bioinorganic Chemistry **(15 Hours)**

Geo-chemical effects on life systems, essential and non-essential elements in bio-systems. Role of metal ions in biological systems. Toxic metal ions, fundamentals of Toxicity and Detoxification or chelation therapy. Fixation of dinitrogen biologically and abiologically, biotransformation of non-metallic inorganic compounds. Na-K, ATPase or sodium pump. Natural and synthetic oxygen carriers and their mechanism. Non-heme Iron-sulfur proteins. Electron transport proteins. Transport and storage of metal ions in vivo. Designing of chelating agents and metal chelates as medicines. Recent advances in cancer chemotherapy using chelates. Photo-induced therapy. Futuristic aspects of organo transition metal complexes in bio-inorganic chemistry.

Unit-2: Introduction to Medicinal Chemistry **(15 Hours)**

History of Medicinal Chemistry. Structure, sites, and functions of proteins, nucleic acids, carbohydrates, and lipids. General mechanism of drug action on enzymes (inhibition of active site, allosteric site, non-competitive inhibitors, transition-state inhibitors and suicidal substrates); agonists, antagonists, allosteric modulators, partial agonists and inverse agonists; receptors (including all types of receptors, i.e., ion channel receptors, GPCRs & their signal transduction mechanism, kinase-linked receptors, and enzymes), nucleic acids (including DNA targeting agents via intercalation, alkylation, chain termination, topoisomerase inhibition, chain cutters & RNA targeting agents via antisense therapy, RNA interference (siRNA); lipids (tunnelling molecules and ion carriers) and carbohydrates (antigens, antibodies, and cyclodextrins). Drug affinity, efficacy, potency, and therapeutic index. Drug metabolism (Phase I and Phase II) and inactivation.

Unit-3: Irreversible Thermodynamics and transport phenomenon **(15 Hours)**

Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations.
Entropy production-specific examples of entropy production, non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications.
Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein-Smoluchowski equation.

References (Theory)

1. M. N. Hughes, *The Inorganic Chemistry of Biological Processes*, Wiley, 2nd Ed., 1981.

2. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Cengage Learning India Private Limited, New Delhi, 2010.
3. D. F. Shriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, Oxford Univ. Press, 2nd Ed., 1998.
4. V. K. Ahluwalia and Madhu Chopra, *Medicinal Chemistry*, Anes Student Edition, 2008
5. A. Kar, *Medicinal Chemistry*, New Age Int. Pvt. Ltd; 2007.
6. N. K. Dunlap, and D. M. Huryn, *Medicinal Chemistry*, Garland Science, New York, 2018.
7. G. L. Patrick, *An Introduction to Medicinal Chemistry,* Oxford University Press, 1995.
8. T. L. Lemke and D. A. William, *Foye's Principles of Medicinal Chemistry*, 5th Ed., USA, 2002.
9. A. Gringuage, *Introduction to Medicinal Chemistry*, Wiley-VCH, 1997.
10. E. Stevens, *Medicinal Chemistry - The Modern Drug Discovery Process*, Pearson, 2014.
11. R. Silverman and M. W. Holladay, *The Organic Chemistry of Drug Design and Drug Action*, Academic Press, 3rd Edn., 2014.
7. R. P. Rastogi, *Introduction to Non-Equilibrium Physical Chemistry*, Elsevier B.V., 2008.
8. A. Katchalsky and P. F. Curran, *Non-Equilibrium Thermodynamics in Biophysics*, Harvard University Press, Cambridge, 1965.
9. P. W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edn, Oxford University Press, 2006.
10. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, 3rd edn, University Science Books, 2001.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR spectroscopy, magnetic susceptibility etc. Selection can be made from the following or any other from the existing literature.

i. Metal acetylacetonates
ii. Cis and trans isomers of $[Co(en)_2Cl_2]Cl$
iii. Preparation of transition metal complexes of triphenyl phosphine, e.g, $[Ni(PPh_3)_2Cl_2]$, $Ni(NCS)_2(PPh_3)_2$.
iv. (N,N)-bis(salicyldehyde)ethylenediamine Salen H_2; and its cobalt complex [Co(Salen)].
v. Vanadyl acetylacetonate.

2. Synthesis, purification and characterisation of APIs and pharmacophores like 5,5-diphenylhydantoin (Phenytoin), Nitrazepam 2-phenylimidazo[1,2-a]pyridine and their analogs.
3. Green Synthesis of 1,4-Dihydropyridines through Catalyst-Free Multicomponent Hantzsch Reaction.
4. Demonstrate the Fourier's Law (Temperature gradient → heat flow) of Heat Conduction in a non-equilibrium steady state via heating a metallic rod.
9. Demonstrate diffusion of dye in water governed by Fick's Laws of Diffusion (Concentration gradient → mass transport) using a camera or optical sensor.

10. Demonstrates the Seebeck Effect (Temperature gradient → electrical voltage) using a thermocouple (two different metals), voltmeter and hot and cold reservoirs.
11. Demonstrate solvent transport through a semi-permeable membrane driven by osmotic pressure differences (Chemical potential gradient → solvent flow).
12. Demonstrate Joule Heating (Electric current → heat production) using a Resistor and thermal sensor.
13. Demonstrate Soret Effect (Thermal Diffusion against Temperature gradient → concentration gradient) using a binary liquid mixture.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. A. S. Batsanov and J. A. K. Howard, *Acta Crystallogr.*, 2001, **57**, 308–309.
2. G. Garton, D. E. Henn, H. M. Powell and L. M. Venanzi, *J. Chem. Soc.* 1963, 3625–3629.
3. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd ed., 1997.
4. J. Springbørg and C. E. Schaffer, *Inorg. Synth.*, 1973, **14**, 63–77.
5. R. A. Rowe and M. M. Jones, *Inorg. Synth.*, 1957, **5**, 113–116.
6. R. B. Lauffer, R. H. Heist and L. Que, *Inorg. Chem.*, 1983, **22**, 50–55.
7. J. D. Woollins, *Inorganic Experim*ents, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 3rd rev. ed., 2010.
8. M. Seco*, J. Chem. Ed.*, 1989, **9**, 779-780.
9. V. K. Ahluwalia and R. Agarwal, *Comprehensive Practical Organic Chemistry*, Universities Press Pvt. Ltd., 2010.
10. R. P. Rastogi, *Introduction to Non-Equilibrium Physical Chemistry*, Elsevier Science, 2007.
11. Y. Demirel, *Nonequilibrium Thermodynamics: Transport and Rate Processes in Physical and Biological Systems*, Elsevier Science, 2002.
12. J. L. Plawsky, *Transport Phenomena Fundamentals*, 4th edn, CRC Press, 2020.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE (DSC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

		Credit distribution of the		

Course title & Code	Credits	course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Frontiers in Bioinorganic(II), Medicinal Chemistry (II),Fast Chemical Processes CH-DSC-402	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To learn about the (i) role of metal ions in DNA and RNA replication and transcription, (ii) nuclear medicines and their applications, e.g., imaging, diagnostics, radiotherapy, etc.
- To explore key drug classes like antibiotics, antivirals, anti-AIDS therapies, anti-histamines, anti-inflammatory and analgesic agents, anticancer and antihypertensive drugs with focus on their molecular mechanisms of action, physiological absorption, distribution, metabolism and elimination.
- Introduce surface phenomena, surfactants, micellization, electrokinetic effects, interfaces, and surface catalysis, along with analytical techniques for surface studies.
- Explain fast reactions and apply theoretical and experimental approaches to understand kinetics in solid-state and solution systems.

Learning outcomes: At the completion of this course, the students should be able to:

- assess application of inorganic based compounds as drugs for the treatment of various diseases including radioactive isotopes and other radio-pharmaceuticals in medical diagnosis and treatment.
- understand important classes of drugs, such as antibiotics, antivirals, anticancer, and antidiabetic agents and their mechanisms of action.
- apply various strategies for molecular screening, drug design, and lead optimization for different classes of drugs
- analyse surfactant behaviour, micellization, surface films, catalytic activity, and electrode kinetics using appropriate thermodynamic and electrochemical principles.
- apply surface characterization and rapid kinetics techniques to interpret kinetic data for solution and solid-state reactions.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Advanced Bioinorganic Chemistry-II **(15 Hours)**

Fundamentals of inorganic biochemistry. Metal ions as antioxidants, metal ion enhancing catalytic activity of enzymes (Biocatalysts). Inhibitions as competitive and non-competitive, metals and metalloproteins. Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA. Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter. Metals in the regulation of biochemical events. Metal complexes as probes of structure and reactivity with metal substitution. Bioinorganic chips and biosensors. Nuclear medicines.

Unit-2: Drug Discovery and Development (15 Hours)

Drug discovery, development, design, and delivery systems. General introduction to antibiotics; mechanism of action of beta-lactam antibiotics mainly penicillin, classification of penicillins (natural, synthetic and beta-lactamase inhibitors) their resistance and SAR, non-lactam antibiotics (synthesis of sulfonamides and their mechanism of action and SAR, fluoroquinolones and quinolones. including synthesis of ciprofloxacin). General introduction to viruses and their life cycle; antiviral drugs in general, anti-HIV drugs (NRTIs, NNRTIs, and protease inhibitors; development of Saquinavir) Neurotransmitters, classes of neurotransmitters, and drugs affecting cholinergic and adrenergic mechanisms. Anti-histamines, anti-inflammatory, anti-analgesics, anticancer, anti-hypertensive, and anti-diabetic drugs.

Unit-3: Surfaces, Catalysis, and Fast Chemical Processes (15 Hours)

Surface phenomena: Surface active agents, classification of surface-active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, Surface films (electrokinetic phenomena), catalytic activity at surfaces. Electrode/ electrolyte interface; electrical double layer, electrode kinetics, Nernst equation. Application of PES, ESCA and Auger spectroscopy to the study of surfaces.

Fast reactions: Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method. Kinetics of solid-state reactions.

References (Theory)

1. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Univ. Science Books, 1994.
2. S. J. Lippard, *Progress in Inorganic Chemistry*, Wiley-Interscience, Vols. 18 and 38, 1991.
3. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, Wiley, New York, 1994.
4. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.

5. A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, U. N. Dhur and Sons, Kolkata, 2nd Edn, 2002.
6. A. K. Das, *Bioinorganic Chemistry*, Books & Allied (P) Ltd., Kolkata, 2007.
7. E. Ochiai, *Bioinorganic Chemistry: A Survey*, Academic Press, Elsevier, 2009.
8. R. R. Crichton, *Biological Inorganic Chemistry: A New Introduction to Molecular Structure*, Elsevier, New York, 2nd Edn., 2012.
9. R. M. Roat-Malone, *Bioinorganic Chemistry: A short Course*, Wiley, New York, 2nd Edn., 2013.
10. V. K. Ahluwalia and Madhu Chopra, *Medicinal Chemistry*, Anes Student Edition, 2008
11. A. Kar, *Medicinal Chemistry*, New Age Int. Pvt. Ltd; 2007.
12. N. K. Dunlap, and D. M. Huryn, *Medicinal Chemistry*, Garland Science, New York, 2018.
13. G. L. Patrick, *An Introduction to Medicinal Chemistry,* Oxford University Press, 1995.
14. T. L. Lemke and D. A. William, *Foye's Principles of Medicinal Chemistry*, 5th Ed., USA, 2002.
15. A. Gringuage, *Introduction to Medicinal Chemistry*, Wiley-VCH, 1997.
16. E. Stevens, *Medicinal Chemistry - The Modern Drug Discovery Process*, Pearson, 2014.
17. R. Silverman and M. W. Holladay, *The Organic Chemistry of Drug Design and Drug Action*, Academic Press, 3rd Edn., 2014.
18. K. J. Laidler, *Chemical Kinetics*, 3rd edn, Benjamin Cummings, 1997.
19. J. M. Thomas and W. J. Thomas, *Principles and Practice of Heterogeneous Catalysis*, John Wiley & Sons, 1996.
20. I. Chorkendorff and J. W. Niemantsverdriet, *Concepts of Modern Catalysis and Kinetics*, Wiley-VCH, 2003.
21. P. W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edn, Oxford University Press, 2006.
22. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, 3rd edn, University Science Books, 2001.
23. D. J. Shaw, *Introduction to Colloid and Surface Chemistry*, 2nd edn, Butterworths, 1970.
24. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6th edn, Wiley-Interscience, 1997.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR spectroscopy, magnetic susceptibility etc. Selection can be made from the following or any other from the existing literature.

i. Mn, Cu and Zn Salen complexes.

ii. *trans*-bis glycinato copper (II) complex.

2. Multistep Synthesis and characterization of APIs and pharmacophores like Multistep Synthesis of Diphenhydramine and its analogues, Umbelliferon and its derivatives.

3. Isolation and characterisation of APIs like ibuprofen and Naproxen from tablets and further functional group modifications.

4. Determine spectrophotometrically the reaction mechanism and rate constant of a fast-photochemical reactions using Flash photolysis.
5. Determine conductometrically the reaction mechanism and rate constant of neutralization reaction between strong acid and strong base.
6. Determine spectrophotometrically the reaction mechanism and rate constant of the Iodine Clock Reaction by studying the time-dependent color change due to the formation of iodine–starch complex.
7. Determine spectrofluorimetrically the reaction mechanism and rate constant of the quenching of florescence of riboflavin by copper ions (quencher).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. F. Basolo, B. M. Hoffman and J. A. Ibers, *Acc. Chem. Res.*, 1975, **8**, 384–392.
2. D. A. Köse, E. Toprak, A. Kaşarcı, E. Avcı, G. A. Avcı, O. Şahin and O. Büyükgüngör, *Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry,* 2016, **46**, 1109–1118.
3. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, 5th Ed., 2017.
4. G. Marr and B. W. Rockett, *Practical Inorganic Chemistry*, Van Nostrand Reinhold Company, London, 1972.
5. J. D. Woollins, *Inorganic Experiments*, Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 3rd ed., 2010.
6. V. K. Ahluwalia and R. Agarwal, *Comprehensive Practical Organic Chemistry*, Universities Press Pvt. Ltd., 2010.
7. S. K. Upadhyay, *Chemical Kinetics and Reaction Dynamics*, Springer, 2006.
8. M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford University Press, 2021.
9. J. I. Steinfeld, J. S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics*, Prentice Hall, 1989.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DSE

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Organotransition Metal Chemistry and Catalysis CH-DSE-401	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- Fundamental understanding of the organometallic compounds, their bonding, and with their practical utility in industries.

Learning outcomes: At the completion of this course, the students should be able to:

- have the knowledge about the organometallic compounds, bonding and their catalytic applications for industrial purpose.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: (15 Hours)

General introduction, Structure and bonding, Survey of organometallic complexes according to ligands. π bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds and their M.O. diagrams.

Unit-2: (15 Hours)

Metal-carbon multiple bonds. Fluxional organometallic compounds including π-allyl complexes and their characterization. Metallacycles, unsaturated nitrogen ligands including dinitrogen complexes. Futuristic aspects of organotransition metal chemistry.

Unit-3: (15 Hours)

Transition metal catalysts for organic transformations and their application in hydrogenation (using symmetric and chiral organometallic catalysts), isomerization, olefin oxidation, carbonylation, and polymerization reactions. C-C Coupling Reactions (Allylic alkylation, Heck, Suzuki, Stille, Sonogashira and Stille reactions), C-heteroatom Coupling Reactions (Hydroamination and Hydrosilylation), Olefin metathesis reaction, Water gas shift and Fischer-Tropsch reactions and Reppe Syntheses.

References (Theory)

1. C. Elschenbroich, *Organometallics*, Wiley-VCH, 3rd Ed., 2005.

2. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 4th Ed., 2005.
3. B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals*, Universities Press, 2010.
4. J. F. Hartwig, *Organotransition Metal Chemistry: From Bonding to Catalysis*, University Science Books, 2010.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Syntheses and characterization of acetyl-, and 1,1´-diacetyl ferrocene.
2. Synthesis and characterization of N,N´-dimethylaminomethylferrocene.
3. Synthesis and characterization of ferrocene carboxaldehyde and its subsequent reactivity
4. Copper(I) catalyzed click reactions.
5. Synthesis and characterization of dichloro(p-cymene)ruthenium(II) dimer.
6. Syntheses of biaryls from Suzuki coupling reactions.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. M. A. Bennett, T. N. Huang, T. W. Matheson and A. K. Smith, *Inorg. Synth.*, 1982, **21**, 74–78.
2. U. Pokharel, H. Flores and L. Siddon, *J. Chem. Edu.,* 2025, **102**, 4530–4537.
3. F. Himo, T. Lovell, R. Hilgraf, V. V. Rostovtsev, L. Noodleman, K. B. Sharpless and V. V. Fokin, *J. Am. Chem. Soc.,* 2005, **127**, 210-216.
4. P. J. Graham, R. V. Lindsey, G. W. Parshall, M. L. Peterson and G. M. Whitman, *J. Am. Chem. Soc.,* 1957, **79**, 3416–3420.
5. W. Shaoyan, Z. Zhiqiang, Z. Hu, Y. Wang, P. Lei and H. Chi, *J. Environ. Sci.,* 2009, **21**, S124–S126.
6. D. Lednicer and C. R. Hauser, *Org. Synth.,* 1960, **40***,* 31.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course
		Lecture	Tutorial	Practical		

						(if any)
Chemistry of Inorganic Materials CH-DSE-402	**04**	**03**	**—**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To introduce the basics of solid-state chemistry including structural aspects and the various properties of crystalline solids and their origin with appropriate examples.

Learning outcomes: At the completion of this course, the students should be able to:

- comprehend the various aspects of solid-state materials chemistry, basic understanding of structure-property correlation.
- familiarize with the fundamental concepts and for learning the chemistry behind the applications of solids.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Introduction to Solid State Crystal Structures, Crystal Chemistry and Defects (15 Hours)

Basics of crystal chemistry and structures, density, symmetry, symmetry elements, Schoenflies and Hermann-Mauguin notations, unit cells, fractional coordinates, crystal systems, space groups, Miller indices, interplanar distances, basic crystallography, PXRD.

Examples for structural types, NaCl, NiAs, fluorite, antifluorite, ZnS (polymorphs), $CdCl_2$, CdI_2, spinel, inverse spinel, rutile, perovskites (various types) and antiperovskites.

Defects (different classifications and dimensional), non-stoichiometry, including solid solutions, ionic conductors, and solid electrolytes.

Unit-2: Defects, Bonding in Solids and Electronic Properties (15 Hours)

Basics, origin of bands, band structure, density of states, electrical conductivity, conductors, semiconductors (*n*- and *p*-type) bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors and band gaps determination.

Basic concepts of dielectric, piezoelectric, ferroelectric and thermoelectric materials.

Superconductors, structures and crystal chemistry of high-T_c copper oxide-based examples.

Unit-3: Optical, Magnetic Properties and Structure-Property Correlation (15 Hours)

Luminescence and phosphorescence of solid materials, phosphors, solid-state lasers, and inorganic pigments (inorganic chemistry concepts behind the origin of color, correlation to structures and applications)

Behavior of Substances in a magnetic Field, effects of temperature: Curie and Curie–Weiss laws, magnetic moments, mechanisms of ferro-and antiferromagnetic ordering. Super exchange, transition metal monoxides, transition metal dioxides, spinels, garnets, ilmenites and perovskites, magneto plumbites. Applications: structure–property relations, transformer cores, permanent magnets, magnetic information storage, recent developments. Magnetoresistance: giant and colossal, and multiferroics.

References (Theory)

1. P. M. Woodward, P. Karen, J. S. O. Evans and T. Vogt, *Solid State Materials Chemistry*, Cambridge University Press, 2021.
2. A. R. West, *Solid State Chemistry and its Applications*, Wiley, 2nd Ed., 2014.
3. C. N. R. Rao and J. Gopalakrishnan, *New Directions in Solid State Chemistry*, Cambridge University Press, 2nd Ed., 2009.
4. L. Smart and E. Moore, *Solid State Chemistry: An Introduction*, CRC Press, 5th Ed., 2020.
5. A. R. West, *Basic Solid State Chemistry*, John Wiley & Sons Ltd., 2nd Ed., 1999.
6. S. Carron, *Recent Advances in Solid State Chemistry*, Random Exports, 2013.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis of $MMoO_4$ (M^{2+} = Ca, Sr. Ba) with scheelite structure.
2. Synthesis of MWO_4 (M^{2+} = Ca, Sr. Ba) with scheelite structure.
3. Synthesis of metal ions substituted scheelite related oxides to study structural tolerance and physical properties.
4. Synthesis of compounds with spinels and inverse spinels ($MgFe_2O_4$, $NiFe_2O_4$ and $CdFe_2O_4$) to study their structural variations and magnetic properties.
5. Synthesis of oxides, $MTiO_3$, (M^{2+} = Ca, Sr, Ba, Pb) with perovskite structure-study of structure-property correlation.
6. Synthesis of halide (AMX_3; A = Na, K; M = Ni; X = Cl, F) perovskites, study of structure-property correlation.
7. Synthesis of other compounds with ilmenite and apatite related stuctures.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. A. R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons Ltd., 2nd Ed., student edition, 2014.
2. C. N. R. Rao, *Chemical Approaches to Synthesis of Inorganic Materials*, Wiley, 1994.
3. E. A. Moore and L. E. Smart, *Solid State Chemistry: An Introduction*, CRC Press, 5th Ed., 2020.

4. A. I. Vogel, *Textbook of Quantitative Chemical Analysis*, Longman, 5th Ed., 1989.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Analytical Techniques CH-DSE-403	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

Advanced understanding on the principle of operation, sources of error and correct interpretation of results using appropriate analytical techniques will be aimed based on the knowledge gained by students under their UG courses.

Learning outcomes: At the completion of this course, the students should be able to:

- enable advanced analytical techniques along with the instrumentation part to perform optimal use of these techniques efficiently to their advantage and will be useful for getting in chemical industries.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Advanced Spectroscopic Methods (15 Hours)

Infrared spectroscopy, UV-Visible NIR spectroscopy. Raman Spectroscopy for Inorganic materials (e.g metal oxides, metal complexes, graphene, hard carbon etc.), Surface enhanced Raman spectroscopy (SARS) (e.g metal nanoparticles etc.), X-ray fluorescence (XRF) spectroscopy, X-ray Absorption Spectroscopy (XAS), X-ray Absorption Near Edge Structure (XANES), Extended X-ray Absorption Fine Structure (EXAFS), X-ray Emission Spectroscopy (XES). X-ray Photoelectron Spectroscopy (XPS), Auger electron spectroscopy.

Unit-2: Advanced Microscopic Techniques (15 Hours)

Field-Emission Scanning Electron Microscopy (FE-SEM) and High-Resolution Transmission Electron Microscopy (HR-TEM), Energy Dispersive X-ray Spectroscopy (EDX) and Elemental mapping, Atomic and Magnetic Force Microscopy (AFM and MFM).

Unit-3: Advanced Thermal and Coupled Analytical Techniques (15 Hours)

Thermal Conductivity and Diffusivity measurement techniques, Infrared Thermometry, Laser Flash Analysis (LFA), Use of Microwave radiation in Inorganic synthesis, Evaluation of Heat Capacity using DSC, Temperature dependent impedance spectroscopy, Hyphenated techniques: TGA-FTIR, TGA-GC-MS etc.

References (Theory)

1. G. D. Christian, *Analytical Chemistry*, John Wiley & Sons Inc., 6th Ed., 2004.
2. D. A. Skoog, D. M. West, R. J. Holler and T. A. Nieman, *Principles of Instrumental Analysis*, Saunders Golden Sunburst Series, 1997.
3. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle (Eds.), *Instrumental Methods of Analysis*, Wadsworth Publishing, 7th Ed., ISBN 0534081428, 1988.
4. G. N. George and I. J. Pickering, *X-ray Absorption Spectroscopy*, De Gruyter, 2025.
5. S. Hofmann, *Auger- and X-Ray Photoelectron Spectroscopy in Materials Science*, Springer, 2013.
6. J. M. Zuo and J. C. H. Spence, *Advanced Transmission Electron Microscopy: Imaging and Diffraction in Nanoscience*, Springer, 2016.
7. T. M. Tritt, *Thermal Conductivity Theory, Properties, and Applications*, Springer, New York, NY, 2004.
8. E. Barsoukov and J. R. Macdonald, *Impedance Spectroscopy Theory, Experiment, and Applications*, John Wiley & Sons, Inc., 2005.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Synthesis and characterization of CuO and related nanoparticles using UV-Visible-NIR spectroscopy.
2. Synthesis of inorganic materials/compounds using Microwave synthesizer followed by characterization by TGA, and UV-Vis spectroscopy.
3. Use of Raman Spectroscopy for the study of Graphene based materials and assignment of the Raman active bands.
4. Imaging of shape, size and composition of inorganic nanoparticles/metal oxides using FE-SEM and EDX analysis.
5. Measurement of temperature dependent conductivity/impedance of inorganic materials/compounds.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. G. D. Christian, *Analytical Chemistry*, John Wiley & Sons Inc., 6th Ed., 2004.
2. D. A. Skoog, D. M. West, R. J. Holler and T. A. Nieman, *Principles of Instrumental Analysis*, Saunders Golden Sunburst Series, 1997.
3. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle (Eds.), *Instrumental Methods of Analysis*, Wadsworth Publishing, 7th Ed., ISBN 0534081428, 1988.
4. G. N. George and I. J. Pickering, *X-ray Absorption Spectroscopy*, De Gruyter, 2025.
5. S. Hofmann, *Auger- and X-Ray Photoelectron Spectroscopy in Materials Science*, Springer, 2013.
6. J. M. Zuo and J. C. H. Spence, *Advanced Transmission Electron Microscopy: Imaging and Diffraction in Nanoscience*, Springer, 2016.
7. T. M. Tritt, *Thermal Conductivity Theory, Properties, and Applications*, Springer, New York, NY, 2004.
8. E. Barsoukov and J. R. Macdonald, *Impedance Spectroscopy Theory, Experiment, and Applications*, John Wiley & Sons, Inc., 2005.

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DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Nuclear and Radiochemistry CH-DSE-404	**04**	**03**	**01**	**–**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To impart advanced knowledge on nuclear chemistry and radiations.
- To comprehend the construction structure of reactors, interaction of nuclear radiations with matter and applications of radiochemistry.

Learning outcomes: At the completion of this course, the students should be able to:

- learn various aspects of materials including nuclear materials, isotopes, detectors, and applications.
- comprehend nuclear structure and nuclear stability, radioactivity, tracer techniques.
- understand nuclear reactions, different types of reactors, and interactions.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: **(15 Hours)**

Nuclear structure and nuclear stability, Nuclear models, Properties of the Nucleus, Radioactivity and nuclear reactions (including nuclear fission and fusion reactions). Hot atom chemistry, Nuclear fission and fusion reactors. Radioactive Decay Kinetics.

Unit-2: **(15 Hours)**

The interaction of nuclear radiations with matter. Radiation hazards and therapeutics. Detectors and their principles. The direction of radioactivity. The counting errors and their corrections. Nuclear Analytical Methods.

Unit-3: **(15 Hours)**

Tracer techniques and their applications. Isotope dilution and radio-activation methods of analysis. Fission product analysis (e.g., the technique of isolating two or three different fission products of U or Th and determining the yields). Nuclear Medicine, Radio pharmaceuticals.

References (Theory):

1. B. G. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice-Hall, 2nd Ed., 1969.
2. G. Friedlander, J. W. Kennedy, E. S. Marcus and J. M. Miller, *Nuclear & Radiochemistry*, John Wiley & Sons, 1981.
3. W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, John Wiley & Sons, 2nd Ed., 2017.
4. W. D. Loveland, D. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, John Wiley & Sons., 2006.

TUTORIAL COMPONENT **(1 Credit: 30 Hours)**

1. Simulation of Radioactive Decay Using a Chemical Clock Reaction.
2. Computational Modeling of Parent–Daughter Decay Chains.
3. Redox Behavior of Actinide Analogues Using Fe^{3+}/Fe^{2+} or Ce^{4+}/Ce^{3+} Systems.
4. Selective Precipitation and Separation of Fission Product Analogues (Ba^{2+}–Sr^{2+}–Ca^{2+} System).

5. Adsorption of Radionuclide Surrogates on Low-Cost Materials.
6. Simulation of Gamma-Ray Shielding Using UV/Visible Light Attenuation.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Tutorial)

1. G. F. Knoll, *Radiation Detection and Measurement*, John Wiley & Sons Inc. 4th Ed., 2010.
2. G. R. Choppin, J. Rydberg, J.-O. Liljenzin, C. Ekberg, *Radiochemistry & Nuclear Chemistry*, Academic Press, 4^{th} Ed., 2013.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Electrochemistry of Energy Storage Systems CH-DSE-405	**04**	**03**	**–**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To develop a fundamental understanding of thermodynamics and kinetics governing electrochemical energy storage systems.
- To analyze key electrochemical parameters such as voltage, capacity, energy density, and power density using theoretical and graphical tools (e.g., Tafel plots, Ragone plots, cyclic voltammetry).
- To understand the design and working principles of electrochemical cells, including electrodes, electrolytes, separators, and cell configurations.
- To compare and evaluate different battery chemistry, including lead–acid, nickel-based, lithium-ion, sodium-based, and emerging systems.
- To explore advanced electrode materials and their electrochemical storage mechanisms for next-generation batteries.

- To assess practical challenges such as safety risks, dendrite formation, self-discharge, cost, and lifecycle performance.
- To understand sustainability aspects, including battery recycling, reuse, and handling of hazardous materials.

Learning outcomes: At the completion of this course, the students should be able to:

- obtain fundamentals of electrochemical energy storage (Thermodynamics, Kinetics, and Basic Cell Concepts).
- learn battery chemistry and advanced electrode materials.
- understand the future perspectives of energy storage systems.

This syllabus covers foundational electrochemistry, energy storage concepts, electrochemical calculations and performance metrics and battery degradation and safety. This course offers knowledge to the students about types of battery, and their components, and architecture, electrochemical characterization techniques followed by cell design and assembly.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Fundamental Principles of Electrochemical Energy Storage Systems (15 Hours)

Thermodynamics and Kinetics of electrochemical Reactions, Introduction of mechanical, thermal, and chemical energy storage, Electrochemical series of metals, Key determining principles for voltage and capacity in electrochemical cells, Studies of Tafel and Ragone plots, Introductory concepts for calculating capacity, energy density, and power density of battery/devices, Basics of redox potential and Cell voltage, Fundamental concepts of Cyclic Voltammetry, Charge and Discharge, electrochemical impedance spectroscopy of cells, Impact of Self-Discharge of energy storage systems, Concepts of internal short circuits and dendrite formation, Cycle life of device, Kinetics at the electrode/electrolyte interface.

Unit-2: Battery Chemistry and Advanced Electrode Materials (15 Hours)

Primary (non-rechargeable) and Secondary (rechargeable) Batteries, Basic components in batteries: electrodes, electrolytes, separators, binders, and current collectors, Design and assembly of Half/Full Cells. Types of Battery Chemistry: (i) Lead–Acid Battery (ii) Nickel–Cadmium Battery (iii) Nickel–Metal Hydride Battery (iv) Lithium-Ion Battery (v) Sodium-Based Battery Technologies (vi) Rechargeable Zinc-Ion Batteries etc.

Materials: An introduction to advanced cathode and anode materials, along with the electrochemical storage processes that enable their use in battery applications: (i) Lithium metal; (ii) Carbon materials; (iii) Noncarbon materials; (iv) Lithium Nickel Manganese Cobalt Oxide; (v) Lithium Iron Phosphate; (vi) Lithium Cobalt Oxide; (vii) Layered Oxides; (viii) Polyanionic Compounds; (ix) Prussian Blue Analogues etc.

Unit-3: Advanced Energy Storage Systems: Safety, Degradation, Thermal Management, and Applications (15 Hours)

Study of advanced and emerging energy storage technologies including solid-state, lithium–sulfur, and lithium–air batteries, along with supercapacitors and hybrid capacitors; degradation mechanisms and failure analysis covering capacity fading, Solid Electrolyte Interphase (SEI) formation, mechanical degradation, and Calendar life vs cycle life; thermal management of batteries with emphasis on heat generation; safety, cost, and sustainability challenges including recycling and hazardous waste management (especially Li/Na metals); and applications of Energy Storage Systems in electric vehicles (Evs), grid-scale storage (renewable integration), and portable electronic devices.

References (Theory)

1. J.-K. Park, *Principles and Applications of Lithium Secondary Batteries*, Wiley-VCH Verlag GmbH & Co. KGaA, 2012.
2. C. Daniel and J. O. Besenhard, *Handbook of Battery Materials*, Wiley-VCH Verlag & Co. KGaA, 2011.
3. K. B. Oldham, J. C. Myland and A. M. Bond, *Electrochemical Science and Technology Fundamentals and Applications*, John Wiley & Sons, 2013.
4. K. Ozawa, *Lithium-Ion Rechargeable Batteries: Materials, Technology, and New Applications*, Wiley-VCH Verlag GmbH & Co. KGaA, 2009.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Synthesis and characterization of electrode materials.
2. Electrode fabrication methodologies.
3. Half-Cell and Full-Cell Assembly.
4. Measurement of Redox Potentials and Cell Voltages.
5. Electrolyte optimization.
6. Operation and testing of batteries.
7. CV, Charge/discharge and EIS Studies of the fabricated cells.
8. Self-Discharge and Cycle Life Assessment.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. S. J. Dhoble, N. T. Kalyani, B. Vengadaesvaran and A. K. Arof, *Energy Materials Fundamentals to Applications*, Elsevier, 2021.
2. A. F. Zobaa, *Energy Storage - Technologies and Applications*, IntechOpen, 2013.
3. A. J. Bard, *Electrochemical Methods: Fundamentals and Applications*, John Wiley & Sons, 2001.

4. B. Scrosati, K. M. Abraham, W. A. van Schalkwijk and J Hassoun, *Lithium Batteries: Advanced Technologies and Applications*, Wiley, 2013.
5. M. Titirici, P. Adelhelm and Y. Hu, *Sodium-Ion Batteries: Materials, Characterization, and Technology*, Volumes 1 & 2, Wiley-VCH, 2022.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry of Life Processes CH-DSE-406	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To provide knowledge about the chemistry of various biochemical processes essential for sustaining life.
- The students will understand the enzymatic pathways involved in metabolism and disorders caused by compromised enzyme activities.

Learning outcomes: At the completion of this course, the students should be able to:

- explain bioenergetics and metabolic processes in all living organism.
- illustrate enzyme pathways involved in production of cellular energy from carbohydrates, photosynthesis and gluconeogenesis.
- describe lipid metabolism including energy production and calorific values of food.
- classify protein degradation pathways for the formation of different nitrogenous by-products.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Introduction to metabolic processes and carbohydrate metabolism **(15 Hours)**

Catabolism and anabolism, Bioenergetics, ATP- Cellular currency of energy, energy-rich and energy-poor phosphates, role of NADH, NADPH, $FADH_2$, TPP, coenzyme A, lipoic acid and biotin. Carbohydrate metabolism: Glycolysis, Fate of pyruvate under anaerobic (lactic acid and alcoholic fermentation), Fate of pyruvate under aerobic conditions, PDH complex, citric acid cycle, oxidative phosphorylation (electron transport system), gluconeogenesis, pentose phosphate pathway and photosynthesis (Light-dependent and Light-independent reactions).

Unit-2: Lipid Metabolism **(15 Hours)**

Digestion and absorption of lipids, Activation of fatty acids, transport to mitochondria, fatty acid degradation (β-oxidation of even, odd chain and unsaturated fatty acids), Energetics of β-oxidation, ketone bodies, fatty acid anabolism, and calorific values of food. Disorders of lipid metabolism.

Unit-3: Protein Metabolism **(15 Hours)**

Glucogenic and ketogenic amino acids, transamination, oxidative deamination, degradation of amino acids (C3, C4, C5 family), Urea cycle, uric acid and ammonia formation (ammonotelic, ureotelic and uricotelic animals.

References (Theory)

1. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer-Verlag, 2012.
2. D. Nelson and M. M. Cox, *Lehninger Principles of Biochemistry*, W H Freeman & Co., 8th ed., 2021.
3. J. M. Berg, G. Gatto, J. Hines, J. L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman & Co., 10^{th} Edn., 2023.
4. D. Voet and J. G. Voet, *Biochemistry*, Wiley, 4^{th} Edn., 2010.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Spectrophotometric assay of the conversion of NAD to NADH using Lactate and Lactate Dehydrogenase (LDH) enzyme: Lactate + NAD^+ → (LDH) → Pyruvate + NADH
2. Yeast fermentation of sugars.
3. Studying the effect of temperature/pH on the fermentation of sugars.
4. Protein estimation by the UV-spectrophotometric method
5. Salting-in and salting-out of proteins
6. Desalting of Proteins using Sephadex G-25
7. Chemical synthesis of triglycerides *via* Fischer esterification and TLC analysis.
8. Lipid extraction and TLC separation using soy lecithin.
9. Measurement of enzyme activity parameters
10. Lipase-catalysed selective acetylation and deacetylation

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. W. W. Christie and X. Han, *Lipid Analysis: Isolation, Separation, Identification and Lipidomic Analysis*, Elsevier, 2016.
2. M. I. Gurr, J. L. Harwood, K. N. Frayn, D. J. Murphy and R. H. Michell, *Lipids: Biochemistry, Biotechnology and Health*, Wiley-Blackwell, 6th ed., 2016.
3. D. T. Plummer, *An Introduction to Practical Biochemistry*, Tata McGraw-Hill, 3rd ed.,1990.
4. J. Jayaraman, *Laboratory Manual of Biochemistry*, New Age International Publishers, 2011.
5. G. Sattanathan, S. S. Padmapriya and B. Balamuralikrishnan, *Practical Manual of Biochemistry*, Skyfox Publishing Group, 2020.

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DISCIPLINE SPECIFIC ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry of Supramolecules, Terpenes and Steroids CH-DSE-407	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To introduce the fundamental concepts of non-covalent interactions and molecular recognition, host-guest chemistry, binding models, self-assembly and functional supramolecular architectures.
- To discuss terpenes and steroids as natural products with their biosynthetic pathways, chemistry and importance of plant growth hormones, pheromones, steroid hormones, artemisinin and azadirachtin.
- To elaborate total synthesis approaches towards the natural products, and provide the students will gain with hands on training in chemical synthesis and extraction of some readily available natural products in the laboratory.

Learning outcomes: After completing this course, students will be able to:

- describe the principles of supramolecular chemistry and various types of non-covalent interactions, host-guest systems, macrocycles, and binding mechanisms.

- determine binding constants, stoichiometry, and thermodynamic parameters using UV–Vis, NMR titrations, Job's plot, and Benesi-Hildebrand method.
- apply supramolecular principles in chemical sensing, drug delivery, materials design, catalysis, and nanotechnology.
- classify various natural products including terpenes and steroids.
- design total synthesis of various terpenoids and steroids
- experiment on isolation and characterization of fragrance materials from natural sources like leaves, bark and peels of the fruits etc.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Supramolecular Chemistry (15 Hours)

Definition and scope of supramolecular chemistry, Historical development – from molecular to supramolecular chemistry, Concept of molecular recognition and self-assembly, Non-covalent interactions, Hydrogen bonding, π–π stacking and cation–π interactions, van der Waals forces, Electrostatic and hydrophobic interactions, Thermodynamics and kinetics of supramolecular interactions. Concept of host and guest molecules, Binding constants, association/dissociation equilibria. Methods for studying host–guest interactions: NMR, UV–Vis, fluorescence, ITC, Types of hosts: Crown ethers and cryptands, Cyclodextrins, Calixarenes, Cucurbiturils, Cyclophanes, Selectivity and complementarity principles. Molecular Recognition and Self-Assembly - principles, design and synthesis of receptors for ions and neutral molecules, cooperative binding and allosteric effects, Self-assembly processes in solution and solid state, Supramolecular polymers, micelles, vesicles, and gels, Template-directed synthesis. Supramolecular Devices and Materials- Molecular machines and switches, Supramolecular catalysis, Conducting and luminescent supramolecular materials, Applications in nanotechnology and drug delivery, Molecular devices, Ion channels, Novel liquid crystals, Gelators, fibres and adhesives, Dendrimers, organic solids, organic conductors and organic superconductors. Supramolecular approaches to drug design, Biomimetic chemistry and molecular recognition in biology

Unit-2: Terpenoids (15 Hours)

Introduction, classification and importance of terpenes and terpenoids, Isoprene and Special Isoprene rule. Biosynthesis of mono-, sesqui-, di- and triterpenes via Mevalonate (MVA) pathway, starting from acetyl-CoA to IPP and IPP to Squalene and various terpenes. Chemistry and importance of Plant growth hormones, e.g., Gibberellins and Pheromones. Gibberellic acid (GA3): General chemistry, Biosynthesis and structural elucidation. Importance, biosynthesis and General chemistry of Artemisinin and Azadirachtin.

Unit-3: Steroids (15 Hours)

Introduction of Steroids. Classification and importance of steroid hormones. General chemistry, Woodward's total synthesis of Cholesterol and Structural Elucidation of Cholesterol. Biosynthesis of Cholesterol: Squalene to Lanosterol and Lanosterol to Cholesterol. Biosynthesis of Estradiol and Esterone from Cholesterol, Synthesis of Progesterone from Diosgenin by Marker Degradation. Importance and chemistry of Ergosterol, Vitamin D2 and Vitamin D3.

References (Theory)

1. J.-M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.
2. D. Philp and J.F. Stoddart, *Angew. Chem. Int. Ed.*, 1996, **35**, 1155–1196.
3. J.W. Steed and J.L. Atwood, *Supramolecular Chemistry*, Wiley, 2nd Edn., 2009.
4. G. R. Desiraju, *Crystal Engineering: The Design of Organic Solids*, Elsevier, 1989.
5. F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, 1991.
6. Selected review articles from Chemical Reviews, Accounts of Chemical Research, and Nature Chemistry.
7. I. L. Finar, *Organic Chemistry*, Vol. 2, Pearson Education, 2002.
8. T. L. Gilchrist, *Heterocylic Chemistry*, Longman Scientific Technical.
9. A.R. Katritzky and C.W. Rees, *Comprehensive Heterocyclic Chemistry*, Pergaman Press.
10. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, *Natural Products: Chemistry and Biology Significance*, Prentice Hall, 1994.
11. I. L. Finar and A. L. Finar, *Organic Chemistry*, Vol. 2, Addison-Wesley, 1998.
12. I. L. Finar, *Organic Chemistry*, Vol. 1, Longman, 1998.
13. J. Mann, *Secondary Metabolites*, Oxford University Press, Oxford, UK, 1980.
14. J.M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, W.H. Freeman and Co., 9^{th} Edn., 2019.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Host–Guest Binding Constant Determination using UV–Vis or fluorescence titration.
2. Investigate of H-bonded complex formation (e.g., phenol–pyridine systems) using UV–Vis or FTIR monitoring of shifts in characteristic peaks.
3. Preparation of a supramolecular dye sensor
4. Formation of charge-transfer complexes (e.g., TCNQ + donor molecules) and monitoring by UV–Vis charge-transfer bands
5. Formation of donor–acceptor complexes and characterization by UV–Vis CT band
6. Isolation and characterization of Limonene from Citrus Peel by Steam Distillation
7. Isolation and characterization of Eugenol (phenolic terpenoid) from clove oil
8. Isolation and characterization of Menthol from peppermint oil
9. Extraction of Cholesterol from Egg Yolk and to characterize it on the basis of IR, NMR and Mass.
10. Colorimetric estimation of cholesterol by Liebermann–Burchard Reaction
11. Characterization of an unknown terpene using spectroscopic data
12. Separation of terpenes and steroids using Thin-Layer Chromatography (TLC) and Column Chromatography
13. Preparation of Limonene oxide by oxidation of limonene using m-CPBA
14. Oxidation of terpenes (e.g. Citral) using mild oxidising agents

15. Preparation of bornyl acetate by acetylation of borneol using acetic anhydride and acid catalyst.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. -M. Lehn, "*Supramolecular Chemistry: Concepts and Perspectives*", VCH, 1995.
2. J.W. Steed and J.L. Atwood, "*Supramolecular Chemistry*", Wiley, 2nd Ed., 2009.
3. A. I. Vogel, "*A Textbook of Practical Organic Chemistry including Qualitative Organic Analysis*" Longmans Green and Co., Ltd., London, 1966.
4. R.M. Silverstein, G. C. Bassler and T. C. Morril *Spectrometric Identification of Organic Compounds*, Wiley, 5th Edn., 1991.
5. D. H. William and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Springer Nature Switzerland AG, 7th Edn., 2020.
6. H. T. Clarke, *A Handbook of Organic Analysis Qualitative and Quantitative*, Edward Arnold (Pub.), Ltd. London, 1975.

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DISCIPLINE ELECTIVE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Alkaloids, Polyphenols, and Active Pharmaceutical Ingredients (APIs) CH-DSE-408	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To provide a comprehensive understanding of alkaloids, polyphenols and Active Pharmaceutical Ingredients (APIs) with emphasis on their chemistry, biosynthesis, structural elucidation and synthetic strategies.

- To elaborate the isolation and characterization of alkaloids, polyphenols and major therapeutic agents, along with their physicochemical properties, mechanistic pathways and total synthesis approaches.
- Students will also gain knowledge of analytical techniques, quality assessment, industrial practices and regulatory considerations essential for pharmaceutical ingredients and natural products.

Learning outcomes: After completing this course, students will be able to:

- explain the isolation, structure elucidation, and biosynthetic pathways of alkaloids and polyphenols.
- analyze synthetic and retrosynthetic strategies for complex natural products and important APIs.
- describe the therapeutic roles, mechanisms of action, and key physicochemical properties of widely used pharmaceutical agents.
- apply analytical techniques to assess the purity, identity, and quality of natural products and APIs.
- interpret industrial, regulatory, and process-related considerations in the development and evaluation of pharmaceutical compounds.
- experiment on purification and isolation of alkaloids, flavonoids, polyphenols and synthesis of common APIs

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Alkaloids (15 Hours)

(i) Morphine, (ii) Reserpine, (iii) Ergotamine, (iv) Sclerotioloids A–C, (v) Gardflorine A–C, (vi) Lysiformine

The study of the above-mentioned alkaloids, including (a) Basic Introduction - Definition, nomenclature, and general characteristics (basic nature, physical state, optical activity), historical background and significance in medicine and society, occurrence and distribution in nature (plants, fungi, animals) (b) Classification - Pharmacological action (analgesics, stimulants, etc.) and biosynthetic pathways, Based on chemical structure (e.g., presence of specific heterocyclic rings), (c) Isolation and Characterization - General methods for extraction and separation using techniques like solvent extraction, chromatography, and precipitation, Qualitative chemical tests for identification using specific reagents e.g. Dragendorff's, Wagner's) (d) Structural Elucidation and Total Synthesis - General methods for determining the molecular structure by functional group analysis and degradation, Modern spectroscopic techniques used in structure determination, detailed study of the structure, stereochemistry, and total synthesis (e) Biosynthesis - Study of Biosynthesis of alkaloids using thiokinase, mixed function oxygenases, methyl transferases, and amino acid decarboxylases (f) Chemical Reactions - Study of important reactions/rearrangements involved

Unit-2: Flavonoids and related polyphenols (15 Hours)

(i) Apigenin, (ii) Luteolin, (iii) Quercetin, (iv) Diadzen, (v) Myrtucommulone A, (vi) Prenylflavone, (vi) Binaringenin, (vii) Biflavanoids, and (viii) Catechin

The study of the above-mentioned Polyphenols, including (a) Introduction to Polyphenols and Flavonoids - Definition and classification of polyphenols, role in plants, Overview of their importance in the human diet and health benefits, Effect of structural features on their physical and biological properties, including antioxidant potential and solubility, Spectroscopic characteristics (UV, MS, NMR) used for identification and analysis (b) Biological Activities and Health Effects - Antioxidant, anti-inflammatory, anticancer, antimicrobial, antiviral activity, and anti-aging properties (c) Structural Elucidation and Synthesis - General methods for determining the molecular structure, including functional group analysis, Modern spectroscopic techniques used in structure determination, Detailed study of the structures and their synthesis (d) Biosynthetic pathways - Study of biosynthesis of polyphenols and flavonoids (e) Chemical Reactions Study of important reactions/rearrangements involved

Unit-3: Active Pharmaceutical Ingredients (APIs) (15 Hours)

Introduction, physicochemical characterization and synthesis of the following APIs.

i. Paracetamol (Acetaminophen), Ibuprofen, Aspirin, Tramadol, Diclofenac: Used for pain relief and anti-inflammatory activity

ii. Amoxicillin, Cefdinir: Antibiotics

iii. Amlodipine, Atenolol: Cardiovascular

iv. Metformin: Diabetes

v. Levothyroxine: Thyroid disorders

vi. Tenofovir Alafenamide Fumarate: Antivirals

vii. Amodiaquine, Chloroquine Phosphate: Antimalarial

viii. Lamotrigine: Antidepressants/CNS

xv. Omeprazole: Gastrointestinal

x. Furosemide: Diuretics

xi. Ziftomenib (API of drug Komzifti): Used to treat adults with relapsed or refractory acute myeloid leukemia (AML)

xii. Remibrutinib (API of drug Rhapsido): To treat chronic spontaneous urticaria in adults

xiii. Paltusotine (API of drug Palsonify): To treat acromegaly in adults

References (Theory):

1. I. L. Finar and A. L. Finar, *Organic Chemistry*, Vol. 2, Addison-Wesley, 1998.
2. I. L. Finar, *Organic Chemistry*, Vol. 1, Longman, 1998.
3. J. Mann, *Secondary Metabolites*, Oxford University Press, Oxford, UK, 1980.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Isolation of caffeine from tea leaves and its characterization with different spectroscopic techniques.
2. Isolation and characterization of piperine from black pepper.
3. Isolation and characterization of Eugenol from cloves.
4. Synthetic application of common reactions involved in alkaloids and polyphenols.
5. Synthesis of Eugenol from simple phenol-based compounds.
6. Semisynthetic modification of alkaloid and polyphenol-based natural products.
7. Structural modification/derivatisation of simple alkaloids and polyphenols.
8. Synthesis of Paracetamol from p-aminophenol; purification and melting-point determination.
9. Preparation of Aspirin (Acetylsalicylic acid) and assessment of reaction yield.
10. Synthesis of Ibuprofen derivative or analogues (as per safe laboratory availability).
11. Synthesis of an amide/ester intermediate relevant to antibiotic cores (e.g., β-lactam model compound).
12. Determination of partition coefficient (log P) for selected APIs.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. S. Berger, and D. Sicker, *Classics in Spectroscopy: Isolation and Structure Elucidation of Natural Products*, Wiley-VCH, 2009.
2. I. L. Finar and A. L. Finar, *Organic Chemistry*, Vol. 2, Addison-Wesley, 1998.
3. V. K. Ahluwalia and R. Aggarwal, *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press, 2004.
4. D. L. Pavia, G. M. Lampman, G. S. Kriz, and R. G. Engel, *Organic Chemistry Laboratory Techniques: A Microscale Approach*, Thomson Brooks/Cole, 2005.
5. A. M. Davis and S. E. Ward, *The handbook of medicinal chemistry: Principles and Practice*, Cambridge, UK: Royal Society of Chemistry, 2015.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		

Polymer Chemistry and Role of Catalysis in Chemical Synthesis CH-DSE-409	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To provide understanding of different techniques of polymerization, their molecular weight determination and processing of polymers.
- To elaborate the role of catalysis in the chemical synthesis that provides sustainable industrial methods for the formation of commercially available chemicals.
- To build a strong foundation for job opportunities in chemical industries involved in manufacturing polymer-based materials, fine chemicals and pharmaceuticals.

Learning outcomes: After completing this course, students will be able to:

- describe physicochemical properties and molecular architecture of biopolymers
- explain polymer processing methods
- understand the art of catalysis for homogenous and heterogenous catalysts
- analyse catalysed reactions used for industrial chemical transformations

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Polymer (15 Hours)

Introduction - Polymers and their classification. Synthesis of Polymers - Chemistry of radical, anionic and cationic polymerization; Zieglar–Natta catalysts; Polycondensation and ring opening polymerization. Methods of polymerization - Bulk, solution, suspension and emulsion polymerizations. Geometry of the polymers – Homopolymers, copolymers, branched-polymers, crosslinked polymers, random, alternating, block and graft copolymers, star polymers and dendrimers, tacticity of polymers. Characterization of polymers - Molecular weight determination of polymers, thermal properties of polymers, Glass transition temperature, plasticizers.

Unit-2: Polymer Processing and the Art of catalysis (15 Hours)

Polymer Processing - Injection moulding, compression moulding, blow moulding, Extrusion compounding, elastomer properties, vulcanization, reinforcement, fillers, plasticisers and other additives. The art of catalysis, Thermodynamic data and catalyst designing, metal-catalysed organic reactions, characteristics of transition metals which make them suitable as catalysts, homogeneous and heterogeneous catalysts and their characterization.

Unit-3: Role of Catalysis in Chemical Synthesis (15 Hours)

Catalyst and molecular activation, Catalytic reaction and the 16 electron rule, Catalysts for fine chemical synthesis, transition metal ion catalysts for organic transformations and their applications in epoxidation of alkenes, isomerization of unsaturated molecules, Alkene Metathesis, Oligomerisation and polymerization (Zeigler Natta polymerization), olefin oxidation (Wacker Process), Hydroformylation (oxoreaction) , Fischer-Tropsch Reaction, The water- Gas Shift Reaction, Monsanto Acetic Acid Process, Reppe Carbonylation, Hydrocyanation, activation of C-H bond, Green Chemistry and Catalysis, Computer applications in catalysis research.

References (Theory)

1. F. W. Billmeyer, *Textbook of Polymer Science*, Wiley-Blackwell, 3rd Ed., 1984.
2. G. Odian, *Principles of Polymerization*, Wiley, 4th Ed., 2004.
3. P. Hodge and D. C. Sherrington, *Polymer-supported Reactions in Organic Synthesis*, John Wiley & Sons, 1980
4. J. P. Collman and L. S. Hegedus, *Principles and Application of Organotransition Metal Chemistry*, University Science Books, 1980.
5. C. Elschenbroich and A. Salzer, *Organometallics: A Concise Introduction,* VCH, 1989.
6. S. M. Roberts and G. Poignant, *Catalysis for Fine Chemical Synthesis*, Volume 1-5, John Wiley & Sons, 2002.
7. R. A. Sheldon, A. Isabel and U. Hanefeld, *Green Chemistry and Catalysis*, Wiley-VCH, 2007.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Free-Radical Polymerization of Styrene.
2. Emulsion Polymerization (Styrene or Butadiene-Styrene)
3. Preparation of a Cross-linked Polymer (Gelatin/Polyacrylamide) & Swelling Study
4. Polymer Characterization — FTIR & DSC of Polymers
5. Rheology: Rotational Rheometer — Viscosity vs Shear Rate and Temperature
6. Polymer Blends & Compatibility — Phase Morphology (SEM/Optical)
7. Thermal Degradation / TGA Study — Stability of Polymers
8. Determination of Molecular Weight by Viscometry (Solution) — Mark–Houwink
9. Heterogeneous Catalysis — Hydrogenation of Styrene over Pd/C (bench scale)
10. Homogeneous Catalysis — Suzuki–Miyaura Cross-Coupling ($Pd(PPh_3)_4$)
11. Acid/Base Heterogeneous Catalysis — Esterification over Amberlyst/Zeolite
12. Enzymatic Catalysis — Lipase-Catalyzed Kinetic Resolution (ester hydrolysis)
13. Photocatalysis — Visible-Light Photocatalyzed Oxidation (Eosin Y or TiO_2)
14. Electrocatalysis — Electrochemical Reduction of Nitrobenzene to Aniline
15. Kinetics & Mechanism — Poisoning Study of Heterogeneous Catalyst

16. Catalyst Characterization Practical — XRD, BET, TEM/SEM

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. S. M. Roberts and G. Poignant, *Catalysts for Fine Chemical Synthesis, New Strategies in Chemical Synthesis and Catalysis*, Wiley & Sons, 2002.
2. D. G. Hundiwale, *Experiments in Polymer Science*, New Age International Private Limited, 2008.
2. T. A. Osswald, *Understanding Polymer Processing: Processes and Governing Equations*, Carl Hanser Verlag GmbH & Co., 2010.
3. A. I. Vogel, *Vogel's Textbook of Practical Organic Chemistry*, Wiley, 5th Edn., 1989.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Quantum Chemistry CH-DSE-410	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:
- Provide an advanced understanding of quantum chemistry, this course covers state-of-the-art methods for solving complex many-body systems.
- Explore modern computational techniques, students will gain the skills needed to design and analyze contemporary materials.
- Understand higher-order and degenerate perturbation theory, second quantization, density functional theory (DFT), quantum statistics, Hartree–Fock theory, and post–Hartree-Fock methods.

Learning outcomes: After completing this course, students will be able to develop understanding of:

- many-electron systems—including perturbation theor:y and variational principles—along with quantum statistics and tunnelling phenomena relevant to chemical and biological processes.
- second quantization, density functional theory, Hartree–Fock self-consistent-field approach, as well as various semi-empirical and post–Hartree–Fock methods, with emphasis on their applications in chemistry.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Quantum Mechanics of Many-Electron Systems (15 Hours)

Perturbation theory: second order for non-degenerate states and applications, first order for degenerate states. Orbital and spin angular momentum operators of many-electron systems, L-S and J-J couplings, Pauli matrices.

Hartree product, Antisymmetrization, Slater determinantal wavefunctions. Matrix elements for one and two electron operators. Secular equation for many-electron Slater determinantal functions.

Unit-2: *Ab Initio* and Semiempirical Methods (15 Hours)

Hartree-Fock Self-Consistent-Field methods, energy minimization (Lagrange method), Roothaan's equations. Koopmans Theorem, Merits and demerits of Basis sets (Slater, Gaussian and integral transform), Electron correlation, CI theories, Brillouin's theorem

Semiempirical Theories- review of HMO, EHT and PPP methods. ZDO approximation and CNDO, INDO

Unit-3: Density Functional Theory (DFT) (15 Hours)

Thomas-Fermi Model, Hohenberg-Kohn theorem. Nature of electron density distribution and Density Functional Theories (DFT). Density functional interpretation of some concepts (electronegativity, electronegativity equalization, softness and hardness, etc.). Electron correlation in DFT, Kohn-Sham equation and its applications.

References (Theory)

1. J. P. Lowe and K. Peterson, *Quantum Chemistry*, Academic Press, 2005.
2. R. G. Mortimer, *Mathematics for Physical Chemistry*, 2nd edn, Elsevier, 2005.
3. F. L. Pilar, *Elementary Quantum Chemistry*, 2nd edn, Dover Publications Inc., New York, 2001.
4. P. W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edn, Oxford University Press, 2006.
5. P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 3rd edn, Oxford University Press, 1997.
6. I. N. Levine, *Quantum Chemistry*, 5th edn, Prentice Hall Inc., New Jersey, 2000.
7. T. Engel and P. Reid, *Physical Chemistry*, Benjamin-Cummings, 2005.

8. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, 3rd edn, University Science Books, 2001.
9. R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, 2004.
10. M. Springborg, *Methods of Electronic Structure Calculations*, Wiley, 2000.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

1. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).
2. Elements of the C/C++/FORTRAN/BASIC languages, including strings and graphics.
3. Numerical methods and their applications in chemistry
    a) Multiplication of matrices
    b) Jacobi Diagonalization of hermitian matrices
    c) LU decomposition of a matrices
    d) Quick Sort, Bubble Sort algorithm and programming
4. Typical Exercises
    a) Decimal-binary conversion
    b) Numerical differentiation, quadrature and finding roots
    c) pH of a weak acid
    d) Roots of cubic equations (e.g. van der Waals' equation)- iterative, Newton-Raphson, Binary bisection, Regula-Falsi methods.
5. Least-squares fit including graphics

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. Noggle, *Physical Chemistry Using Mathcad*, Newark, DE, 1997.
2. D. Rogers, *Computational Chemistry Using the PC*, 3rd edn, Wiley-Interscience, 2003.
3. C. M. Quinn, *Computational Quantum Chemistry*, Academic Press, 2002.
4. W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes in C: The art of Scientific computing*, Cambridge University Press, 1993.
5. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in FORTRAN 77: The art of Scientific computing*, 2nd Ed., Cambridge University Press, 1993.
6. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 3rd Ed., Cambridge University Press, 2007.

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DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Fluorescence Methods for Chemical and Biomedical Research CH-DSE-411	**04**	**03**	—	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- Introduce the principles of fluorescence and phosphorescence in molecules and biomolecules, along with techniques for recording absorption, emission, and time-resolved spectra.
- Explain factors affecting fluorescence such as solvent polarity, pH, concentration, and quenching.
- Demonstrate applications in biomolecular systems and develop practical skills in fluorescence experiments and data interpretation.

Learning outcomes: After completing this course, students will be able to:

- Measure and interpret absorption and emission spectra, and calculate fluorescence parameters such as Stokes shift, quantum yield, and lifetimes.
- Analyse effects of environment, pH, solvent, concentration, and perform quenching studies (dynamic and static).
- Apply fluorescence techniques to study biomolecular interactions, conformational changes, and energy transfer processes.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Fundamentals of Fluorescence Spectroscopy (15 Hours)

Introduction to fluorescence spectroscopy, Quantum mechanical descriptions and significance, Absorption, emission, and excitation spectra, Stokes shift, Jablonski diagram; Types of fluorophores, and labelling strategies; Instrumentations of spectrofluorometers and its components (detectors, lasers, light sources etc.); Discussion on Steady-state, pico-second and femtosecond time-resolved fluorescence spectroscopy, Discussion on fluorescence quantum yield, lifetime, anisotropy, and solvent effect on fluorescence spectra.

Unit-2: Advanced Fluorescence Methods and Analysis (15 Hours)

Fluorescence quenching, Energy transfer (FRET) principles, and applications; Polarization anisotropy, molecular rotation and binding studies; Solvent relaxation, effect of environment on fluorescence; Advanced fluorescence imaging techniques (epi-fluorescence, Confocal microscopy, total-internal reflection fluorescence (TIRF), Single-molecule fluorescence spectroscopy), fluorescence correlation spectroscopy (FCS)-principles, instrumentation, and data interpretation.

Unit-3: Applications of Fluorescence Spectroscopy (15 Hours)

Study of structure, dynamics, and folding of biomolecules; lipid organization, fluidity, and protein-lipid interactions; Fluorescent proteins and its variants, Optical properties of nanomaterials, live-cell imaging; Specific examples highlighting applications of fluorescence techniques.

References (Theory)

1. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Ed., Springer, 2006.
2. B. Alberts, A. Johnson, J. Lewis, M. Raff, K. Roberts and P. Walter, *Molecular Biology of the Cell*, 5th Ed., Garland Science, 2008.
3. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH Verlag GmbH, 2001.
4. K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, 4th Ed., New Age International Private Limited, 2021.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Recording absorption and emission spectra of different fluorescent dyes (e.g., fluorescein, rhodamine or other dye molecules) and determining Stokes shifts.
2. Measurement of fluorescence quantum yield of dyes using a reference standard.
3. Synthesis of nanomaterials and investigation of its fluorescence properties.
4. Evaluation of solvent effects on fluorescence emission spectra of a dye in polar vs. non-polar solvents.
5. Evaluation of CMC of surfactant molecules (Cationic, anionic and neutral) using fluorescence spectroscopy.
6. Dynamic and static quenching studies using a suitable dye-quencher pair; calculation of quenching constants.
7. Dynamic and static quenching studies in heterogenous medium and calculation of quenching constants.
8. Determine energy transfer efficiency between donor-acceptor dye pairs.

9. Study intrinsic tryptophan fluorescence to monitor protein folding/unfolding.
10. Effect of pH on the fluorescence properties of pH-sensitive molecules.
11. Record the fluorescence spectra of a weak acid (α-naphthol or others) at different pH and determine the dissociation constant in the excited state.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Ed., Springer, 2006.
2. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH Verlag GmbH, 2001.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Chemical Kinetics CH-DSE-412	**04**	**03**	**__**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- Understand kinetic rate expressions and how to design experiments to determine them.
- Gain exposure to advanced topics in kinetics and reactor design relevant to post graduate-level research and industry. with an emphasis on more sustainable chemical and energy conversion systems
- Develop problem-solving methodologies and creative thinking skills for Chemical reactions.
- Develop computer skills for mathematical modelling of reactive systems to broadly apply to a wide range of real-world problems.

Learning outcomes: After completing this course, students will be able to understand:

- the importance of chemical kinetics in optimizing chemical processes
- designing new materials and drugs, ensure safety, and understand natural phenomenon like biological and environmental reactions.
- understanding the importance of this branch for developing and optimizing enzymes and catalysts.
- use reaction dynamics at microscopic level.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Theories of Reaction Rates (15 Hours)

Theories of Reaction rate: Arrhenius theory, Collision theory. Activated Complex theory.
Potential energy surfaces: attractive and repulsive forces, theoretical calculations of rate constant.
Hinshelwood's Treatment, Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular reactions.

Unit-2: Chemical & Enzyme Kinetics of Complex Reactions (15 Hours)

Complex reactions: Reversible first order reaction, Consecutive first order reaction, Chain reactions and oscillatory reactions, Principle and applications of Photochemical reactions, Homogeneous catalysis.
Enzyme kinetics: Factors Affecting Enzyme Activity. Michaelis-Menten mechanism (single and double intermediates). King-Altman method for working out the kinetics of complex enzyme reactions.
Enzyme inhibition- types of inhibition, products inhibition. Usefulness of inhibitors: Computer simulation in chemical kinetics.

Unit-3: Reaction Dynamics (15 Hours)

Reaction Dynamics: Importance of reaction dynamics. Molecular beams, principle of crossed-molecular beams. Molecular encounters and principal parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity). Influence of reactant vibrational and rotational energy. Dependence of collisional cross-section on translational energy.
Probing the transition state, Dynamics of barrierless chemical kinetics in solution, dynamics of unimolecular reactions.

References (Theory)

1. K. J. Laidler, *Chemical Kinetics*, 3rd edn, Benjamin Cummings, 1997.
2. M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford University Press, 1997.
3. R. J. Silbey, R. A. Alberty and M. G. Bawendi, *Physical Chemistry*, 4th edn, Wiley, 2005.
4. A. G. Marangoni, *Enzyme Kinetics*, Wiley-Interscience, 2005.
5. P. L. Houston, *Chemical Kinetics and Reaction Dynamics*, 2nd edn, Dover Publications, 2006.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Determine the rate constant of reaction between hexacyanoferrate and thiosulphate in the absence and presence of metal catalysts like silver or gold.
2. Study the kinetics of decolourisation of Crystal violet in alkaline medium.
3. Study the kinetics of oxidation of ethanol by potassium dichromate. Determine the order, rate constant, energy of activation and possible mechanism for the reaction.
4. Study the kinetics of hydrolysis of 4-nitrophenyl ethanoate in the presence of base.
5. Study the pH dependent kinetic study of oxidation of D-glucose by enzyme glucose-oxidase (GOD).
6. Determine the velocity constant for the mutarotation of D(+) glucose and determine the order of the reaction and the equilibrium concentrations of the two forms.
7. To determine the order and the rate constant of the reaction between Potassium iodide and hydrogen peroxide in acidic environment. Determine the activation energy and other thermodynamic parameters of this reaction.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, 18th Ed., R. Chand & Co., 2018.
2. J. N. Gurtu, *Advanced Physical Chemistry Experiments*, Pragati Publications, 2008.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		

Advanced Molecular Spectra CH-DSE-413	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives: Students will understand and explain

- To deliver advanced insight into vibrational, electronic, and ESR spectroscopy, as well as group theory
- Its roles in elucidating molecular structures.

Learning outcomes: By the end of this course, students will be able to:

- Basic comprehension of vibrational, electronic, and ESR spectroscopy for characterizing atomic and molecular systems.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Vibrational and Electronic spectroscopy (15 Hours)

Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules: BF3, NH3. Square planar, trigonal bipyramid, framework and cage molecules. Jahn-Teller distortions.
Electronic spectroscopy: Electronic spectroscopy of transition metal complexes. Octahedral and tetrahedral complexes, Correlation diagrams for octahedral fields and fields of lower symmetry.
Electronic spectroscopy of organic molecules - benzene, effect of substitution- pyridine, pyrimidine, pyrazine, methyl substitution. Vibronic analysis.

Unit-2: Electron Spin Resonance spectroscopy (15 Hours)

Basic principles. Relaxation and Line Widths. Zero-field splitting and Kramer's degeneracy. *g*-factor for paramagnetic ions. *g*-factor for organic radicals. Factors affecting the *g*-factor.
Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra.

Unit-3: Applications of ESR spectroscopy (15 Hours)

Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and *o*-, *m*- and *p*-xylene radical ions from HMO theory. Study of unstable paramagnetic species, Kinetic studies of electron transfer reactions, Spin-labelling studies of biomolecules.

References (Theory)

1. D. C. Harris and M. D. Bertolucci, *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Publications, New York, 1990.
2. D. M. Bishop, *Group Theory and Chemistry*, Clarendon Press, Oxford, UK, 1973.

3. R. Kakkar, *Atomic & Molecular Spectroscopy*, Cambridge University Press, 2015.
4. D. N. Satyanarayana, *Handbook of Molecular Spectroscopy: From Radio Waves to Gamma Rays*, I. K. International Publishing House, 2015.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. Record the UV spectra of a weak acid (p-nitrophenol in 1:4 ethanol: water mixture) at different pH and determine the dissociation constant in the ground state.
2. Record the UV spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the ground state.
3. Record the fluorescence spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the excited state. Comment on the difference in the two values using MO theory.
4. Record the UV spectra of methyl orange at different pH and determine its dissociation constant.
5. Study the effect of surfactant on the *pKa* value of methyl orange.
6. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron(III) by Job's method of continuous variation. Determine the concentration equilibrium constant and extinction coefficient for the charge transfer complex by applying the Benesi-Hildebrand equation.
7. Repeat Expt. 4 for salicylate ions in place of thiocyanate ions.
8. Record the UV spectra of benzene, pyridine and pyrimidine in methanol. Compare and discuss the various transitions involved in terms of MO theory.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., 2015.
2. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th edn, Brooks/Cole, 2017.
3. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, 2nd revised edn, Holt, Rinehart & Winston of Canada Ltd., 1988.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Computational Methods in Chemistry CH-DSE-414	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- This course offers a solid foundation in programming languages such as BASIC, FORTRAN, and C, and provides comprehensive training in empirical and semi-empirical electronic structure calculations and simulations.

Learning outcomes: After completing this course, students will be able to:

- Students will be able to learn various programming languages that are required for different types of molecular simulations and electronic structure calculations.
- They will be able to write independent programs and correctly compile them.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Computational Tools and Pattern Recognition (15 Hours)

Introduction to LINUX/UNIX and shell scripts. Some illustrative numerical methods in chemistry: numerical differentiation, integration and solution of ODE, matrix inversion and diagonalization, interpolation. Pattern recognition techniques and molecular graphics.

Unit-2: Computational Chemistry Methods (15 Hours)

Basics of electronic structure calculations, Molecular Mechanics, Monte Carlo and Molecular Dynamics simulations. Use of some packages to study molecular electronic structures and molecular modelling (GAMESS, MOPAC, molecular dynamics packages, etc.)

Unit-3: Chemoinformatics and Drug Design (15 Hours)

Basic ideas on structure-activity relationships, drug and catalysis design, etc. Development of some simulation programs and use of the internet for chemical information retrieval. Chemoinformatics.

References (Theory)

1. A. Hinchliffe, *Modelling Molecular Structures*, 2nd edn, John Wiley & Sons, 2003.

2. H.-D. Höltje, W. Sippl, D. Rognan and G. Folkers, *Molecular Modeling: Basic Principles and Applications*, 2nd edn, Wiley-VCH, 2003.
3. A. R. Leach, *Molecular Modelling: Principles and Applications*, 2nd edn, Pearson Education, England, 2001.
4. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran/C*, 2nd edn, Cambridge University Press, 1996.
5. E. Lewars, *Computational Chemistry*, Kluwer Academic Publishers, 2003.
6. F. Jensen, *Introduction to Computational Chemistry*, Wiley, 2007.
7. C. J. Cramer, *Essentials of Computational Chemistry*, John Wiley & Sons, England, 2002.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).
2. Elements of the C/C++/FORTRAN/BASIC languages, including strings and graphics.
3. Numerical methods and their applications in chemistry
    e) Multiplication of matrices
    f) Jacobi Diagonalization of hermitian matrices
    g) LU decomposition of a matrices
    h) Quick Sort, Bubble Sort algorithm and programming
4. Typical Exercises
    a) Decimal-binary conversion
    b) Numerical differentiation, quadrature and finding roots
    c) pH of a weak acid
    d) Roots of cubic equations (e.g. van der Waals' equation)- iterative, Newton-Raphson, Binary bisection, Regula-Falsi methods.
5. Least-squares fit including graphics.
6. Numerical solution of differential equations (e.g. in kinetics).
7. Intrapolation & interpolation of data.
8. Calculate Entropy (*S*) from C_p data.
9. Calculate Enthalpy (*H*) from C_p data.
10. Calculate Free Energy (*G*) from C_p data.
11. Verification of Nernst Heat Theorem.
12. Gauss-Siedel method and its use in solving simultaneous equations (e.g. Lambert-Beer's law).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. J. Noggle, *Physical Chemistry Using Mathcad*, Newark, DE, 1997.
2. D. Rogers, *Computational Chemistry Using the PC*, 3rd edn, Wiley-Interscience, 2003.
3. C. M. Quinn, *Computational Quantum Chemistry*, Academic Press, 2002.
4. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 3rd edn, Cambridge University Press, 2007.
5. W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes in C: The Art of Scientific Computing*, Cambridge University Press, 2nd edn., 1992.
6. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran 77: The Art of Scientific Computing*, Cambridge University Press, Cambridge, 2nd edn., 1992.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC ELECTIVE (DSE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Solid State Chemistry CH-DSE-415	**04**	**03**	**--**	**01**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives

- In-depth understanding of crystal structures and diffraction methods for analyzing crystalline and amorphous materials.

Learning outcomes: After completing this course, students will be able to:

- The fundamental concepts of symmetry and crystal structure as explored through diffraction and scattering techniques.
- To determine the structures of crystalline, amorphous, organic materials, and proteins.
- The electronic and magnetic properties of metals and semiconductors.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Scattering and Diffraction Theory (15 Hours)

Unit cells, and crystal symmetry; Relation of the crystal symmetry to the symmetry observed in a diffraction experiment for primitive, orthorhombic, tetragonal, trigonal, hexagonal, and cubic crystal systems. Concept of Reciprocal space.
Interaction of radiation with condensed matter and how this can be used in generalized crystallography. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, Structure factor and its relation to intensity and electron density, Fourier synthesis. Phase problem, Patterson synthesis. Heavy atom method. Direct method. Refinement, R factor. Fourier refinement. Least squares refinement. Determination of absolute configurations (Bijvoet method). Chemical interpretation of results. Estimation of errors. Effects of thermal motion, limitations. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

Unit-2: Electronic properties and Band Theory **(15 Hours)**

Metals, insulators and semiconductors, electronic structure of solids- band theory, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors.
Magnetic properties- Classification of materials: Quantum theory of paramagnetics - cooperative phenomena - magnetic domains, Hysteresis.

Unit-3: Organic Electronic Materials and their Characterization **(15 Hours)**

Organic solids: Electrically conducting solids, organic charge transfer complexes, organic metals, new superconductors.
Electron Microscopy: Fundamentals of electron microscopy as a useful subsidiary technique for crystallographers; Examples of its application in materials science and macromolecular structural biology.
Electron diffraction: Scattering intensity *versus* scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

References (Theory)

1. E. A. Moore and L. Smart, *Solid State Chemistry: An Introduction*, 2nd edn, Chapman & Hall, 1996.
2. G. Rhodes, *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models*, 3rd edn, Elsevier, 2006.
3. W. Massa, *Crystal Structure Determination*, 2nd edn, Springer, 2004.
4. B. E. Warren, *X-Ray Diffraction*, Dover Publications, 1990.
5. D. E. Sands, *Introduction to Crystallography*, Dover Publications, 1994.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Preparation of oxide materials (For example, ZnO, TiO_2) or semiconducting materials (CdSe, ZnSe, In_2S_3) by using any solid-state synthesis technique or any soft chemical approach.
2. Determination of crystal phase using powder diffraction pattern of prepared or known samples.
3. Calculation of crystallite size from the powder X ray diffraction pattern of prepared materials using Debye Scherrer equation.
4. Calculation of lattice strain (tensile or compressive) from the powder X ray diffraction pattern of prepared materials using Williamson-Hall plot.
5. Determination of cell parameters (a,b,c and α,β,γ) from the powder X ray diffraction pattern of prepared materials.
6. Determination of band gap of a semiconducting nanoparticle (in solution) using UV visible spectrophotometer.
7. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).
8. Determination of magnetic properties using Vibrating Sample Magnetometer working at room temperature and with magnetic field ranging of 1Tesla (students can use the machine at USIC, University of Delhi).
9. Studying photocatalytic degradation of environmentally pollutant dye (Crystal Violet, Rhodamine B, methyl orange etc.) by any semiconducting (In_2S_3, CdSe, ZnO- any of one) or metallic nanoparticles under visible light irradiation and using UV-Visible spectrophotometer.
10. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
11. Determination of glass transition temperature of a given salt (e.g. $CaCl_2$) conductometrically.
12. Thermogravimetric and Differential Thermal analysis (TGA and DTA) of an as prepared sample.
13. Measurement of photoluminescence properties of semiconducting nanomaterials (at least one) using fluorescence spectroscopy.
14. Demonstration: Sample preparation, observation and visualization of internal structure of as synthesized nanoparticles using transmission electron microscope (TEM) instrument.
15. Demonstration: Visualization of diffraction rings and identification of hkl planes of as synthesized nanoparticles from selected area electron diffraction (SAED) data using transmission electron microscope (TEM) instrument.
16. Demonstration: Observation of elemental/chemical composition of as synthesized nanoparticles from energy dispersive x-ray spectroscopic (EDX) data using transmission electron microscope (TEM) or Scanning electron Microscope (SEM) instrument.
17. Demonstration: Sample preparation, observation and visualization of surface morphology of as synthesized nanoparticles using scanning electron microscope (SEM) instrument.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. C. N. R. Rao, A. Müller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH GmbH & Co., Weinheim, 2007.
2. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry Experiments*, Pragati Prakashan, 2011.
3. B. D. Khosla, V. C. Garg and A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co., New Delhi, 2015.
4. G. N. Mukherjee, *University Handbook of Undergraduate Chemistry Experiments*, University of Calcutta, 2003.
5. I. M. Watt, *The Principles and Practice of Electron Microscopy*, Cambridge University Press, Cambridge, 2nd edn., 1997.
6. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, Springer, New York, 3rd edn., 2006.
7. C. J. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 6th edn, Tata McGraw-Hill, New Delhi, 2025.
8. R. F. Egerton, Physical Principles of Electron Microscopy: An Introduction to SEM, TEM and AFM, Springer, New York, 2nd edn., 2016.
9. W. Kemp, *Organic Spectroscopy*, 3rd edn, Palgrave Macmillan, London, 1991.
10. Y. Waseda, E. Matsubara and K. Shinoda, *X-Ray Diffraction Crystallography: Introduction, Examples and Solved Problems*, Springer, Berlin, 2nd edn., 2011.

Assessment methods: All examination and assessment methods shall be in line with the University of Delhi guidelines issued from time to time.

Techniques of Research Writing

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite of the course (if any)
		Lecture	Tutorial	Practical		
Techniques of Research Writing CH-SBC-4301	**02**	**01**	**-**	**01**	UG	**--**

Course objectives:

- To teach the effective techniques for research writing, communication and publishing ethics.

Learning outcomes: At the completion of this course, the students should be able to:

- improve scientific communication.
- communicate experimental results.
- know ethics in Research and publishing.
- prepare important components of a research paper
- design an experiment to publishing the results.

THEORY COMPONENT (1 Credit: 15 Hours)

Unit-1:

Recording, Writing and Presentation Skills of the research findings: Understanding the importance of recording the scientific data, its writing and presentation.

Writing Process & Disseminations and Ethics: Structure, writing while researching, Study the significance, Guide for authors, Revising-Editing-and-Proofing. Ethical principles in research writing. Scientific Misconduct. Consequences of unethical practices. Authorship. Data Management: Ethical data storage.

The Anatomy of a Chemistry Research Paper: IMRaD Structure, Reporting Chemical Data, The Abstract and Title, Preparing supplementary Information for a research paper, Dissertation Writing, Structure of a Review paper.

Technical writing and Style Guidelines: The Style Guide, Grammar for Science, Visual Representation, Numbers and Units.

The Publication Ecosystem: Peer Review, Journal Metrics, Predatory publishing, Copyright.

References (Theory)

1. C. D. Manning, P. Raghavan and H. Schütze, *Introduction to Information Retrieval*, Cambridge University Press, 2008.
2. W. C. Booth, G. G. Colomb and J. M. Williams, *The Craft of Research*, University of Chicago Press, 4th ed., 2016.
3. H. P. Stern, *The scientific publishing handbook: A Practical Guide to Writing and Publishing a Scientific Paper*, Springer, 2019.
4. F. Ecarnot, M.-F. Seronde, R. Chopard, F. Schiele, N. Meneveau, *Writing a scientific article: A step-by-step guide for beginners*, European Geriatric Medicine 6 (2015) 573–579.
5. S. Gao, A short comment on how to write research papers for STM journals, Inorganic Chemistry Frontiers, 1 (2014) 518-520.

6. G. M. Whitesides, *Whitesides' Group: Writing a Paper*, Advanced Materials, 16 (2004) 1375-1377.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Create a library and generate a bibliography with Mendeley or other software.
2. Draw a Graphical Abstract for a hypothetical paper using drawing software.
3. Write a formal "Experimental Section" for a synthesis performed in the lab, including full spectral characterization data formatting.
4. Prepare a Cover Letter to an Editor and format a manuscript file according to a specific journal's "Guide for Authors."
5. Submit a sample text, interpret the similarity report, and rewrite the flagged sections to reduce similarity.
6. Prepare a supporting information for publication and Review Only.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. M. Coghill and L. R. Garson, *The ACS style guide: Effective Communication of Scientific Information*, American Chemical Society, 3rd Ed., 2006.
2. C. D. Manning, P. Raghavan and H. Schütze, *Introduction to Information Retrieval*, Cambridge University Press, 2008.
3. W. C. Booth, G. G. Colomb and J. M. Williams, *The Craft of Research*, University of Chicago Press, 4th Ed., 2016.
4. National Academies of Sciences, Engineering, and Medicine, *Fostering Integrity in Research*, The National Academies Press, 2019.
5. H. P. Stern, *The Scientific Publishing Handbook: A Practical Guide to Writing and Publishing a Scientific Paper*, Springer, 2019.
6. E. Wager and S. Kleinert, *Good Publication Practice for Communicating Science and Technology: An Instructional Manual,* World Association of Medical Editors (WAME), 2011.
7. C. D. Manning, P. Raghavan and H. Schütze, *Introduction to Information Retrieval*, Cambridge University Press, 2008.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Quantitative Analyses of Alloys CH-SBC-401	**02**	**00**	—	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	--

Course objectives:

- To analyze the metal ions and insolubles accurately from various alloys through extractions followed by complexometric and gravimetric experiments.

Learning outcomes: At the completion of this course, the students should be able to:

- learn and simultaneously execute the principles complexometric titrations using suitable buffers and indicators. Some insolubles will be estimated through gravimetric titrations.

PRACTICAL COMPONENT **(2 Credit: 60 Hours)**

Suggested/Recommended List of Experiments:

1. To estimate calcium and magnesium in a given ore by complexometric titrations using EDTA.
2. To estimate copper and zinc in a given ore by iodometric and complexometric titrations using sodium thiosulphate and EDTA solution.
3. To estimate the metal ions in Bronze.
4. To estimate the metal ions in Brass.
5. To estimate the metal ions in Dolomite.
6. To estimate the metal ions in Cement.
7. To estimate the metal ions in Gun metal.
8. To estimate the metal ions in Solder.
9. To estimate Aluminum in a sample solution by complexometric titration.
10. To estimate zinc, manganese and magnesium in a sample solution by complexometric titration.
11. To estimate Fe^{3+} and Cr^{3+} in a sample solution by complexometric titration.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's text book of quantitative chemical analysis,* Longman Scientific & Technical, 5th Ed., 1989.
2. G. D. Christian, P. K. Dasgupta and K. A. Schug, *Analytical Chemistry*, Wiley, 7th Ed., 2013.
3. D. C. Harris, *Quantitative Chemical Analysis*, W. H. Freeman and Company, 7th Ed., 2006.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Instrumental Analysis-II CH-SBC-402	**02**	**00**	**-**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

The objective of the course is to teach instrumental analysis.

Learning outcomes: At the end of this course the student will be able to:

- understand fundamental principles behind modern analytical, spectroscopic, thermal, electrochemical, and separation techniques used in chemistry.

PRACTICAL COMPONENT **(2 Credit: 60 Hours)**

Suggested/Recommended List of Experiments:

Any three/four techniques covered in the semester out of the following syllabus:

1. Synthesis and analysis of basic structural types using powder X-ray diffraction patterns, indexing simple cubic, tetragonal and orthorhombic PXRD patterns and crystallite size determination..
2. Morphology examination of solids through FESEM, TEM, and electron diffraction imaging.
3. Synthesis and thermal analysis of decomposable inorganic complexes.
4. Synthesis and PXRD characterization of MOFs materials.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. G. Brauer, *Handbook of Preparative Inorganic chemistry*, Vol. 1 and 2, Academic Press, New York, 2nd ed., 1967.
2. G. Marr and B. W. Rockett, *Practical Inorganic Chemistry*, Van Nostrnad Reinhold, London, 1972.
3. G. Pass and H. Sutcliffe, *Practical Inorganic Chemistry*, Chapman and Hall, 2nd Ed., 1985.
4. J. D. Woolins, *Inorganic Experiments*, Wiley – VCH Verlag GmbH and Co., 2003.
5. G. D. Christian, P. K. Dasgupta and K. A. Schug, *Analytical Chemistry (An Indian Adaptation)*, Wiley India Pvt. Ltd., 2020.
6. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, Cengage Learning Publishers, 7th ed., 2016.
7. Willard, Merritt, Dean and Settle, *Instrumental Methods of Analysis*, CBS Publishers & Distributors; 7th Ed., 2004.
8. B. K. Sharma, *Instrumental Methods of Chemical Analysis*, Krishna Prakashan Media, 25th ed., 2005.
9. Z. G. Khan, *Practical Instrumental Method of Analysis*, Birla Publications Pvt. Ltd., Delhi, 2022.
10. G. H. Jeffery, J. Bassett, J. Mendham and R C. Denney, *Textbook of Quantitative Chemical Analysis*, Longman, 5th ed., 1989.
11. G. D. Christian, *Analytical Chemistry*, John Wiley & Sons, 6th Ed., 2004.
12. N. G. Graham and J. P. Ingrid, *X-ray Absorption Spectroscopy*, DE Gruyter, 2025.
13. M. Z. Jian and C. H. S. John, *Advanced Transmission Electron Microscopy: Imaging and Diffraction in Nanoscience*, Springer; 2016.
14. M. T. Terry, *Thermal Conductivity: Theory, Properties, and Applications*, Springer New York, 2004.
15. E. Barsoukov and J. R. Macdonald, *Impedance Spectroscopy: Theory, Experiment, and Applications*, A John Wiley & Sons, 2005.
16. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Academic Science, 2008.

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SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Qualitative analysis of binary mixture of organic compounds CH-SBC-403	**02**	**00**	**--**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

To provide experimental skills for various separation and purification techniques which will strengthen the opportunities in academia and industry.

Learning outcomes: After completing this course, students will be able to:

- demonstrate chemical and physical methods applied for separation of binary mixture of organic compounds of varied functionalities.
- experiment synthetic methods for chemical modification of separated compounds.
- characterize organic compounds by detailed spectroscopic studies.

PRACTICAL COMPONENT **(2 Credits: 60 Hours)**

Suggested/Recommended List of Experiments:

1. Qualitative Analysis of a binary mixture of Organic compounds
2. Separation and qualitative analysis of mixtures containing two components by chemical and physical methods (using acids, weak and moderate bases, water, ether).
3. Characterization of separated organic compounds by synthetically derivatizing them.
4. Application of spectral data (IR, UV, NMR and mass) for structural elucidation of the compounds separated.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. A. I. Vogel, *Vogel's Textbook of Practical Organic Chemistry*, Wiley, 5th Edn., 1989.
2. F. G. Mann and B. C. Saunders, *Practical Organic Chemistry*, Orient Longmans, 4th Ed., 1990.
3. V. K. Ahluwalia, P. Bhagat and R. Aggarwal, *Laboratory Techniques in Organic Chemistry*, I. K. International Publishing House, 2005.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SKILL BASED COURSE (SBC)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Hands on Modelling and Designing Drugs CH-SBC-404	**02**	**00**	**__**	**02**	B. Sc. (Major in Chemistry) and 10+2 with Mathematics	**--**

Course objectives:

- To introduce students to quantum chemical methods (HF and DFT), molecular modelling, and molecular dynamics techniques for studying molecular structure, properties, and reactivity.
- To develop practical skills in computational tools for geometry optimization, spectral analysis, docking studies, and biomolecular visualization.
- To enable understanding of structure–property relationships, intermolecular interactions, and drug–receptor binding through computational simulations and data analysis.

Learning outcomes: By the end of this course, students will be able to:

- perform geometry optimization, frequency calculations, and conformational analysis, and interpret computational results in terms of molecular structure and spectroscopy.
- analyse biomolecular systems using visualization, docking, and database tools to identify binding interactions, active sites, and structure–activity relationships.
- carry out molecular dynamics simulations and evaluate thermodynamic and transport properties (e.g., RMSD, RDF, diffusion coefficient) to understand molecular behavior in different environments.

PRACTICAL COMPONENT (2 Credit: 60 Hours)

Suggested/Recommended List of Experiments:

1. Perform geometry optimization of small molecules (e.g., H_2O, NH_3, CO_2, benzene, etc.) using HF and DFT methods and compare optimized bond lengths, angles, and total energies
2. Carry out frequency calculations to confirm optimized structures (minimum vs transition state), assign vibrational modes and interpret IR spectra and compare it with experimental values.
3. Study conformers of ethane, butane and cyclohexane: calculate relative energies and identify the most stable conformer and plot potential energy vs dihedral angle.

4. Perform Mulliken/NBO charge analysis and correlate electron distribution with molecular and bond polarity.
5. Visualization of biomolecules using software such as PyMOL/Chimera; identification of secondary structures, active sites, and ligand-binding pockets.
6. Downloading and analyzing protein structures from the Protein Data Bank and obtaining ligand structures from chemical databases (e.g., PubChem, DrugBank) and performing structure optimization.
7. Geometry optimization and energy minimization of small molecules using molecular modelling tools and determination of ligand-binding pockets and key interacting residues in proteins.
8. Performing docking simulations using docking software (e.g., AutoDock, AutoDock Vina).
9. Interpretation of binding energies, hydrogen bonding, hydrophobic interactions, and ligand orientation and visualizing them using molecular visualization tools.
10. Comparative analysis of a series of ligands and their docking scores to understand SAR.
11. Screening a small ligand library against a target protein using docking-based approaches.
12. Evaluation of compounds using Lipinski's rule of five and other pharmacokinetic parameters.
13. Selection of a target protein, docking of multiple ligands, and identification of potential inhibitors with interaction analysis.
14. Simulate a box of 1000 water molecules using the TIP3P model, observe how density evolves from an initial arbitrary value to ~1.0 g/cc during NPT equilibration and plot temperature vs time to verify thermostat performance.
15. Investigate solvation behaviour and structural stability of a small peptide in water, and to analyse intermolecular interactions from MD trajectories by monitoring RMSD and RDF.
16. Perform MD simulations of bulk water and correlate molecular motion in simulations with experimentally measurable transport properties, such as diffusion, by calculating mean square displacement and diffusion coefficient.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. R. Leach, *Molecular Modelling: Principles and Applications*, 2nd edn, Prentice Hall, Harlow, 2001.
2. H.-D. Höltje, W. Sippl, D. Rognan and G. Folkers, *Molecular Modeling: Basic Principles and Applications*, 3rd edn, Wiley-VCH, Weinheim, 2008.
3. J. B. Brown, *Drug Design and Discovery: Principles and Applications*, Wiley, 2012.
4. K. Roy, S. Kar and R. N. Das, *Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment*, Academic Press, 2015.
5. J. M. Haile, *Molecular Dynamics Simulation: Elementary Methods*, Wiley-Interscience, 1992.
6. T. Lengauer, *Bioinformatics: From Genomes to Drugs*, Wiley-VCH, Weinheim, 2007.
7. A. Hinchliffe, *Modelling Molecular Structures*, 2nd edn, John Wiley & Sons, 2003.

8. E. Lewars, *Computational Chemistry*, Kluwer Academic Publishers, 2003.
9. F. Jensen, *Introduction to Computational Chemistry*, Wiley, 2007.
10. C. J. Cramer, *Essentials of Computational Chemistry*, John Wiley & Sons, England, 2002.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Metals in Medicine CH-GE-401	**04**	**03**	**--**	**01**	UG	**--**

Course objectives:

- To teach about the role of metal ions in various therapeutic and diagnostic agents.

Learning outcomes: At the completion of this course, the students should be able to:

- learn about various metals present in commercially available medicines.
- understand the role of metal ions in medicines and diagnostic processes.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Bio Roles of Metals **(15 Hours)**

Metals having bio roles: Fe, Cu, Zn, Mn, Cr(III), V, Mo, W, Co, Ni, Na, K, Mg and Ca (Brief knowledge).Toxicity of essential metal ions at high concentrations and toxicity of heavy metals. Antidotes for detoxification. Transition of traditional mineral medicine to modern metallodrugs (efforts should be made to study an Indian perspective). Chemical structure, Commercial name, Name of the disease it is made for and its brief mechanism of action shall be taught for all the mentioned metals below.

Unit-2: Therapeutic Agents and Radiopharmaceuticals (15 Hours)

Diagnostic and therapeutic agents with Pt (Cisplatin) and Ga for cancer Au (auranofin) for arthritis and V for diabetes.

Radiopharmaceuticals and MRI contrast agents: ^{99m}Tc for heart, brain and bone imaging, ^{123}I radiopharmaceuticals, $BaSO_4$ for X-ray contrast agent, Gd (III) for MRI contrast agents.

Unit-3: Metal as Ingredient in Commercial Brand of Medicines and Multivitamins (15 Hours)

Li_2CO_3 (Camcolit) for manic-depressive illness, $NaHCO_3$ (Alka-seltzer) for heartburn, $Al(OH)_3$ (Gaviscon) for heartburn, As (melarsoprol) for sleeping sickness, Bi subsalicylate (pepto-Bismol) for heartburn and diarrhea, Bi subcitrate (De-nol) peptic ulcer, Zinc oxide with Fe_2O_3 (Calamine lotion) as antimicrobial agent. Cyanocobalamin (Co), Ferrous fumerate (Fe), Magnesium oxide (Mg), Zinc Sulfate (Zn), Magnanese sulphate (Mn), Copper Sulfate (Cu), Sodium selenite (Se) and Chromium trichloride(Cr).

References (Theory)

1. J. C. Dabrowiak, *Metals in Medicine*, Wiley-Blackwell, 2009.
2. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, The MIT Press, 1994.
3. C. Jones and J. Thornback, *Medicinal Applications of Coordination Chemistry*, Cambridge, UK: Royal Society of Chemistry, 2007.
4. Z. Guo, and P. J. Sadler, *Angew. Chem. International Edition*, 1999, **38**, 1512-1531.
5. I. Bertini, H. B. Gray, E. Stiefel and J. Valentine, *Biological Inorganic Chemistry: Structure and Reactivity*, University Science Books, 2007.
6. M. Gielen, and E. R. T. Tiekink, *Metallotherapeutic Drugs and Metal-based Diagnostic Agents: The Use of Metals in Medicine*, John Wiley & Sons, 2005.
7. K. H. Thompson and C. Orvig, *Metal Ions in Biological Systems*, 2004, **41**, 221-252.
8. A. Casini and A. Pöthig, *ACS Central Science*, 2024, **10**, 242-250.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

Suggested/Recommended List of Experiments:

1. To estimate the acidity of commercially available antacids volumetrically.
2. To estimate the concentration of Fe in commercially available medicines volumetrically.
3. To estimate the concentration of calcium in commercially available medicines by complexometry and flame photometry.
4. To estimate the concentration of bismuth in commercially available medicines by complexometry.
5. To estimate the concentration of iron in commercially available medicines by spectrophotometry.
6. To estimate the concentration of calcium in commercially available medicines by flame photometry.

7. To estimate the concentration of calcium and magnesium in milk complexometrically.
8. To estimate the concentration of zinc in commercially available medicines complexometrically.
9. To estimate the concentration of aluminium in commercially available deodorant complexometrically.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. P. G. McCormick, *J. Chem. Educ.* 1973, **50**, 136.
2. R. M. Steinert, M. E. Heikes, J. T. Mitchell-Koch, G. A. Baker and K. R. Mitchell-Koch, *J. Chem. Educ.,* 2022, **99**, 3723−3730.
3. J. Mendham, *Vogel's Quantitative Chemical Analysis*, Pearson Education Asia, 6th Ed., 2009.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Chemistry for Mitigation of Environmental Challenges CH-GE-402	**04**	**03**	**-**	**01**	UG	**--**

Course objectives:

- To provide an advanced, interdisciplinary understanding of circular economy frameworks, materials science of waste, state-of-the-art recycling technologies.
- To engage in analytical thinking, research critique, and real-world application oriented learning.

Learning outcomes: At the completion of this course, the students should be able to:

- understand natural chemical cycles, pollution sources/impacts (air, water, soil), analytical techniques, and sustainable solutions.
- enable students to analyze environmental problems, apply quantitative skills and interpret data.
- evaluate control measures for issues like smog, water contamination, and agrochemical effects, aligning chemical knowledge with ecological sustainability.

THEORY COMPONENT (3 Credit: 45 Hours)

Unit-1: Intersection of Chemical and Environmental Sciences (15 Hours)

Role of chemical sciences for understanding various aspects of environmental processes; brief overview of different sources of contamination into the environment; basics of environmental toxicology emanating from inorganic and nanomaterial-based pollutants: dose-response, LD50, biodegradation, persistence, bioaccumulation; Conventional and nanotechnology based remediation for wastewater treatment, Basics of Adsorption, Basics of Photocatalysis, Basics of membrane filtration.

Unit-2: Strategies for Chemical Decontamination of water (15 Hours)

Nano-adsorbents in pollutant removal, photocatalytic treatment of wastewater; Removal of pollutants using nanofiltration technique; Nanomaterial-based disinfection in water treatment, Risk assessment and nanotoxicology, ecological & environmental impact of nanomaterials; Removal of toxic anionic waste, removal of heavy metal ions, Use of metal nanoclusters for removal of arsenic based compounds, removal of radioactive ions, Fundamentals of analytical techniques (AAS, ICP-MS) in context of Environmental remediation.

Unit-3: Chemistry for Recycling: Key to Circular Economy (15 Hours)

Principles of circular economy, relevance of waste management and recycling toward circular economy; Energy recycling: waste heat to electricity using inorganic thermoelectric materials; Plastic recycling: different types of recycling techniques: selective vs. non-selective approaches, depolymerization of common plastics (PET, polyesters, polycarbonates etc.), application of metal and metal oxides in catalytic depolymerization; Recycling of battery materials: selective strategies for separation of lithium and other critical transition metals (such as cobalt and nickel) from battery materials

References (Theory)

1. M. Wiesner and J.-Y. Bottero, *Environmental Nanotechnology: Applications and Impacts of Nanomaterials*, McGraw Hill Professional, 2007.
2. M. Diallo, J. Duncan, N. Savage, A. Street and R. Sustich, *Nanotechnology: Applications for Clean Water*, William Andrew, 2008.
3. J. Lead, and E. Smith, *Environmental and Human Health Impacts of Nanotechnology*, John Wiley & Sons., 2009.

4. S. A. Bandh and F. A. Malla, *Waste Management in the Circular Economy*, Springer, 2024.
5. S. M. Khopkar, *Environmental Pollution Analysis*, Wiley Eastern, 1993.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Estimation of hardness and alkalinity.
2. Analysis of heavy metals by AAS (Pb, Cd, Hg, Cr).
3. Estimation of soil pH, moisture, and organic content.
4. UV-Visible spectrophotometric analysis of dye-based pollutants.

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. S. K. Rai, R. Xalxo, T. K. Patle, A. Verma, R. Chauhan and P. K. Mahish, *ACS Symposium Series*, 2023, Chapter **10**, 167-204.
2. C. N. Sawyer, P. L. McCarty and G. F. Parkin, *Chemistry for Environmental Engineering*, Tata McGraw-Hill Publishing Company Limited., 4th Ed., 2000.
3. M. L. Jackson, *Soil Chemical Analysis*, Prentice-Hall, Inc., 1956.

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Biomolecules, structure and functions-II **CH-GE-403**	**4**	**3**	**0**	**1**	UG	NIL

Course Objectives:

To provide understanding of the structure of carbohydrates and lipids and their involvement in various biological processes.

Learning Outcomes: After completing this course, students will be able to:

- understand the chemical structure of carbohydrates and lipids
- explain various types of carbohydrate, lipids and their mechanism of action
- design small molecule for regulation of carbohydrate transfer protein and use to treat diseases.

THEORY COMPONENT **(3 Credit: 45 Hours)**

Unit-1: Introduction **(15 Hours)**

Carbohydrates - Definition, classification, structure and importance of monosaccharides and oligosaccharides. Polysaccharides: Homopolysaccharides and Heteropolysaccharides, Storage and Structural Polysaccharides, Artificial sweeteners. Lipids - Classification, structure, function and properties of Lipids (Fatty acids, phospholipids, triacyl glycerols, cholesterols, steroids, terpenes, terpenoids), Liposomes. Structure, classification and properties of different type of fatty acids, Vitamins - Water- and fat-soluble vitamins and their functions.

Unit-2: Structure, function of carbohydrates **(15 Hours)**

Structure of receptor sites, Glycolysis, Aldolase, amylose, uronic acid, glycosylamines, N-acetyl-D-glucosamine, Glycolipids and Glycoproteins, carbohydrate antibiotics, Role of carbohydrate in human diseases (Type I and Type II diabetes). Inhibitors of glucose transporters.

Unit-3: Structure, function of lipids **(15 Hours)**

Biological importance of Lipids. Synthesis of lipids: phospholipids and glycolipids, Biological application of lipids, phosphatidylinositol (PI) cycle and receptor protein, regulator of PI cycle such as diacylglycerol kinases.

References (Theory):

1. J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman and Co., 9th Ed., 2019.
2. D. L. Nelson, M. M. Cox and A. L. Lehninger, *Principles of Biochemistry*, W. H. Freeman and Co., International Edition, 2017.
3. S. Kuashik and A. Singh, *Biomolecules: From Genes to Proteins, Berlin*, Boston: De Gruyter, 1st Ed., 2023.
4. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer-Verlag, 1989.

PRACTICAL COMPONENT **(1 Credit: 30 Hours)**

Suggested/Recommended List of Experiments:

1. Qualitative tests for Carbohydrates.
2. Qualitative tests for Lipids.

3. Estimation of sugars by using Fehling solution.
4. Determination of saponification value of the given oil.
5. Determination of iodine number of the given oil
6. Synthesis of osazone of glucose/fructose
7. Synthesis of D-glucopyranose pentaacetate from D-Glucose

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical):

1. S. Kukreti, *Manual of Biochemistry Workshop,* Department of Chemistry, University of Delhi, 2012.
2. A. I. Vogel, *Vogel's Textbook of Practical Organic Chemistry*, Wiley, 5th Ed., 1989.
3. F. G. Mann and B. C. Saunders, *Practical Organic Chemistry*, Orient Longmans, 4th Ed., 1990.

GENERIC ELECTIVE COURSE (GE)

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

<table>
<tr><th rowspan="2">Course title & Code</th><th rowspan="2">Credits</th><th colspan="3">Credit distribution of the course</th><th rowspan="2">Eligibility criteria</th><th rowspan="2">Pre-requisite of the course (if any)</th></tr>
<tr><th>Lecture</th><th>Tutorial</th><th>Practical/ Practice</th></tr>
<tr><td>Computational and AI/ML Methods in Chemistry
CH-GE-404</td><td>04</td><td>03</td><td>---</td><td>01</td><td>UG</td><td>NIL</td></tr>
</table>

Course Objectives:

- Develop a foundation in scientific programming and numerical methods for computational chemistry applications.
- Understand empirical, semi-empirical, and electronic structure methods for molecular simulations.

- Introduce AI/ML concepts and apply them to problems in molecular modelling, quantum chemistry, and catalysis.

Learning Outcomes*:* Students will gain an understanding of

- demonstrate proficiency in scientific programming and numerical methods to solve computational problems in chemistry.
- apply empirical, semi-empirical, and electronic structure methods for molecular simulations and analysis of chemical systems.
- understand and utilize AI/ML concepts and techniques for chemical data analysis, modelling, and prediction.

THEORY COMPONENT (3 Credit, 45 Hours)

Unit-1: Scientific Computing and Numerical Methods (15 Hours)

Programming in scientific languages (FORTRAN/C/C++/Python) for chemical applications. Introduction to the LINUX/UNIX environment and basic shell scripting. Fundamental numerical methods used in chemistry. Finding roots of equations: Bisection, Secant, and Newton–Raphson methods.

Unit-2: Electronic Structure and Simulations (15 Hours)

Electronic Structure Methods: Basic concepts of quantum chemical calculations and their use in determining molecular structures, energies, and properties.
Molecular Modelling and Simulations: Introduction to molecular mechanics, force fields, and basic principles of molecular dynamics simulations.
Basic use of standard software (e.g., GAMESS, MOPAC, etc.) for electronic structure calculations and molecular modelling.

Unit-3: Basics of AI and Data Analytics (15 Hours)

Introduction to AI/ML in Chemistry: Basic concepts of AI/ML, including data preprocessing, model training and evaluation, and types of learning (supervised and unsupervised) with emphasis on challenges in chemical data.
AI/ML Models and Techniques: Overview of common models such as linear regression, kernel ridge regression, and neural networks including basic ideas of deep learning.
Applications of AI/ML: Illustrative applications in healthcare, finance, transportation, and education, with emphasis on chemical and scientific research such as drug discovery, and enhancement of quantum chemical calculations, along with emerging trends in AI.

References (Theory)

1. A. Hinchliffe, *Modelling Molecular Structures*, 2nd edn, John Wiley & Sons, 2003.

2. H.-D. Höltje, W. Sippl, D. Rognan and G. Folkers, *Molecular Modeling: Basic Principles and Applications*, 2nd edn, Wiley-VCH, 2003.
3. A. R. Leach, *Molecular Modelling: Principles and Applications*, 2nd edn, Pearson Education, England, 2001.
4. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in Fortran/C*, 2nd edn, Cambridge University Press, 1996.
5. F. Jensen, *Introduction to Computational Chemistry*, Wiley, 2007.
6. C. J. Cramer, *Essentials of Computational Chemistry*, John Wiley & Sons, England, 2002.
7. J. P. Janet and H. J. Kulik, *J. Chem. Educ.*, 2021, **98**, 2892–2898.
8. C. J. Heard, *J. Chem. Educ.*, 2024, **101**, 2957–2959.
9. J. N. Wei, D. Duvenaud and A. Aspuru-Guzik, *Chem. Rev.*, 2021, **121**, 9816–9872.

PRACTICAL COMPONENT (1 Credits: 30 Hours)

Suggested/Recommended List of Experiments:

1. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).
2. Write a program to compute the area and circumference of a circle, given the radius
3. Write a program to compute to check whether a number is positive, negative, or zero.
4. Write a program to compute *p*H of a weak and strong acid.
5. Write a program to compute convert Celsius to Fahrenheit or vice versa.
6. Calculate the sum of the first 10 natural and prime numbers using a loop.
7. Write a program to find the maximum and minima for a set of numbers.
8. Fit a polynomial curve using Excel or spreadsheets (linear, quadratic, cubic, quartic, etc) to find a trendline
9. Examine interpolation to find the missing data using Excel or spreadsheets.
10. Examine extrapolation to predict future values or trends using Excel or spreadsheets.
11. Least-squares fit including graphics using Excel or spreadsheets.
12. Numerical solution of differential equations (e.g. in kinetics).

(Note: Depending on availability of time, additional experiments/assignments may be included during the semester)

References (Practical)

1. V. Rajaraman, *Computer Programming in C*, 2nd edn, PHI Learning Pvt. Ltd., New Delhi, 2012.
2. Y. P. Kanetkar, *Let Us C*, 15th edn, BPB Publications, New Delhi, 2016.
3. V. Rajaraman, *Computer Programming in Fortran 77*, PHI Learning Pvt. Ltd., New Delhi, 1997.
4. S. J. Chapman, *Fortran 90/95 for Scientists and Engineers*, 2nd edn, McGraw-Hill Higher Education, New York, 2004.

5. J. M. Zelle, *Python Programming: An Introduction to Computer Science*, 4th edn, Shroff Publishers & Distributors Pvt. Ltd., New Delhi, 2017.
6. M. Schatzman, *Numerical Analysis: A Mathematical Introduction*, Oxford University Press, Oxford, 2002.
7. J. N. Wei, D. Duvenaud and A. Aspuru-Guzik, Chem. Rev., 2021, *121*, 9816–9872.
8. a) https://jupyter.org/, b) https://colab.research.google.com/, c) https://www.python.org/, d) https://numpy.org/, e) https://scikit-learn.org/stable/, f) https://pytorch.org/

Assessment methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.