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UNIVERSITY OF DELHI

Master of Science (M. Sc.) in Chemistry

(Effective from Academic Year 2025-26)

ABOUT THE DEPARTMENT

The Chemistry teaching started in 1922 with three constituent colleges St. Stephens, Hindu and Ramjas. The chemistry teaching was confined to a two year course for B. Sc. Degree department and the teaching up to I.Sc. Level was conducted in the constituent colleges of the University. In October 1933, the University offices and Library shifted to the Viceregal Lodge Estate and the chemistry department made an inconspicuous beginning in the Viceregal kitchen which was used for conducting the lectures and practical classes. In 1942, new Laboratories and lecture rooms were constructed and visionary faculty members were invited by special efforts of illustrious Vice Chancellor, Sir Maurice Gwyer. In June 1949, Professor TR Seshadri took over as head of the department and owing to his untiring effort, the research activities gradually increased, and the department attained formidable reputation in the international scene as one of the finest schools of chemistry. In 1963, the University Grants Commission recognized the department of chemistry as a Centre of Advanced Study for the Chemistry of Natural Products. In 1965, the department of chemistry was recognized as a Centre of Advanced Study in Chemistry. In eighties several faculty members joined the department and the department expanded rapidly in terms of both research and teaching and a large number of small independent groups started flourishing. Various faculty members made significant contributions in computational chemistry, biopolymers, physical chemistry of polymers, organic synthesis, medicinal chemistry, apart from the structure elucidation of natural products, biotransformations, chemical communications, structure investigation of metal complexes, organometallic chemistry and analytical chemistry. After the year 2000 new group of faculty members joined the department with specialization in newer areas that included biomolecular structures, synthesis of nucleosides, medicinal chemistry, electrochemistry and material chemistry. With advent of the new era of materials and nanomaterials other young and energetic faculty members have also joined the department. With this input the department is marching forward in newer areas of research and teaching. The Department of Chemistry is well known for its excellence in teaching and research. The faculty members of the department are engaged in state of the art research as well as guiding the Ph.D., M. Tech. M. Sc. and Post Doctoral Students. The Department has made great strides by revising and updating the M. Sc. syllabus time and again. A thoroughly updated and revised M. Sc. syllabus has been implemented in the year 2009. In the international year of chemistry, the Department started new project work in M. Sc. syllabus where students have exposure of writing the project and also develop communication skills. Advanced level optional courses are also offered at the Ph.D. levels and these courses are taught semester wise. Collaborative research programmes with many research laboratories and research institutes in Delhi and outside India are also operating very successfully with mutual benefit. The Department has distinguished itself as a centre for innovative and pioneering research in a wide range of areas in chemistry and chemistry interfacing with physical and biological sciences. It has attained the status of a DST-FIST Sponsored department by DST in 1982. The department is recognized as one of the best performing chemistry department in the country by DST in the International Year of Chemistry (2011).

1st Year of PG Curricular Structure for 2 Year M. Sc. Under NEP-2020

Semester	**DSC** (2T + 2P)	**DSE** (3T + 1P)	**Skill-based course/workshop/specialised laboratory/hands-on learning** (2 Credits= 1T+1P)	Dissertation/ Academic Project/ Entrepreneurship	Total credits
I	DSC-1 **(CH-DSC-101)** DSC-2 **(CH-DSC-102)** DSC-3 **(CH-DSC-103)** **(3 x 4 credits = 12 credits)**	**DSE-1* and DSE-2*** **(2 x 4 credits = 8 credits)** ***Note:** 1. DSE Course Options for M.Sc. Chemistry Students: Students enrolled in the M.Sc. Chemistry program will have the option to choose two DSE (Discipline Specific Elective) courses from the following combinations: Set-1: CH-DSE-104 and CH-DSE-105 Set-2: CH-DSE-104 and CH-DSE-106 Set-3: CH-DSE-105 and CH-DSE-106 2. Allocation of Sets: Each of the above three sets will be allotted to one-third of the total admitted students in this combination on the basis of Academic merit and Preferences submitted by the students. **Or** **DSE-1*** and **GE-1** (choose only one GE course offered by other Departments) **(2 x 4 credits = 8 credits).** Provision for Opting DSE-1 and GE-1 Combination 1. Students enrolled in the M.Sc. Chemistry programs are required to choose one Discipline Specific Elective (DSE) course from the options CH-DSE-104, or CH-DSE-105, or CH-DSE-106 and each of the above three DSE papers will be allotted to one-third of the total admitted students in this combination based on Academic merit and Preferences submitted by the students. 2. A provision has been made to allow a maximum of 25% of the total allocated students to opt for a combination of: One DSE course (as listed above), and One Generic Elective (GE) course offered by other departments (subject to the terms and conditions of the respective departments). 3. The allotment of the DSE-GE combination will on the basis of Academic merit, and Preferences submitted by the students.	**SEC-1#** **2 Credits** **Note:** 1. SEC Course Options for M.Sc. Chemistry Students: Students pursuing the M.Sc. program in the Chemistry Department will be required to choose one Skill Enhancement Course (SEC) from the following options: CH-SEC-107, CH-SEC-108, CH-SEC-109* and CH-SEC-110* *Only one course will be offered from among CH-SEC-109 and CH-SEC-110, depending on availability and departmental decision. 2. Each SEC paper will be allotted to one-third of the total number of allocated seats to the department on the basis of Academic merit and Preferences submitted by the students.	Nil	22

II	DSC-4 **(CH-DSC-201)** DSC-5 **(CH-DSC-202)** DSC-6 **(CH-DSC-203)** (3 x 4 credits = 12 credits)	**DSE-3* and DSE-4* (2 x 4 credits = 8 credits)** **Note:** 1. DSE Course Options for M.Sc. Chemistry Students: Students enrolled in the M.Sc. Chemistry program will have the option to choose two DSE (Discipline Specific Elective) courses from the following combinations: Set-1: (CH-DSE-204 and CH-DSE-205) Set-2: (CH-DSE-204 and CH-DSE-206) Set-3: (CH-DSE-205 and CH-DSE-206) 2. Allocation of Sets: Each of the above three sets will be allotted to one-third of the total admitted students in this combination on the basis of Academic merit and Preferences submitted by the students **Or** **DSE-2*** and **GE-2** (choose only one GE course offered by other Departments) **(2 x 4 credits = 8 credits).** Provision for Opting DSE-2 and GE-2 Combination 1. Students enrolled in the M.Sc. Chemistry program are required to choose one Discipline Specific Elective (DSE) course from the options CH-DSE-204, or CH-DSE-205, or CH-DSE-206 each of the above three DSE papers will be allotted to one-third of the total admitted students in this combination based on Academic merit and Preferences submitted by the students. 2. A provision has been made to allow a maximum of 25% of the total allocated students to opt for a combination of: One DSE course (as listed above), and One Generic Elective (GE) course offered by other departments (subject to the terms and conditions of the respective departments). 3. The allotment of the DSE-GE combination will on the basis of Academic merit, and Preferences submitted by the students.	**SEC-2# 2 Credits** **Note**: SEC Course Options for M.Sc. Chemistry Students: 1. Students pursuing the M.Sc. program in the Chemistry Department will be required to choose one Skill Enhancement Course (SEC) from the following options: CH-SEC-207, CH-SEC-208, CH-SEC-209*, CH-SEC-210* *Only one course will be offered from among CH-SEC-209 and CH-SEC-210, depending on availability and departmental decision. 2. Each SEC paper will be allotted to one-third of the total number of allocated seats to the department on the basis of Academic merit and Preferences submitted by the students.	Nil	22

General Elective Table*

	Pool of GE offered (3T + 1P)*		
Ist Semester (GE-I)	**CH-GE-111**	**CH-GE-112**	**CH-GE-113**
IInd Semester (GE-II)	**CH-GE-211**	**CH-GE-212**	**CH-GE-213**

*Provision for Admitting Students from Other Departments to GE Courses Offered by the Department of Chemistry

1. Admission Provision: A provision has been made to admit up to 25% of the total seats allocated to the Department of Chemistry for Generic Elective (GE) courses to students from other departments of the university. Admission will be on the basis of Academic merit, and Preferences submitted by the students.

2. Allocation of Seats to GE Courses: The three GE courses offered by the Department of Chemistry in each semester will be allotted to one-third of the total admitted students.

Distribution of Courses and credits for M. Sc. Chemistry Semester I & II under NEP-2020

DISCIPLINE SPECIFIC CORE COURSES (DSC) FOR SEMESTERS- I & II			
Semester	**Name of the Course**	**Course Code**	**Credits**
I	Stability constants of metal complexes and their applications	**CH-DSC-101**	**T=2** **P=2**
	Reactive Intermediates in Organic Chemistry	**CH-DSC-102**	**T=2** **P=2**
	Principles of quantum chemistry and approximate methods.	**CH-DSC-103**	**T=2** **P=2**
II	Chemistry of *d*- and *f*- block elements	**CH-DSC-201**	**T=2** **P=2**
	Advanced Organic Spectroscopy	**CH-DSC-202**	**T=2** **P=2**
	Statistical Mechanics and Thermodynamics	**CH-DSC-203**	**T=2** **P=2**
POOL OF DISCIPLINE SPECIFIC ELECTIVES (DSE) FOR SEMESTERS- I & II			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
I	Supramolecular chemistry and Photoinorganic Chemistry	**CH-DSE-104**	**T=3** **P=1**
	Advanced Stereochemistry of Organic Compounds	**CH-DSE-105**	**T=3** **P=1**
	Mathematical methods in Chemistry	**CH-DSE-106**	**T=3** **P=1**
II	Group Theory and its Applications in Chemistry	**CH-DSE-204**	**T=3** **P=1**

	Methods in Organic Synthesis	**CH-DSE-205**	**T=3** **P=1**
	Electrochemistry, Macromolecules and Chemical Kinetics by Statistical Thermodynamics	**CH-DSE-206**	**T=3** **P=1**
POOL OF SKILL ENHANCEMENT COURSES (SEC) FOR SEMESTERS- I & II			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
I	Introduction to Basic Lab Safety and Softwares for Research work	**CH-SEC-107**	**T=1** **P=1**
	Best Practices in Chemical Laboratory Safety	**CH-SEC-108**	**T=1** **P=1**
	Introduction to Computer Programming and Numerical Methods	**CH-SEC-109**	**T=1** **P=1**
	Electrochemical Energy Devices and Technologies	**CH-SEC-110**	**T=0** **P=2**
II	Hands-on Training of Analytical Instruments	**CH-SEC-207**	**T=1** **P=1**
	Hands-on Training of Separation Techniques	**CH-SEC-208**	**T=1** **P=1**
	Recent Trends in Advanced Molecules and Materials	**CH-SEC-209**	**T=1** **P=1**
	Concepts and Applications of Artificial Intelligence and Machine Learning in Chemistry	**CH-SEC-210**	**T=1** **P=1**
POOL OF GENERIC ELECTIVE COURSES (GE) FOR SEMESTERS- I & II			
Semester	**Name of the Course**	**Type of Courses**	**Credits**
I	Basics of Mineral Chemistry	**CH-GE-111**	**T=3** **P=1**

	Introduction to Drug Discovery and Development	**CH-GE-112**	**T=3** **P=1**
	Biophysical and Nanomedicinal Chemistry	**CH-GE-113**	**T=3** **P=1**
II	Introductory Chemistry of The Earth's Atmosphere	**CH-GE-211**	**T=3** **P=1**
	Medicines and Therapeutics in Daily Life	**CH-GE-212**	**T=3** **P=1**
	Modern Materials of Chemistry and Physics	**CH-GE-213**	**T=3** **P=1**

NOTE: GE courses will be offered to students of other Departments only up to 25 % of the total allocated seats of the Chemistry Department based on the merit and preferences given by the students.

Assessment Method:

The assessment of all courses will follow the guidelines prescribed by the University.

For Practical Chemistry papers, the assessment will be carried out as follows:

50% of the total marks will be based on Continuous Evaluation (including regular performance, records, viva, etc.).

50% of the total marks will be based on the End Semester Examination.

SEMESTER-I

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		
Stability constants of metal complexes and their applications **CH-DSC-101**	**04**	**02**	—	**02**	U.G. Chemistry	--

Course objectives

The objectives of this course are as follows:

- To impart advanced knowledge on the analytical chemistry aspects of complexometric titrations.
- To comprehend the stability, reactions of supra molecular complexes of alkali metal and other univalent ions.

Learning outcomes

After completing the course, the students will be able to:

- Define stability constant, differentiate between overall and stepwise stability constants and identify factors influencing the stability of metal complexes.
- Students will learn how the nature of the metal ion, the ligand, and the chelate effect impact stability.
- Students will understand various techniques used to measure stability constants, including potentiometry (pH measurement), spectrophotometry, and other analytical methods and hence, will be able to calculate the concentrations of metal ions, ligands, and complexes, using the stability constants.
- Students will learn how knowing the stability constants of metal complexes can be useful for applications, in the fields of Analytical Chemistry, Biochemistry, Environmental Science, Medicinal Chemistry, and so on.

THEORY COMPONENT **(2 Credit: 30 Hours)**

UNIT 1: **(15 Hours)**

INTRODUCTION TO METAL COMPLEX FORMATION, COMPLEX FORMATION FUNCTIONS AND THEIR DETERMINATION BY VARIOUS METHODS

Stoichiometric and thermodynamic equilibrium constants, Stepwise and overall formation constants, trends in stepwise formation constants, conditional equilibrium constants; factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect and thermodynamic origin (statistical and non-statistical factors influencing stability of complexes in solution); role of the hydrogen ion concentration in complex formation.

Formation functions, φ, n and αC and relationship between different functions. Calculation of protonation and stability constants. Determination of formation constant by: Graphical Methods: using sets of data {φ, [A]}; {αC, [A]} and {n, [A]}. Curve fitting method, Elimination method, Numerical method.

UNIT 2: **(15 Hours)**

DETERMINATION OF STABILITY CONSTANTS AND APPLICATIONS OF COMPLEX FORMATION WITH EXAMPLES

Potentiometric method, Method of corresponding solutions, Ion exchange method-cation and anion exchange, Solvent extraction, Polarographic method and Spectrophotometric methods, which include Job's method of continuous variation, Logarithmic method, Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskii's method.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction, etc. Simultaneous titrations, stepwise titrations, replacement titrations, back titrations); analysis of mixtures of metals. Use of masking and demasking agents in complexometric titrations.

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

EXPERIMENTS:

1. Quantitative analysis of mixtures of metal ions by complexometric titrations (mixture of two metals) with the use of masking and de-masking agents.

2. Any other relevant experiment from time to time during the semester.

ESSENTIAL/RECOMMENDED READINGS (Theory)

1. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).

2. Khopkar, S.M., Basic Concepts of Analytical Chemistry 3rd Edition, Publisher: New Age International Publishers (2008), ISBN: 9788122420920, 8122420923.

3. Hartley, F. R., Burgess, C. & Alcock, R. M. Solution Equilibria. Prentice-Hall: Europe (1980).

4. Srivastava and Mishra, Fundamental of Analytical Chemistry (First Edition, 2016)

5. Robinson, J.W, Undergraduate Instrumental Analysis, CRC Press (2014).

6. Inczedy, J. Analytical applications of complex equilibria Halsted Press: New York, NY (1976).

7. Vogel, A. I. Vogel's Qualitative Inorganic Analysis - 7th ed. (revised by G. Svehla) Longmans (1996) ISBN 058-221866-7.

SUGGESTED READINGS (Practical)

1. Vogel, A. I. Vogel's Qualitative Inorganic Analysis - 7th ed. (revised by G. Svehla) Longmans (1996) ISBN 058-221866-7.

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 (CH-DSC-102)

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		
Reactive Intermediates in Organic Chemistry **CH-DSC-102**	**4**	**2**	**0**	**2**	U.G. Chemistry	NIL

Course Objectives:
1) To learn and understand the involvement of intermediates, their role in reaction mechanisms, predict their behaviour, and apply this knowledge to organic synthesis.
2) To develop experimental skills of various separation and purification techniques and preparative TLCs and study of reactions involving different reactive intermediates.

Learning Outcomes: At the completion of this course, the students should be able to:
1) Understand the structure-reactivity pattern of reactive intermediates involved in organic reactions.

2) Write the mechanism of organic reactions involving reactive intermediates and apply these reactions in organic synthesis.
3) The students will acquire knowledge of:
i) Chromatographic separation and identification of organic compounds.
ii) Purification, Crystallization, and different Distillation processes.
iii) Synthesis using substitution and condensation reactions

SYLLABUS OF CH-DSC-102

THEORY COMPONENT **(2 Credit: 30 Hours)**

UNIT 1: **(15 Hours)**

INTRODUCTION

A review of reaction mechanisms, including methods of determination.
Linear free energy relationships and their applications (Hammett equation and modifications).

CARBOCATIONS

Non-classical carbocations, stability and reactivity of bridgehead carbocations, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, C-C bond formation involving carbocations. Generation and application of Contemporary Carbocations: (i) Electrochemically generated carbocations (ii) Allenyl and propargylic Cations (iii) Superelectrophilic Carbocations: Charge Migration and Remote Functionalization (iv) Boronic Acids (a Lewis Acid) generated carbocations.

CARBANIONS

Generation, structure, stability, and reactivity including molecular rearrangements. Ambident ions, and their general reactions; HSAB principle and its applications.

UNIT 2: **(15 Hours)**

FREE RADICALS

Generation, structure, stability and reactions, cage effects; radical-cations including Hofmann–Löffler–Freytag & radical anions, Bergmann cyclization, allenyl radicals and their application in organic synthesis, other radical cyclization reactions.

CARBENES

Formation and structure, reactions involving carbenes, N-heterocyclic carbenes (NHC), and carbenoids.

NITRENES

Generation, structure, and reactions of nitrenes and nitrenoids.

ARYNES

Generation and reactivity of arynes and nucleophilic aromatic substitution reactions.

PRACTICAL COMPONENT (2 Credits: 60 Hours)

EXPERIMENTS

i) Analytical and preparative TLCs (mixtures containing three or more compounds, natural extracts and use of different developing agents)

ii) Preparations involving stereochemical aspects (geometrical isomers and stereoisomers) and different reactive intermediates:
(a) Condensation reaction,
(b) Bromine addition,
(c) Carbene addition,
(d) Nucleophilic and Electrophilic substitution reaction,
(e) Rearrangement reactions involving carbocations and carbanions
iii) Identification of organic compounds using UV and IR

ESSENTIAL/RECOMMENDED READINGS

Theory

1. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th edition, Springer, New York, 2007.
2. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition 2005, Cambridge University Press.
3. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2007.
4. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, 2nd edition
5. Peter Sykes, A guidebook to mechanisms in organic chemistry

Practical

1. Vogel, A. I. (2012), Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing House Pvt. Ltd, New Delhi

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 /Practice		
Principles of Quantum Chemistry and Approximate Methods **CH-DSC-103**	04	02	-	02	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives:

- To provide a foundation in the fundamental quantum mechanical principles and associated mathematical framework.
- To explore and solve exactly solvable quantum systems, including particle models, harmonic oscillators, etc.
- To understand angular momentum and its applications to atomic and molecular systems.
- To learn and apply approximate methods such as variational techniques and perturbation theory to complex quantum problems.
- To study quantum mechanical approaches to chemical bonding and molecular orbital theory, including applications to conjugated and polyatomic systems.

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

- Acquire a foundational understanding of key quantum chemistry concepts and the mathematical tools necessary to describe chemical phenomena.
- Apply mathematical techniques to solve problems in quantum chemistry.
- Understand and utilize quantum mechanical principles to evaluate the properties of atomic and molecular systems.
- Interpret and predict the chemical properties and behavior of atomic and molecular systems based on quantum theory.
- Connect theoretical quantum concepts with real-world chemical applications.

Theory Course Contents: **Credit 2 (30 hours)**

Unit I: **15 hours**

A. Postulates of Quantum mechanics, Linear and Hermitian operators, Turn-over rule, Commutation of operators and Heisenberg's Uncertainty principle (qualitative discussion). *Some exactly soluble problems*: Particle in a Ring, 2D and 3D box. Degeneracy, Jahn-Teller distortion, and accidental degeneracy. Simple harmonic oscillator problem by factorization method (step-up, step-down Ladder operators), Calculation of various average values utilizing step-up and step-down operators or recursion relations.

B. Angular momentum operators and their commutation relations, utilization of raising and lowering operators for eigenvalues and eigen-functions of rigid rotator; H-atom (qualitative discussion), Radial distributions, Radial density, and nodes.

Unit II: **15 hours**

A. *Approximate methods:* First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom), Ground and excited state of helium atom. Pauli's Exclusion principle.

B. *Chemical bonding:* Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments and their equivalence limit. Configuration Interaction. Extension of MO theory to other systems- Homonuclear and heteronuclear diatomic, polyatomic.

C. *HMO method and its applications:* π-Electron approximation, Huckel Molecular Orbital Theory of conjugated systems, Calculation of properties- Delocalization energy, electron density, bond order, non-alternant hydrocarbons, cyclic molecules.

Recommended Texts:

1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
3. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
4. Cohen-Tannoudji, Claude, Bernard Diu, and Franck Laloë F., Quantum Mechanics (Translated by G. G. Levine and D. S. Constable), vols-I&II, Wiley-Interscience, New York (1977).
5. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
6. Atkins, Peter, and Ronald Friedman. Molecular Quantum Mechanics, Oxford University Press, 5th ed. (2011).
7. Sakurai, J. J. and Napolitano, J. Modern Quantum Mechanics, 2nd Ed., Addison-Wesley, (2011).
8. Merzbacher, E. Quantum Mechanics, John Wiley & Sons, 3rd Edition, (1998).
9. Landau, L. D. and Lifshitz, E. M. Quantum Mechanics: Non-Relativistic Theory, Vol. 3, Pergamon Press, 3rd Edition (English), (1977).
10. Messiah, A. Quantum Mechanics, North-Holland Publishing Company, 1961, Reprinted by Dover Publications (2014).

<u>Practical Components</u>: **Credit 2**

Chemical Kinetics

1. Determine the specific rate constant for the acid catalysed hydrolysis of methyl acetate by the *Initial Rate Method*. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
2. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
3. Study the saponification of ethyl acetate with sodium hydroxide volumetrically.

Conductometry

1. Determine the Cell Constant of the given conductivity cell at room temperature and study the equivalent conductance versus square root of concentration relationship of a strong electrolyte (KCl or NaCl) and weak electrolyte (acetic acid).
2. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
3. Determine the equivalent conductance, degree of dissociation and dissociation constant (K_a) of acetic acid.
4. Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.
5. Study the conductometric titration of potassium sulphate solution vs. barium chloride solution
6. Study the conductometric titration of (a) Acetic acid vs. sodium hydroxide, (b) Acetic acid vs. ammonium hydroxide, (c) HCl vs. NaOH. Comment on the nature of the graphs.
7. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.

Potentiometry

1. Titrate hydrochloric acid and sodium hydroxide potentiometrically.
2. Determine the dissociation constant of acetic acid potentiometrically.
3. Titrate oxalic acid and sodium hydroxide potentiometrically.
4. Titrate a mixture of (a) Strong and weak acids (Hydrochloric and acetic acids); (b) Weak acid (acetic acid) and dibasic acid (oxalic acid) (c) Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide.
5. Titrate a solution of Mohr's salt against potassium permanganate potentiometrically. (ii). Titrate a solution of Mohr's Salt and potassium dichromate potentiometrically.

<u>Recommended Texts/References:</u>

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
2. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
3. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International 2 Revised ed edition (1 February 1988).

DISCIPLINE SPECIFIC ELECTIVE COURSES

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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		
Supramolecular & Photoinorganic Chemistry **CH-DSE-104**	**04**	**03**	—	**01**	U.G. Chemistry	--

Course objectives

The Objectives of this course are as follows:

- To comprehend the fundamental knowledge of supramolecular chemistry and its importance.
- To impart advanced knowledge the crystal engineering and catalysis of supramolecular complexes and their applications.
- Knowledge of various Photochemical electron transfer in metal complexes and their applications.

Learning outcomes

After completing the course, the students will be able to:

- Demonstrate the role of supramolecular chemistry in understanding of molecular bonding and structure.
- Interpret the supramolecular interactions in proteins and enzymes.
- Elucidate the understanding of self-assembly of biological molecules.
- Understand various types of photochemical reactions of coordination compounds and solar energy conversion in semiconductor systems.

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

UNIT 1: **(8 Hours)**

FUNDAMENTALS OF SUPRAMOLECULAR CHEMISTRY

Classification of Molecules, Large Molecules, Supermolecules, and Supramolecules, Nomenclature, Thermodynamic and Kinetic selectivity, Supramolecular interactions, Chelate, macrocyclic, and macro-bicyclic effects, High dilution synthesis, Template synthesis.

UNIT 2: **(15 Hours)**

CRYSTAL ENGINEERING

Introduction to Tectons and Synthons and their classification; Hydrogen bonds, strong, moderate, weak H-bonds; acidity and basicity of hydrogen bonds and hydrogen bonding Synthons; Use of H-bonds in crystal engineering and molecular recognition.

SELF-ASSEMBLY & MOLECULAR RECOGNITION

Introduction to self-assembly; biological examples of self-assembly; self-assembly in synthetic systems; self-assembly in coordination complexes; Supramolecular host design, Macrocyclic versus acyclic hosts, Catenanes; Rotaxanes.

SUPRAMOLECULAR CATALYSIS

Introduction; supramolecular interactions in proteins and enzymes for the control of their function; enzyme mimics; artificial enzymes; supramolecular catalysis in synthetic systems.

UNIT 3: **(22 Hours)**

PHOTOINORGANIC CHEMISTRY

Introduction to inorganic photochemistry, Redox reactions of transition metal complexes in excited states, excited-state electron transfer, Marcus-Hush model, Photochemical electron transfer in $[Ru(bipy)_3]^{2+}$, $[Os(bpy)_3]^{2+}$ and $[Fe(bpy)_3]^{3+}$ complexes, Role of spin-orbit coupling, life-times of excited states in these complexes, Photochemical supramolecular devices, devices for photo-induced energy or electron transfer, photo-chemically driven molecular machines.

ENERGY CONVERSION

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in semiconductor supported metal oxide systems, water-photolysis, Nitrogen fixation and CO_2

reduction. Supramolecular photochemistry in natural and artificial systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

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

EXPERIMENTS:

1. Synthesis, characterization (XRD, IR, UV, TGA, etc.) of semiconductors metal oxides and their photocatalytic applications.
2. Synthesis of a series of Cr(III) complexes (with ligands of varying ligand field strength), electronic spectral interpretation.
3. Synthesis, spectral studies and crystal structure of Ru(II) and Os(II) complexes.
4. Any other relevant experiment from time to time during the semester.

ESSENTIAL/RECOMMENDED READINGS (Theory)

1. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).
2. Khopkar, S.M., Basic Concepts of Analytical Chemistry 3rd Edition, Publisher: New Age International Publishers (2008), ISBN: 9788122420920, 8122420923.
3. Eldik, R. V.; Stochel G. Advances in Inorganic Chemistry: Inorganic Photochemistry, Volume 63, 1st Edition, Academic Press (2011)
4. Hartley, F. R., Burgess, C. & Alcock, R. M. Solution Equilibria. Prentice-Hall: Europe (1980).
5. Atwood, J. L. & Steed, J. W. Supramolecular Chemistry: A Concise Introduction John Wiley & Sons (2000).
6. Lehn, J. M. Supramolecular Chemistry: Concepts & Perspectives, Print ISBN:9783527293124 Wiley-VCH (2006).
7. Principles and Applications of Photochemistry, B. Wardle, John Wiley, 2009
8. Ligand Field Theory and Its Applications; B. A. Figgis and M. A. Hitchman; Wiley India, 2000
9. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
10. Inorganic Chemistry, Principles of structure and reactivity; 4th edn; J. E. Huheey, E. A. Keiter and R. L. Keiter. Pearson Education Inc.2003
11. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
12. Photochemistry, C. J. Wayne and R. P. Wayne; Oxford University Press; 1996.

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 (CH-DSE-105)

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 Stereochemistry of Organic Compounds **CH-DSE-105**	**4**	**3**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives: To impart knowledge of advanced concepts of stereochemical principles and asymmetric synthesis of organic compounds, and provide hands-on training in the synthesis and resolution of chiral compounds through laboratory experiments.

Learning Outcomes: Students will develop the ability to analyse the spatial arrangements, and study the properties and reactivity of stereoisomers through the knowledge of symmetry and chirality in organic molecules, gained through this course. The students will be able to predict and design different methods to attain enantioselectivity and diastereoselectivity in a reaction and examine the factors guiding the observed stereoselectivities. Students will attain hands-on training in synthesis, resolution, and optical purity determination of chiral compounds through laboratory experiments that would enhance employability in the chemical, especially pharmaceutical, industry where synthetic organic chemists work on stereo-selective synthesis of industrially relevant compounds.

SYLLABUS OF CH-DSE-105

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

UNIT 1: **(15 Hours)**
MOLECULAR SYMMETRY AND CHIRALITY
Symmetry operations and symmetry elements, point group classification, and symmetry number.

STEREOISOMERISM
Classification, racemic modification, molecules with one, two or more chiral centres; Assigning configuration (D/L, R/S, E/Z and P/M). Axial, planar, and helical chirality;

stereochemistry of allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds, and cyclophanes.

TOPICITY AND PROSTEREOISOMERISM

Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres. Simple chemical correlation of configurations with examples, quasiracemates.

UNIT 2: (15 Hours)

CYCLOSTEREOISOMERISM

Configurations, conformations and stability of cyclohexanes (di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

MOLECULAR DISSYMMETRY AND CHIROPTICAL PROPERTIES

Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

UNIT 3: (15 Hours)

ASYMMETRIC INDUCTION

Cram's, Prelog's, and Felkin-Ahn models; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

ASYMMETRIC SYNTHESIS

Significance and basic principles, stereoselective and stereospecific synthesis: Enantioselective and diastereoselective reactions. Methods of asymmetric synthesis: Resolution – Classical resolution, kinetic resolution, and dynamic kinetic resolution of racemic compounds/*meso*-compounds by resolving agents. Development in asymmetric synthesis from prochiral substrates using chiral auxiliaries, chiral reagents, and chiral catalysts.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

EXPERIMENTS

(i) Determination of optical purity of organic compounds such as tartaric acid, glucose, phenylalanine, proline, and limonene etc. by polarimeter.
(ii) Classical resolution of racemic compounds such as cis-/trans-1,2-diaominocyclohexane or 1-phenyl ethylamine by using a resolving agent.
(iii) Synthesis of racemic BINOL.
(iv) Resolution of racemic BINOL using (1*R*,2*R*)-diaminocyclohexane and determination of optical purity by polarimeter.
(v) *cis*-/*trans*- Isomerisation of alkenes.

(vi) Asymmetric aldol reaction catalysed by (L)-proline/(L)-prolinamide.
(vii) Oxidative kinetic resolution of secondary alcohols by using (1*R*,2*R*)-Jacobsen Mn(III) salen complex using an oxidant
(viii) Determine the Cotton effect of chiral compounds by CD.

ESSENTIAL/RECOMMENDED READINGS

1. Eliel, E. L. Stereochemistry of Carbon Compounds, Textbook Publishers (2003).
2. Nasipuri, D. N. Stereochemistry of Organic Compounds: Principles & Applications, South Asia Books (1994).
3. Kalsi, P. S. Stereochemistry: Conformation and Mechanism, New Age International Pvt. Ltd. (2022)
4. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998).
5. Bruice, P. Y. Organic Chemistry, Pearson Education, (2020)
6. Sengupta, S. Basic Stereochemistry of Organic Molecules, Oxford University Press (2018)
7. Clayden, J; Greeves, N.; Warren, S. Organic Chemistry, Oxford University Press, (2014)
8. Gawley, R. E.; Aube, J. Principles of Asymmetric Synthesis (Tetrahedron series in Organic Chemistry), Pergman, (1996).
9. Catalytic Asymmetric Synthesis I. Ojima, Ed.; VCH: New York, (1993).
10. Schanz, H.; Linseis, M. A.; Gilheany, D. G. Improved resolution methods for (R,R)- and (S,S)-cyclohexane-1,2-diamine and (R)- and (S)-Binol. Tetrahedron: Asymmetry, 2003, 14, 2763.
11. Walsh, P. J., Smith, D.K.; Castello, C. Resolution of Trans-Cyclohexane-1,2-diamine and Determination of the Enantiopurity Using Chiral Solid Phase HPLC Techniques and Polarimetry. J. Chem. Educ. 1998; 75, 11, 1459.

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 /Practice		
Fundamentals of Mathematics for Chemistry **CH-DSE-106**	**04**	**03**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objective:

- To develop a sound foundation in mathematical methods essential for basics in study and research of Chemistry.
- To understand the application of linear algebra, multivariable calculus, differential equations, Fourier and other integral transforms, and statistical methods.
- To focus on mathematical approaches relevant to quantum chemistry, thermodynamics, kinetics, spectroscopy, and data analysis.
- To advance analytical skills to formulate and solve mathematical models of complex chemical systems.
- To prepare students to interpret experimental data quantitatively and engage in computational and theoretical chemical research.

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

- Recognize and apply basic calculus concepts, including differentiation and integration in quantum chemistry, thermodynamics, electrochemistry, and kinetics.
- Solve differential equations relevant to physical chemistry problems.
- Understand basic linear algebra, including vectors and matrices, to describe molecular structures and quantum systems.
- Apply elementary statistics for analyzing chemical data and phenomena.
- Interpret functions of several variables and use partial derivatives in thermodynamics and physical chemistry contexts.

Theory Course Contents: **Credit 3 (45 hours)**

Unit I: **15 hours**

A. Operators and Eigen-vectors: Linear operator and geometrical interpretation, Linear vector spaces; linear independence (qualitative discussion on Wronskian), basis vectors, inner product, Dirac bra-ket notation, hermitian conjugates (differential operators). Orthonormal sets. Completeness.

B. Vectors: Differentiation and integration of vectors, scalar and vector fields, divergence &

curl, theorems on line, surface, and volume integrals. Transformation of rectilinear cartesian to curvilinear spherical polar coordinates.

Unit II: **15 hours**

A. Differential calculus: Ordinary differential equations (ODE), ordinary and singular points of an ODE, and Partial differential equations (PDE), general solution of homogeneous equations. Power series solutions- particle in a box model, solutions of Associated Legendre polynomials- for integer *l* and second solution, harmonic oscillator, Laguerre, and associated Laguerre polynomials. Linear ODE of hypergeometric functions (qualitative discussion); Generating functions-recursion formulae and orthonormality: Hermite, Legendre, and Laguerre Polynomials.

B. Determinant and matrices: Properties of determinants and Laplace expansion (qualitative discussion). Matrices- diagonal, symmetric and anti-symmetric, hermitian and anti-hermitian, orthogonal, and unitary matrices, normal matrices, Eigenvectors and eigenvalues of Hermitian and unitary matrices, Cayley-Hamilton theorem, degenerate eigenvalues, Diagonalization of matrices (change of basis and similarity transformation).

Unit III: **15 hours**

A. Fourier sine-, cosine-, and exponential series. Fourier transform, Dirac delta function, Fourier sine and cosine transforms, applications of Fourier transforms. Laplace transform, theorems and Inverse Laplace transform, Solution of initial value problems using Laplace transform.

H-atom (quantitative discussion), Virial theorem, Hyper-virial theorem, and its applications to harmonic oscillator and H-like atoms.

B. Algebra of spin: Stern-Gerlach experiment, concept of spin operators and spin-eigenfunctions, two-electron spin systems; Pauli Exclusion Principle, Hartree product, antisymmetrization operator and Slater determinantal wavefunctions (qualitative discussion). Multiconfiguration calculations and Hartree-Fock theory (qualitative discussion).

Recommended Texts/References:

1. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).

2. Cohen-Tannoudji, Claude, Bernard Diu, and Franck Laloë F., Quantum Mechanics (Translated by G. G. Levine and D. S. Constable), vols-I&II, Wiley-Interscience, New York (1977).

3. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).

4. Atkins, Peter, and Ronald Friedman. Molecular Quantum Mechanics, Oxford University Press, 5th ed. (2011).

5. Howard Anton, Elementary Linear Algebra, John Wiley & Sons (2010).

6. Mortimer, Robert G., Mathematics for Physical Chemistry, 3rd ed., Academic Press (2010).

7. Arfken, George B., Hans J. Weber, and Frank E. Harris. Mathematical Methods for Physicists, 7th ed., Academic Press (2012).

8. Kreyszig, E., Advanced Engineering Mathematics, John Wiley & Sons, Inc. (2006).

9. Boas, Mary L., Mathematical Methods in the Physical Sciences, 3rd ed., Wiley (2005).

Practical Components **Credit 1**

1. Plot atomic orbitals (Spherical Harmonics *S(θ) versus θ* using polar graph paper. Students will be provided with the p-, d-, and f- functions.
2. Plot wavefunctions $\psi_n(x)$, and probability densities $|\psi_n(x)|^2$ for the 1D harmonic oscillator at different energy levels over the domain $-\infty < x < +\infty$.
3. Calculate the bond length of conjugated dye molecules (e.g., cyanine, β-carotene, etc.) using the particle-in-a-1D-box model.
4. Assign IR bands using symmetry considerations and selection rules for various molecules.
5. Develop familiarity with computational tools for analysis of experimental data:
   (a) Word processing, electronic spreadsheets etc.
   (b) Data processing software, mathematical packages, etc.
   (c) Chemical structure drawing, and molecular modelling, etc.
6. Perform statistical treatment of error analysis, including:
   (a) Null hypothesis testing,
   (b) T-test, F-test, Q-test (criteria for rejection of hypothesis),
   (c) Statistical analysis of laboratory data.
7. Determine standard deviation, mean and maximum absolute errors, root-mean-square deviation (error), and correlation coefficient of linear straight-line plots.

Recommended Texts/References:

1. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
2. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
3. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International 2 Revised ed edition (1 February 1988).

SKILL ENHANCEMENT COURSES

SKILL ENHANCEMENT COURSE (SEC)

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		
Introduction to Basic Lab Safety and Softwares for Research work **CH-SEC-107**	**02**	**01**	—	**01**	U.G. Chemistry	--

Course Objectives:

The course is designed to provide the fundamental understanding of the principle of operation, interpretation and learning of chemistry related softwares and Spectral Analysis, which will be highly helpful especially for their higher studies.

Learning Outcomes:

The students will be to:

1. Be aware of their and lab safety.
2. Analyze, interpret and index experimental data/theoretical data collected after various characterizations of their inorganic materials. It will enhance understanding of chemical concepts, improve problem-solving skills and the ability to utilize various tools in research and analysis.
3. Understand reaction mechanisms, visualizing molecular interactions, quantitative analysis, data interpretation, report writing and presentation, access to scientific literatures, software proficiency etc.

THEORY COMPONENT (1 Credit: 15 Hours)

Unit-I **(15 Hours)**

Types of personal protections (such as eye protection, gloves, lab coats, fire extinguishers etc.) their use, and limitations. Physical hazards like fire safety, electrical safety, glassware safety, radiation safety etc. Materials Safety Data Sheet (MSDS) file of all the available chemicals. Disposal of chemical waste, handling of hazardous chemicals, Identification of corrosives, flammables, and toxic substances etc. Handling and storing chemicals, including segregation and labelling.

ChemDraw: Widely used for creating 2D and 3D chemical structures, reactions, and pathways.

Origin: A data analysis and graphing software used for visualizing and analyzing data from experiments.

Chemsketch: To draw chemical structures, such as inorganic, organic, organometallic, polymers etc.

Vesta: A 3D visualization tool for structural data files, including those from crystallography. Chemical Databases and their utility.

X-pert High-score: Widely used to analyze X-ray diffraction (XRD) data with various applications such as phase identification, crystallographic analysis, cluster analysis, and Rietveld calculations.

International Centre for Diffraction Data (ICDD): Used to identify crystalline phases in materials using X-ray diffraction (XRD) data. It allows researchers to compare experimental XRD patterns against a vast database of reference patterns to determine the composition and structure of unknown materials.

Inorganic Crystal Structure Database (ICSD): To search, visualize, and analyze crystal structures. Valuable software for materials scientists, crystallographers, and other researchers who need precise information about the arrangement of atoms in solids. **Scifinder and Web of Science:** Databases and search engines for Chemical Literature.

Mendeley: To organize, manage, and cite research papers, articles, and other sources.

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

EXPERIMENTS:

1. Use of ChemDraw to create 2D and 3D chemical structures.
2. Data analysis and interpretation using Origin for 2D and 3D graphs, performing statistical analysis, signal processing, curve fitting and peak analysis.
3. Drawing, editing, and visualizing chemical structures, reaction drawing, molecular property calculations using Chemsketch software
4. Modeling and visualizing crystal structures, including unit cells, atomic positions, and bonds, handling of multiple structural models using Vesta software.
5. Hands on training on X-pert High-score software for XRD analysis.

6. To search, analyze and curating chemical information, as well as for accessing spectral data, synthetic methods, and safety information using ChemSpider, and Mendeley.

Reference (Theory):

1. Handbook for Laboratory Safety, Benjamin R. Sveinbjornsson and Sveinbjorn Gizurarson, Copyright © 2022 Elsevier Inc. ISBN 978-0-323-99320-3

2. Laboratory Safety for Chemistry Students, Robert H. Hill and David Finster, Wiley–Blackwell (20 August 2010). ISBN-13 : 978-0470344286.
3. https://csl.du.ac.in/
4. https://www.youtube.com/watch?v=hhfckQtdfKw

References (Practical):

1. https://www.youtube.com/watch?v=fHEe7AZ7sS0
2. https://www.youtube.com/watch?v=8tCUg2B523o
3. https://share.google/NiP4QGBFQFT8wZnZm
4. https://www.youtube.com/watch?v=TwVyvh628wE
5. https://www.acdlabs.com/resources/free-chemistry-software-apps/chemsketch-freeware/ (Freeware software)
6. https://www.youtube.com/watch?v=l06ljePcg8U
7. https://www.youtube.com/watch?v=CpW7khVmSAE
8. https://www.youtube.com/watch?v=dASaENblC_4
9. https://www.youtube.com/watch?app=desktop&v=TpuL4NgCMYc&t=0s
10. https://www.youtube.com/watch?v=lST-yMe322Y
11. https://www.youtube.com/watch?v=Go-BdmnYusU
12. https://www.youtube.com/c/mendeley/videos
13. https://www.youtube.com/watch?v=PJXnfBSq4Lg

*Students are encouraged to participate in various chemistry related workshops/conferences and submit their certificates and learning outcomes (1 page).

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

SKILL ENHANCEMENT COURSE (CH-SEC-108)

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		
Best Practices in Chemical Laboratory Safety **CH-SEC-108**	**2**	**1**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives: For a majority of students, chemistry laboratory safety is limited to a set of safety precautions explained by the instructors during a chemistry practical class. These safety precautions, though important are not sufficient to prepare a student for a research laboratory or an industrial job in the field of chemistry. This course aims to provide an in-depth knowledge on the best practices in chemistry laboratory safety. The students will be made aware of the need for safety culture through various documented laboratory accidents and near misses. This course will delve into recognition of hazards, risk assessment and its minimization in a chemistry laboratory through lectures, hands on learning/ demonstration and activities. This course will also prepare the students for responding to a chemical emergency.

Learning Outcomes:

After the completion of this course the students will develop a positive attitude towards safe laboratory practices. They will be able to recognise the potential hazards in a chemistry laboratory, assess these hazards by GHS, SDSs and other resources and will be able to minimise the risks. This course will also prepare them to respond to any emergencies in a chemistry laboratory. The students will also learn about chemical laboratory safety through hands on training, demonstration and activities. This advance course on best practices in chemistry laboratory safety will make students more employable in the field of chemistry in both academia and industry.

SYLLABUS OF CH-SEC-108

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

UNIT 1: **(15 Hours)**

LABORATORY SAFETY CULTURE

Understanding RAMP strategy, ethics and safety, learning from lab incidents.

RECOGNIZING HAZARDS

Globally Harmonized System of Classification and Labelling of Chemicals (GHS) and Safety Data Sheets (SDSs); toxicity, corrosives, carcinogens, biological hazards, hazards of nanomaterials, flammable chemicals, incompatible chemicals, explosion hazards, reactive and unstable chemicals, gas cylinders, cryogenic liquid tanks, cryogenic hazards, low- or high-pressure systems.

ASSESSING RISK

Understanding Occupational Exposure Limits (OEL), assessing chemical exposure, risk assessment for new experiments.

MINIMIZING RISK

Strategies to minimise risk, Personal Protective Equipment (PPE), fume hood, common laboratory safety measures in a chemistry laboratory, handling chemical wastes, management of chemicals in a laboratory- chemical inventory, storage and chemical security.

PREPARE FOR EMERGENCIES

Responding to emergencies in a chemistry laboratory, chemical spills, fire emergencies, first-aid.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

1. Demonstration/ hands on learning of the:
   a. Appropriate use of common laboratory devices and equipment (e.g., Bunsen burners, laboratory ovens, magnetic stirrers, U.V. chambers, centrifuges, vacuum pumps, rotary evaporators, refrigerators, freezers etc.).
   b. Proper use of a safety shower and an eyewash.
   c. Basic first aid procedures for common minor laboratory accidents
   d. Proper disposal of “sharps” and prevention of lacerations while handling glassware.
   e. Proper techniques for cleaning up minor spills (acid, base, or organic spill) in the laboratory.
   f. Appropriate use of PPE in response to a minor chemical spill.
   g. Proper use of the fire extinguisher.
   h. Storage protocols for laboratory chemicals (incompatible chemicals, flammables and corrosives)

2. Understanding Risk Assessment in a laboratory through activities.

3. Safety Data Sheet practice for a few commonly used laboratory chemicals.

ESSENTIAL/RECOMMENDED READINGS

1. Laboratory Safety for Chemistry Students by David Finster and Robert Hill. https://institute.acs.org/acs-center/lab-safety/education-training/college-univ-guidelines/laboratory-safety-for-chemistry-students-etextbook.html
2. Hill, R.H.; Finster, D.C. Laboratory Safety for Chemistry Students, 2nd Ed; Wiley: Hoboken, NJ, 2016.
3. Guidelines for Chemical Laboratory Safety in Academic Institutions, ACS Committee on Chemical Safety, Washington, DC., 2016. www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/acs-safety-guidelines-academic.pdf?logActivity=true
4. Safety in academic chemistry laboratories 8th edition best practices for first- and second-year university student. https://www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/safety-in-academic-chemistry-laboratories-students.pdf
5. Prudent practices in the laboratory: Handling and management of chemical hazards, Updated version. Washington, DC: The National Academies Press. https://doi.org/10.17226/12654.
6. United Nations. Globally Harmonized System of Classification and Labelling of Chemicals (GHS), Fifth revised edition, ST/SG/AC.10/30/Rev.5; New York and Geneva, 2013.
7. Bretherick's Handbook of Reactive Chemical Hazards, 8th Edition; Urben, P., Ed.; Elsevier, 2017.

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

SKILL ENHANCEMENT COURSE (SEC)

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		
Introduction to Computer Programming and Numerical Methods CH-SEC-109	**02**	**01**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives

- To introduce the evolution of programming languages and the rationale behind structured programming.
- To familiarize students with the syntax, compilation/execution process, and development environments for programming, variables, data types, operators, expressions, and program structure
- Understand the fundamental principles and need for numerical methods in solving mathematical problems.
- Develop the ability to implement numerical methods using programming tools.

Learning Outcome

1) Write, compile, and execute basic programs using appropriate IDEs and compilers across different platforms.
2) Design modular code using user-defined functions, input/output operations, control statements and formatted data handling
3) Explain the concepts and importance of numerical methods in computational problem-solving.
4) Apply numerical techniques for solving equations
5) Implement numerical methods using suitable programming languages or tools.

Theory Component **Credit: 1 (15 hours)**

Unit I:

A. Computer Programming: Evolution of programming languages; Importance of structured programming; Syntax overview and compilation/execution flow; IDEs and compilers.
Variables and Data Types (constants; variables, and declarations); Integer, real, double, character, logical, Mix-mode arithmetic and type conversion; Comments and program structure; Operators and Expressions, Logical and arithmetic expressions, Built-in (library) functions; Control Structures (Conditional branching, Loops), Input/Output Operations, Concepts of Functions, Procedures, and Modular Programming; Arrays and Strings
B. Finding roots of an equation, Iterative method, Successive bisection method, Method of false position and Newton-Raphson method.

Recommended Texts/References:

1) Rajaraman, V., *Computer Programming in C*. PHI Learning; 2nd edition (2019)
2) Kanetkar, Y. P. *Let us C*, BPB Publications; 15th edition (2024)
3) Rajaraman, V., *Computer Programming in Fortran 90 and 95*. 2nd Edition, PHI Learning (1997)
4) Chapman, S. J., *Fortran 90/95 for Scientists and Engineers*, McGraw-Hill Higher Education; 2nd edition (2003)
5) Zelle, J. M. *Python Programming: An Introduction to Computer Science*, 4th Edition, Shroff Publishers & Distributors Pvt. Ltd. (2024)
6) Schatzman, M., *Numerical Analysis: A Mathematical Introduction*, 1st edition, Oxford University Press. (2002).
7) Press, W. H., Teukolsky, S. A., Vetterling, W. T. and Flannery, B. P., *Numerical Recipes: The Art of Scientific Computing*, Vol 1, 3rd Edition, Cambridge University Press (2007).

Lab Components **Credit: 1**

1) Write a program to compute (i) the area and circumference of a circle, given the radius, (ii) to check whether a number is positive, negative, or zero, (iii) *H* and *S* from *Cp* from given data, (iv) *p*H of a weak and strong acid, (v) convert Celsius to Fahrenheit or vice versa, (vi) leap year checker, (vii) palindrome checker, (viii) Fibonacci series
2) Write a function to compute the factorial of a number.
3) Write a program to reverse a given string.
4) Calculate the sum of the first 10 natural and prime numbers using a loop.
5) Write a program to check whether a given number is even or odd.
6) Write a program to find the maximum and minima for a set of numbers.
7) Write a program to find a root using the bisection method.
8) Write a program for false position method for root-finding.
9) Write a program to solve a nonlinear equation using the fixed-point iteration (simple iteration) method
10) Use the Newton-Raphson method to solve systems of simultaneous nonlinear equations.
11) Implement and compare the Bisection and Newton-Raphson methods for solving nonlinear equations.
12) Write a program to compare Bisection, Regula Falsi, and Newton-Raphson methods on the same function.

Recommended Texts/References:

1) Rajaraman, V., *Computer Programming in C*. PHI Learning; 2nd edition (2019)
2) Kanetkar, Y. P. *Let us C*, BPB Publications; 15th edition (2024)
3) Rajaraman, V., *Computer Programming in Fortran 90 and 95*. 2nd Edition, PHI Learning (1997)
4) Chapman, S. J., *Fortran 90/95 for Scientists and Engineers*, McGraw-Hill Higher Education; 2nd edition (2003)
5) Zelle, J. M. *Python Programming: An Introduction to Computer Science*, 4th Edition, Shroff Publishers & Distributors Pvt. Ltd. (2024)
6) Schatzman, M., *Numerical Analysis: A Mathematical Introduction*, 1st edition, Oxford University Press. (2002).
7) Press, W. H., Teukolsky, S. A., Vetterling, W. T. and Flannery, B. P., *Numerical Recipes: The Art of Scientific Computing*, Vol 1, 3rd Edition, Cambridge University Press (2007).

SKILL ENHANCEMENT COURSE (SEC)

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		
Electrochemical Energy Devices and Technologies **CH-SEC-110**	02	0	-	02	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives:

- To learn process of making contemporary electrochemical energy devices and their testing methodology. Course is developed through videos of process of making and assembling Li ion batteries, Dye-sensitized Solar Cell, and associated devices.

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

- Know how to assemble and test an electrochemical energy device of various kinds.

Lecture Demonstration Course Contents**:** **(Credit 2; 60 Hours)**

1. Assembling and testing of liquid-electrolyte based Li-ion Rechargeable Battery and its working mechanism.
2. Assembling and testing of All solid-electrolyte based Li-ion Rechargeable Battery and its working mechanism.
3. Demonstration of Dye-sensitized Solar cell and its working mechanism.
4. Principle of electrolysis and demonstration of Hydrogen Production.
5. Demonstration of Supercapacitor and its working mechanism.

Recommended Texts/References:

1. Electrochemical Energy: Advance Materials and Technologies, Edt P.K. Shen, C-Y Jiang, X. Sun, J. Zhang, CRC Press, 2016
2. Bockris, John O'M. and Reddy, A.K. N. Vol 1: Modern Electrochemistry , Ionics, 2nd Edition Springer (1998)
3. Bockris, John O'M., Reddy, A.K. N. and Gamboa-Aldeco, M. Modern Electrochemistry, Vol 2A, Fundamental of Electrodes, 2nd Edition Springer (2000)

GENERIC ELECTIVE COURSES

Generic Elective (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		
Basics of Mineral Chemistry **CH-GE-111**	**04**	**03**	—	**01**	B.Sc. (any stream)	NIL

Course objectives:

Introducing students to the naturally occurring inorganic solids called as the minerals that are formed by complex processes over wide-ranging temperatures and pressures.

That the study of the minerals is essentially learning about their chemistry, physical and chemical properties.

Learning outcome:

Upon successful completion of this course, the students will be able to:

- Recognize the relevance of inorganic chemistry concepts to understand the minerals.
- The development of the structural chemistry of a vast majority of the inorganic solids is related to the various mineral structural families.

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

Unit-1: INTRODUCTION, PHYSICAL PROPERTIES OF MINERALS AND ELEMENTS OF CRYSTAL CHEMISTRY **(15 Hours)**

Definition of Mineral, Economic importance of minerals, Naming of minerals

Crystal form and Crystal Habit, Intergrowths, Twins and striations, State of aggregation, Properties depending on light, Luster, Color and streak, Play of colors, Luminescence, Fluorescence and Phosphorescence, Cleavage, Parting and Fracture, Hardness, Tenacity, Specific Gravity and its determination, Magnetism, Radioactivity, Piezoelectricity.

Chemical Composition of earth's crust, Bonding forces in crystals, Atomic and Ionic radii, Examples of common structure types, NaCl structure, CsCl structure, Sphalerite (ZnS) structure, CaF_2 structure, Rutile (TiO_2) structure, Perovskites (ABO_3) structure, spinel (AB_2O_4) structure, Silicate structures, Substitutional solid solution, Interstitial solid solution, Omission solid solution.

Unit-2: MINERAL REACTIONS, STABILITY AND BEHAVIOR (15 Hours)

Reaction in an Igneous regime, reaction under metamorphic conditions, Reaction in a weathering environment, Ultra-high-pressure reactions, Mineral stability, one -, two-, three- or more component diagrams, mineral reactions involving H_2O or CO_2, Eh-pH diagrams, Polymorphic reactions, Origin of color, Magnetic properties and Radioactivity.

Unit-3: CRYSTAL STRUCTURE OF ROCK-FORMING SILICATES (15 Hours)

Classifications, structures and properties. Nesosilicates, Sorosilicate, Cyclosilicates, Inosilicates, Phyllosilicates, Tectosilicates including aluminosilicates and Zeolite group.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

EXPERIMENTS:

1. Analysis: Few qualitative analysis experiments to confirm the presence of frequently occurring (e.g. Na, K, Mg, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Al, Si, Pb, F, Cl, Br, I, S) cations and anions in minerals along with few quantitative estimation experiments.
2. Physical characterization methods, IR, UV-Visible experiments, and PL (Photo Luminescence) Emission. Simple inorganic compounds may be used to draw the analogy with the minerals.
3. Powder X-Ray diffraction. Experiments to demonstrate the identification using the literature available as data base; XRF analysis. Demonstration experiments if possible to detect the using simple minerals or analogs ($CaCO_3$ mixed with $MgCO_3$)

4. Magnetic property measurements at RT.
5. Any other relevant experiment from time to time during the semester.

References (Theory):

1. The 22nd Edition of the Manual of Mineral Science, Cornelis Klein, John Wiley & Sons, Inc. New York, 2002.
2. Inorganic Chemistry (Fifth Edition), Shriver & Atkins, 2010, Oxford University Press
3. Vogel's Qualitative Inorganic Analysis – Arthur. I. Vogel, Imperial College, Longmans, Green and Co, London, New York, Toronto, 1937 or 7th Edition – G. Svehla and B. Ravisankar, Pearson Education 2008.
4. Textbook of quantitative chemical analysis – Arthur. I. Vogel, Longman Publisher, 5th edition 1989.
5. Quantitative Chemical Analysis 7th Edition Daniell C. Harris, Freeman & Company, New York 2007.

References (Practical)

1.Textbook of quantitative chemical analysis – Arthur. I. Vogel, Longman Publisher, Latest edition.

2.Quantitative Chemical Analysis 7th Edition Daniell C. Harris, Freeman & Company, New York 2007.

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 (CH-GE-112)

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		
Introduction to Drug Discovery and Development **CH-GE-112**	**4**	**3**	**0**	**1**	B.Sc. (any stream)	NIL

Course Objectives:

Understand what drugs are and how they are processed in the body, and how molecular characteristics impact the success of pharmaceutical drugs. Gaining knowledge about the molecular interactions that form the basis of drug-target interactions. Understanding the factors that enhance such interactions to make more effective therapeutics. Understand and predict how drugs are metabolized at the molecular level, including functional groups that are metabolic liabilities and those that are toxic. Discuss and describe modern strategies to identify chemical compounds from large chemical libraries that may serve as a source for new drugs.

Learning Outcomes:

1. Develop knowledge of the process through which potential new therapeutics are identified.
2: Develop an understanding of important drug discoveries.
3: Develop knowledge of modern drug discovery techniques and methodologies.
4: Understanding the various approaches to screen and design.
5: Present advanced knowledge to demonstrate understanding of drug discovery and development.
6. The students will acquire the following skills through experiments:
 i) Synthesis of the common APIs, involving functional group manipulations.
 ii) Use purification techniques to purify common APIs.

SYLLABUS OF CH-GE-112

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

UNIT 1: (15 Hours)

KEY CONCEPTS FOR DRUG DEVELOPMENT

Introduction and role of medicinal chemistry, difference between a drug and medicine, history and development, drug discovery approaches, drug targets (lipids, proteins including enzymes and receptors, nucleic acids and carbohydrates), drug-receptor interaction, mode of actions, agonist, antagonist, reverse agonist, therapeutic index, random/non-random screening, pharmacophore, Lipinski rule (rule of five), role of chirality in drug discovery (thalidomide history).

UNIT 2: (15 Hours)

PROCESS OF DRUG DEVELOPMENT

Lead discovery, lead modification, bioisosterism, optimizing drug-target interactions, structure-activity relationship, concept of prodrug, pharmacokinetics, pharmacodynamics, drug metabolism (ADME), drug administration routes, toxicity, clinical trials, repurposing of drugs, me-too drugs, aspirin, paracetamol, remdesivir.

UNIT 3: (15 Hours)

THERAPEUTICS IN ACTION

General introduction to antibiotics, mechanism of action of β-lactam antibiotics, non-β-lactam antibiotics, quinolones, antiviral drugs, gene therapy, anti-sense therapy, and drug resistance.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

EXPERIMENTS

1. Separation and Purification techniques: Distillation, Recrystallization, Chromatography
2. Synthesis of APIs
    - 2.1 Synthesis of aspirin
    - 2.2 Synthesis of sulphanilamide
    - 2.3 Synthesis of paracetamol
3. Isolation of APIs from tablets
    - 3.1 Isolation of paracetamol
    - 3.2 Isolation of naproxen
4. Isolation of biologically active natural products from plant materials
    - 4.1 Isolation of caffeine from tea leaves
    - 4.2 Isolation of curcumin from turmeric
    - 4.3 Isolation of eugenol from clove oil
    - 4.4 Isolation of lycopene from tomato

ESSENTIAL/RECOMMENDED READINGS

Theory

1. V. K. Ahluwalia and Madhu Chopra, Medicinal Chemistry, Anes Student Edition, 2008.
2. S. K. Gupta, Drug screening methods, New Delhi: Jaypee Brothers Medical Publishers (P) Ltd; 2004.

3. N. K. Dunlap, & D. M. Huryn, Medicinal Chemistry, Garland Science, New York, 2018.
4. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 1995.
5. T. L. Lemke & D. A. William, Foye's Principles of Medicinal Chemistry, 5th Ed., USA, 2002.
6. A. Gringuage, Introduction to Medicinal Chemistry, Wiley-VCH, 1997.
7. E. Stevens, Medicinal Chemistry-The Modern Drug Discovery Process, Pearson, 2014.
8. Richard Silverman, The Organic Chemistry of Drug Design and Drug Action, 3rd Ed, Academic Press.

Practical

1.Vogel, A. I. (2012), Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
3. Reddy, Y. K., Jayaveera, K. N., Subramanyam, S. (2013), Practical Medicinal Chemistry, S. Chand Publication.
4. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press.

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

Generic Elective (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		
Interface Chemistry: Bridging Biophysics, and Nanomedicine **CH-GE-113**	**04**	**03**	**-**	**01**	B. Sc in Science	--

Course Objectives:

- To introduce the fundamental principles of colloidal and surface chemistry, including micellization, adsorption phenomena, and the thermodynamics of self-assembly.
- To develop an understanding of macromolecules and polymers, their synthesis, characterization, and physicochemical properties.

- To explain the structural and thermodynamic properties of biological macromolecules, such as proteins and enzymes, and to apply quantitative models to ligand binding and enzymatic reactions.
- To explore the design, function, and biological interactions of nanomaterials used in diagnostics and drug delivery, including targeting strategies and pharmacokinetics.
- To familiarize learners with modern analytical and optical techniques used in studying biological systems, such as spectroscopy, calorimetry, and microscopy.

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

- Understand of surface chemistry principles, including micellization, adsorption isotherms, and thermodynamics of surfactant systems.
- Analyze the properties, synthesis, and characterization techniques of macromolecules and polymers, including molecular weight determination and polymerization types.
- Interpret the structural and thermodynamic behavior of biological macromolecules, and apply enzyme kinetics models such as the Michaelis-Menten equation and inhibition mechanisms.
- Evaluate the biomedical applications of lipid-, polymer-, and inorganic-based nanomaterials, focusing on drug delivery, diagnostics, cellular uptake, and biological barrier transport.
- Apply modern analytical and optical techniques-including spectroscopy, calorimetry, and microscopy-for studying biomolecular interactions and structures.

Course Contents (Theory): **Credit: 3 (45 hours)**

Unit-I: **15 hours**

A. Surface-active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature. Packing parameters, thermodynamics of micellization.

Adsorption: Gibbs adsorption isotherm, Langmuir and BET isotherms, surface area measurements.

Macromolecules and types of polymerizations, Degree of polymerization, number and mass average molecular masses, Polymer characterization: osmometry, viscometry, light scattering, diffusion.

B. Isoelectric point of amino acids, Configuration, and conformation of biological macromolecules, Thermodynamics of protein folding/stability, Thermodynamics and kinetics of ligand interactions, Macromolecule-ligand binding and cooperativity (including Hill equation).

Unit II: **15 hours**

Lipid-, polymer-, inorganic-based and hybrid nanomaterials for biomedical applications. Nanomaterials in optical, magnetic-resonance, radio and other diagnostics. Encapsulation and release of drugs, DNA, and other active agents. Interaction of nanomaterials with mammalian and pathogenic cells. Endocytosis, phagocytosis and other cell-entry mechanisms. In vitro assays: cell viability, ROS determination, etc. Routes of administration of nanoparticles in the body. Delivery of nanoparticles across biological barriers: RES barrier, blood-brain barrier, skin barrier, mucosal barrier, etc. Bioavailabilty, PK/PD of nanomaterials in the body. Passive and active targeting. Long-term fate and toxicological aspects of nanomaterials in the body.

Unit III: **15 hours**

A. Enzyme catalysis: Michaelis-Menten equation (with derivation), Lineweaver-Burk plot, define the turnover number and Michaelis constant, Enzyme inhibition-reversibility and products inhibition.

B. Basic principles and applications of analytical and optical techniques in biological systems: Absorption and fluorescence spectroscopy, Isothermal Titration Calorimetry (ITC), Linear and Circular Dichroism (CD), Optical Microscopy (Basic principles and Instrumentations).

Recommended Texts/References:

1. Wilson, K. & Walker, J., Principles and Techniques of Biochemistry and Molecular Biology, Eight Editions, 2018.
2. Lehninger, Principles of Biochemistry Seventh Edition, 2017.
3. Voet, D.; Voet, J. G.; Pratt, C. W. Voet's Principles of Biochemistry Fifth Edition, 2018.
4. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, Third Edition, 2006.
5. Carraher, C. E., Introduction to Polymer Chemistry, Fourth Edition, 2017.
6. Prasad, P. N. Introduction to Nanomedicine and Nanobioengineering. Wiley, 2012.
7. Webster, T. J. Nanomedicine Technologies and Application (2nd Edition), ScienceDirect, 2023.
8. Jain. K. K. The Handbook of Nanomedicine. Springer, 2017

Practical Components: **Credit 1**

1. (a) Determination of critical micellar concentration (cmc) of surfactant solutions and (b) calculation of thermodynamic parameters of micellizations.
2. Study the kinetics of the reaction of crystal violet with sodium hydroxide.
3. Determination of molecular weight of polymers
4. Determination of isoelectric points of amino acids.
   a) Neutral, b) Basic and c) acidic amino acids
5. Study of the oscillating reaction using a redox system.
6. Develop familiarity with computational tools for analysis of experimental data:
   (a) Word processing, electronic spreadsheets etc.
   (b) Data processing software, mathematical packages, etc.
   (c) Chemical structure drawing, and molecular modelling, etc.
7. Determine standard deviation, mean and maximum absolute errors, root-mean-square deviation (error), and correlation coefficient of linear straight-line plots using experimental data.

Recommended Texts/References:

1. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
2. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).

3. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
4. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International 2 Revised ed edition (1 February 1988).

SEMESTER- II

DISCIPLINE SPECIFIC CORE COURSES

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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		
Chemistry of *d*- and *f*- block elements **CH-DSC-201**	**04**	**02**	—	**02**	U.G. Chemistry	**--**

Course objectives

The Objectives of this course are as follows:

- To learn about the fundamental structural and bonding aspects of d- and f-block metal chemistry.
- Imparting knowledge of the physical properties of these metal complexes.

Learning outcomes

After completing the course, the students will be able to:

- Interpret the experimental electronic absorption spectra
- Establish the structure property correlation for magnetic metal complexes
- Elucidate stability of various metal complexes based on the bonding aspects

THEORY COMPONENT **(2 Credit: 30 Hours)**

UNIT 1: **(15 Hours)**

BONDING AND STRUCTURAL ASPECTS IN *d* AND *f*-BLOCK METAL COMPLEXES

Brief discussion on Crystal Field Theory (CFT), splitting in octahedral, tetrahedral, square planar and trigonal bipyramidal and square pyramidal crystal field; application of crystal field stabilisation energy (CFSE) in different thermodynamic aspects, the Irving–Williams series; static and dynamic Jahn-Teller distortion**;** Molecular orbital theory (MOT) for octahedral, tetrahedral and square planar complexes; Ligand Field Theory (LFT) for complexes with σ-donor, π- donor and π- acceptor ligands**;** Angular Overlap Model (AOM) for quantitative assessment of bonding in the metal complexes. Structural diversity in transition and lanthanoid based complexes, structural isomerism and stereoisomerism inmetal complexes;Dewar-Chatt-Duncanson model for structure and bonding in complexes containing π-acceptor ligands; metal-metal bonds, cluster compounds of *d*-block elements, poly-oxometallates of Ruthenium, Osmium and Molybdenum.

UNIT 2: (15 Hours)

PHYSICAL PROPERTIES OF *d*- AND *f*-BLOCK COMPLEXES

d- and *f*-Orbitals and oxidation states, electronic configuration, microstates, Term symbol, Russel-Saunders scheme, spin-orbit coupling, Hund's rule for ground state term symbol. Electronic absorption spectra of octahedral and tetrahedral complexes, Interpretation of electronic absorption spectra: Orgel diagram, Tanabe-Sugano diagram; determination of Dq, Racah parameters, Nephelauxetic parameter; Quantum non-crossing rule, Selection rules, charge transfer absorption, fluorescence and phosphorescence spectra of *d*- and *f*- block metal complexes; Magnetic properties of transition metal and lanthanide complexes; Introduction to transition and lanthanide metal based single molecular magnets (SMMs), Relativistic effects affecting the properties of heavier transition elements; application of lanthanoid shift reagents in NMR spectroscopy.

PRACTICAL COMPONENT (2 Credit: 60 Hours)

EXPERIMENTS:

1. Qualitative analysis of mixtures of salts including rare element salts (soluble and insoluble) containing eight radicals including interfering ions.
2. Synthesis of lanthanide and cerium complexes and their analysis: Magnetic moments, IR, NMR
3. Synthesis and characterization of iron/chromium complexes: IR, electronic spectra and magnetic susceptibility
4. Utilization of coordination chemistry to demonstrate invisible ink in laboratory.

5. Colour effects due to ligand-exchange in nickel complexes: Demonstration of ligand-field strength in the spectrochemical series.

6. Any other relevant experiment from time to time during the semester.

ESSENTIAL/RECOMMENDED READINGS (Theory)

1. Shriver, D. F., Atkins, P. W. & Langford, C. H. Inorganic Chemistry, 2nd Ed., Oxford Univ. Press (1998).
2. Purcell, K. F. & Kotz, J. C. Inorganic Chemistry, W. B. Saunders and Co.: N. Y. (1985).
3. Wulfsberg, G. Inorganic Chemistry Univ. Science books: Viva Books: New Delhi (2000)
4. Mabbs, F. E. & Machin, D. J. Magnetism and Transition Metal Complexes Chapman and Hall: U.K. (1973).
5. Drago, R. S. Physical Methods in Chemistry W. B. Saunders Co.: U.K. (1982).

SUGGESTED READINGS (Theory)

1. Housecroft, C. E. and Sharpe, A. G. Inorganic Chemistry, Pearson (2018).
2. Miessler, G. L.; Fischer P. J. and Tarr D. A. Inorganic Chemistry, Pearson (2018).
3. Dutta, R. L. and Syamal, A. Elements of Magnetochemistry, Affiliated East-West Publishers (1993).

ESSENTIAL/RECOMMENDED READINGS (Practical)

- Svehla, G. Vogel's Textbook of Macro and Semi-micro Qualitative Inorganic Analysis, 5th Edition (1979)

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 (CH-DSC-202)

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 Organic Spectroscopy **CH-DSC-202**	4	2	0	2	U.G. Chemistry	NIL

Course Objectives: Understanding of spectroscopic principles and advanced techniques of NMR and Mass, and their application in the structural elucidation of organic compounds.

Learning Outcomes*:* Students will gain an understanding of the basic principles of NMR spectroscopy, such as chemical shift, coupling constant, and anisotropy, and describe how they are affected by molecular structure, and identify organic compounds by analysis and interpretation of spectral data. At the end of this course the students will be able to analyse an unknown organic compound by interpreting its UV-Vis, IR, ^{1}H NMR, ^{13}C NMR, 2D-NMR, and mass spectral data. The students will synthesise organic compounds and will characterise these with the help of IR, NMR (^{1}H and ^{13}C NMR) and mass spectral data, D_2O exchange, DEPT and 2D-NMR techniques.

SYLLABUS OF CH-DSC-202

THEORY COMPONENT **(2 Credit: 30 Hours)**

UNIT 1: **(15 Hours)**

PROTON MAGNETIC RESONANCE SPECTROSCOPY

Basics of NMR with focus on ^{1}H, ^{13}C, ^{19}F, ^{31}P nuclei; chemical shift and spin-spin coupling; coupling patterns; chemical and magnetic equivalence; proton exchange; and factors affecting the coupling - First and non-first order spectra; simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents) and NOE experiment; study of dynamic processes by Variable temperature (VT) NMR; Applications of PMR in structural elucidation of simple and complex compounds.

UNIT 2: **(15 Hours)**

CARBON-13 NMR SPECTROSCOPY

Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling, noise decoupling, broadband decoupling; deuterium, fluorine, and phosphorus coupling; NOE signal enhancement, offresonance, proton decoupling, structural applications of CMR; DEPT and INEPT experiments; introduction to 2D-NMR; COSY, HETCOR, HSQC, HMBC, NOESY, HOESY, ROESY spectra.

MASS SPECTROMETRY

Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms: singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; Nitrogen rule; Ionization methods (EI, CI, FAB, ESI, APCI and MALDI), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-, β-, allylic and benzylic cleavage; McLafferty rearrangement, ortho effect etc.

STRUCTURE ELUCIDATION USING SPECTROSCOPIC DATA

Structure elucidation of organic compounds using IR, NMR, and Mass Spectral data.

PRACTICAL COMPONENT (2 Credits: 60 Hours)

EXPERIMENTS

Note: All the synthesized compounds will be characterized with the help of IR, NMR (^{1}H and ^{13}C NMR) and mass spectral data. D_2O exchange, DEPT and 2D-NMR will also be performed wherever necessary.

1. Acetylation/benzoylation reactions of arylamines, phenols, hydroquinone, salicylic acid, carbohydrates.
2. Synthesis of heterocyclic compounds.
3. Identification of exchangeable protons by D_2O exchange experiments.
4. Identification of $-CH_3$, $-CH_2$, CH and quaternary carbons by DEPT and APT experiment.
5. Identification of inter and intramolecular hydrogen bonding by IR and NMR.
6. Application of the coupling constant to identify cis- and trans-isomers, diastereotopic protons in organic compounds by NMR.

ESSENTIAL/RECOMMENDED READINGS

Theory

1. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991, reprinted 2002).
2. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds John Wiley & Sons (2014).
3. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy Cengage Learning (2015).
4. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007.

Practical

1. Vogel, A. I. (2012), Quantitative Organic Analysis, Part 3, Pearson Education.
2. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.

3. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
4. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
5. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press

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 /Practice		
Fundamentals of Statistical Mechanics and Thermodynamics **CH-DSC-203**	**04**	**02**	**-**	**02**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objective:

- To develop a foundation in the core principles of classical and quantum statistical mechanics.
- To understand the concept of ensembles and their role in statistical mechanics.
- To explain how statistical methods connect macroscopic thermodynamic behavior with microscopic quantum systems.
- To apply these principles to systems such as ideal gases and monoatomic crystals.
- To study the Third Law of Thermodynamics and its implications using statistical mechanics.

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

- Learn the fundamental principles of statistical mechanics linking microscopic properties to macroscopic observables.
- Understand the concept of ensembles and their significance in statistical mechanics.
- Explore the applications of the Boltzmann distribution in various physical systems.
- Understand and apply Bose-Einstein and Fermi-Dirac statistics.

- Students will be able to gain knowledge about monoatomic crystals and chemical equilibrium through molecular partition functions.

Theory Course Contents: **Credit 2 (30 hours)**

Unit I **15 Hours**

A. Fundamentals: Idea of microstates and macrostates. Concept of distributions- Binomial & multinomial distributions for non-degenerate and degenerate systems, Thermodynamic probability and most probable distribution. Lagrange's undetermined multipliers. Stirling's approximation

B. Ensemble Concepts, Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Molecular partition function and its importance. Assembly partition function.

Unit II: **15 Hours**

A. Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy.

B. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures. Strongly and weakly degenerate Fermi and Bose gases (Qualitative discussion)
Einstein theory and Debye theory of heat capacities of monatomic solids.
Third law of thermodynamics, Residual entropy.

Recommended Texts/References:

1. McQuarrie, D. A. *Statistical Mechanics*, Viva Books Pvt. Ltd.: New Delhi (2003).
2. Reif, Frederick., Fundamentals of Statistical and Thermal Physics, McGraw-Hill, (1965).
3. Huang, Kerson, Statistical Mechanics, 2nd ed., Wiley (1987).
4. Pathria, R. K., and Paul D. Beale, Statistical Mechanics, 3rd ed., Elsevier (2011).
5. Pal, Palash B., Statistical Mechanics: Principles and Applications, Narosa Publishing House, (2008).
6. Bagchi B., Statistical Mechanics for Chemistry and Material Science, CRC Press (2018).
7. Landau, L. D. and Lifshitz, E. M. Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed. (2005).
8. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).

Practical Components: **Credit 2**

CHEMICAL KINETICS

1. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the

Initial Rate Method.

2. Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.

CONDUCTOMETRY

1. Study the conductometric titration of a mixture of a strong and weak acid.
2. Titrate a moderately strong acid (salicylic/ mandelic acid) by the, (a) salt-line method and (b) double alkali method.
3. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
4. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
5. Titrate magnesium sulphate against $BaCl_2$ and its reverse titration.
6. Estimate the concentration of each component of a mixture of $AgNO_3$ and HNO_3 by conductometric titration against NaOH.
7. Determine the degree of hydrolysis of aniline hydrochloride.

POTENTIOMETRY

1. Determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.
2. Determine the mean activity coefficient ($\gamma_{\pm}$) of 0.01 M hydrochloric acid solution.
3. Titrate phosphoric acid potentiometrically against sodium hydroxide.
4. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
5. Titrate potentiometrically solutions of (a) KCl/ KBr/ KI; (b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
6. Titrate Fe^{2+} with Ce^{4+} potentiometrically.
7. Determine zinc in the presence of calcium by potentiometric titration.
8. Verify the Debye-Hückel theory through the solubility of ionic salts.

Recommended Texts/References:

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
2. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
3. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
4. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International, 10th Revised edition (4th August 2021).

DISCIPLINE SPECIFIC ELECTIVE COURSES

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 / Practice		
Group Theory and its Applications in Chemistry **CH-DSE-204**	**04**	**03**	—	**01**	U.G. Chemistry	--

Course Objectives:

The objective of this course is to understand symmetry of molecules and implication of symmetry aspect on molecular properties.

Learning Outcomes:

Upon successful completion of this course, students will be able to:

- Understand the fundamental mathematical concepts of group theory.
- Identify and classify symmetry elements and operations in molecules.
- Assign point groups to molecules systematically.
- Construct and interpret character tables for various point groups.
- Apply group theory principles to predict molecular properties such as polarity and chirality.
- Utilize group theory to simplify and analyze molecular orbitals and chemical bonding.
- Determine selection rules for various spectroscopic techniques (IR, Raman, UV-Vis) based on molecular symmetry.
- Apply group theory to understand and predict vibrational modes of molecules.
- Gain an appreciation for the power of symmetry in various chemical phenomena.

THEORY COMPONENT (3 Credit: 45 Hours)

UNIT I: FUNDAMENTALS OF SYMMETRY AND GROUP THEORY (09 Hours)

Introduction to Symmetry, Symmetry in nature and chemistry, Importance of symmetry in chemical problems, Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation. Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups, and classification.

Group multiplication tables, Systematic assignment of molecular point groups (Schoenflies notation): Low symmetry groups (C_1, C_s, C_i), High symmetry groups (T_d, O_h, I_h), Special symmetry groups (C_{nv}, C_{nh}, D_n, D_{nh}, D_{nd}). Group generators, symmetry of Platonic solids. Relationship between symmetry and physical properties (polarity, chirality, optical activity).

UNIT II: REPRESENTATION THEORY AND CHARACTER TABLES (15 Hours)

Matrix Representation of Symmetry Operations, Representing symmetry operations by matrices, Reducible and irreducible representations, Properties of matrix representations: similarity transformation

Character Tables: Definition and significance of characters, The Great Orthogonality Theorem (GOT) and its consequences, Construction of character tables for simple point groups (e.g., C_{2v}, C_{3v}, C_{2h}, D_{3h}, C_{4v}), Properties of irreducible representations (IRs), Direct product of irreducible representations, Standard reduction formula for reducing reducible representations, position vector and base vector as basis for representation, some properties of vectors

UNIT III: APPLICATIONS IN CHEMICAL BONDING AND MOLECULAR ORBITALS (21 Hours)

Symmetry Adapted Linear Combinations (SALCs): Concept of basis sets and projection operators, Generating SALCs for various ligand types (sigma, pi), Construction of molecular orbitals for polyatomic molecules using SALCs, Examples: water, ammonia, methane, planar MX_3 and octahedral MX_6 complexes.

Symmetry and Bonding in Transition Metal Complexes: Ligand field theory and d-orbital splitting in various geometries (octahedral, tetrahedral, square planar) using group theory, Jahn-Teller effect from a symmetry perspective, Symmetry and bonding in metal carbonyls.

Spectroscopic Applications of Group Theory

Vibrational Spectroscopy (IR and Raman): Normal modes of vibration and their symmetries (3N Cartesian coordinates, internal coordinates), Determination of symmetries of vibrational modes using reducible representations, Selection rules for IR and Raman spectroscopy based on symmetry (activity of vibrational modes), Overtones, Hot bands, Combination bands, Ascent-Descent in Symmetry Relationships, Mutual exclusion principle, Examples: H_2O, CO_2, BF_3, NH_3, SF_6.

Electronic Spectroscopy (UV-Visible spectroscopy):

(i) Symmetry of molecular electronic states, Selection rules for electronic transitions (Laporte selection rule, spin selection rule), Symmetry aspects of charge transfer spectra.

(ii) Symmetry rules for Inorganic reactions, and Construction of correlation diagrams.

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

EXPERIMENTS:

1. Apply group theory to predict the number, symmetry, and IR/Raman activity of vibrational modes in selected ligands andtheir transition metal complexes ($[Co(NH_3)_6]^{3+}$, $[PtCl_4]^{2-}$, etc.).
2. Investigate the change in molecular symmetry and its spectroscopic consequences during structural transformations of metal carbonyl complexes (Octahedral to Tetrahedral Transformation or vice-versa).
3. Synthesize metal oxides (NiO, CuO, etc.) and characterize their vibrational properties using group theory to interpret the obtained spectra.
4. Any other relevant experiment from time to time during the semester.

References:

1. **F.A. Cotton,***Chemical Applications of Group Theory*, John Wiley & Sons, 1991.
2. **A. Vincent,***Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, John Wiley & Sons, 2013.
3. **K.V. Reddy,***Symmetry and Spectroscopy of Molecules*, New Age International Ltd. 2020.
4. **D.C. Harris and M.D. Bertolucci,***Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Publications. 1989.
5. **Davidson, G.** Group theory for chemists. London: Macmillan.1991.
6. Jaffe, H. H. &Orchin, M. Symmetry in Chemistry, Dover Publications (2002).
7. Hatfield, W. E. & Parker, W. E. Symmetry in Chemical Bonding & Structure. C. E. Merrill Publishing Co. USA (1974).
8. Garg, B.S. Chemical Applications of Molecular Symmetry and Group Theory, Macmillan Publishers India Ltd (2012).

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 (CH-DSE-205)

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		
Methods in Organic Synthesis **CH-DSE-205**	**4**	**3**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives: The students will acquire knowledge on various metal catalyzed coupling reactions, reducing agents, oxidizing agents, protecting and deprotecting reagents and their applications in organic synthesis. To equip students with the knowledge and skills to design a synthesis.

Learning Outcome: Students will gain an understanding of the basic principles of metal catalyzed coupling reactions, reducing agents, oxidizing agents, protecting and deprotecting reagents and their applications in organic synthesis. Students will learn various synthetic methodologies employed in organic synthesis. After completing this course, the students will be able to design synthetic routes and execute them.

SYLLABUS OF CH-DSE-205

THEORY COMPONENT (3 Credit: 45 Hours)

UNIT I (15 Hours)

C-C, C-N, C-S, AND C-O BOND FORMATION REACTION

Introduction of various bond formation reactions at sp, sp^2 and sp^3 carbons, challenges in Csp^2-C, N, S, O bond formation reaction, Catalytic cycles for aromatic C-C, C-N, C-S, and C-O bond formation, Ligands, mono-, bi- and multidentate phosphine ligands and their uses in various catalytic reaction, Role of Pd, Cu and Ni based catalysts in C-C, C-N, C-S, and C-O bond formation (Applications: Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling, Buchwald-Hartwig amination reactions).

C-H BOND ACTIVATION REACTION

Metal-catalysed C-H bond activation reaction at sp^2 carbon, Catalytic cycle involved in N-directed C-H activation reaction, Pd and Ru mediated N-Directed C-H activation reaction for C-C bond formation reactions

UNIT 2 **(15 Hours)**

Synthesis and applications of BuLi, Grignard reagent, organoaluminium, and organozinc reagents, lithium organocuprates, lower and higher order cuprates, organosilicon compounds.

REDUCTIONS

Stereochemistry, stereo-selection, and mechanism of catalytic hydrogenation and metal-liquid ammonia reductions.

HYDRIDE TRANSFER REAGENTS

Sodium borohydride, sodium cyanoborohydride, Triacetoxyborohydride, lithium aluminium hydride (LAH), and alkoxy-substituted LAH reducing agents, DIBAL.

HOMOGENEOUS HYDROGENATIONS

Mechanisms and applications using Rh, Ru, and other metal complexes for homogeneous hydrogenation.

UNIT 3 **(15 Hours)**

OXIDATIONS

Scope of the oxidizing reagents with relevant applications and mechanisms: Ceric Ammonium Nitrate, Sodium perborate, Tetramethyl piperidin-1-oxyl (TEMPO), Thallium nitrate, Selenium dioxide, Phase-transfer-catalyst (PTC), Crown ethers, Oxone, and sulphur. Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification & Swern Oxidation); Lead Acetate, Phenyliodine (III) diacetate (PIDA), Dess Martin periodinane, Tetrapropylammonium perruthenate, Ruthenium tetroxide. Sharpless Asymmetric epoxidation, Asymmetric hydroxylation, and aminohydroxylation.

Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN.

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

EXPERIMENTS

(i) TLCs (mixtures containing three or more compounds, and use of different visualizing/developing reagents).
(ii) Protection and deprotection reactions of carboxylic acids, amines, alcohols, 1,2-diols, aldehydes/ketones, etc.
(ii) Oxidation reactions of alcohols, aldehydes, etc.
(iii) Reduction reactions of aldehydes/ ketones, carboxylic acids, carbon-carbon multiple bonds, nitro compounds
(iv) Metals/ metal salts catalysed coupling reactions
(v) Bromination reactions involving allylic/ benzylic bromination and aromatic substitution reactions
(vi) Diazotisation reactions for substitutions and couplings

(vii) Condensation reactions
(viii) Esterification, transesterification and hydrolysis reactions
(ix) Preparation of phenoxyacetic acids and 2,4-D (2, 4-dichlorophenoxyacetic acid)

ESSENTIAL/RECOMMENDED READINGS

Theory

1. Carruthers, W. *Modern Methods of Organic Synthesis* Cambridge University Press (1996).
2. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
3. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).

Practical

1. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
2. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi
3. Vogel, A. I. (**2012**). Quantitative Organic Analysis, Part 3, Pearson Education
4. Furniss, B. S., Hannaford, A. J., Smith, P.W.G., Tatchell, A. R. (**2012**), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson
5. Ahluwalia, V.K., Dhingra, S. (**2004**), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.

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 /Practice		
Electrochemistry, Macromolecules and Chemical Kinetics: Statistical Approach **CH-DSE-206**	**04**	**03**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objective:

- To provide a comprehensive understanding of electrolytes and electrochemical interfaces through the principles of Statistical Mechanics and Thermodynamics.
- To introduce foundational concepts in macromolecular science and chemical kinetics.
- To explore the structure, synthesis, and properties of macromolecules such as polymers and biopolymers.
- To examine chemical reaction mechanisms, rate laws, and kinetic modeling of chemical systems.
- To develop the ability to analyze and design macromolecular and reactive systems in industrial and biological contexts.

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

- Apply the Boltzmann distribution and statistical thermodynamics to analyze ionic systems and interpret activity coefficients in electrolyte solutions.
- Describe the structural features, classifications, and physical properties of macromolecules.
- Model chemical reaction rates, mechanisms, and rate laws in both homogeneous and heterogeneous systems using principles of chemical kinetics.
- Explain the role of catalysis-including enzyme and heterogeneous catalysis—and solve problems involving chain reactions, photochemical kinetics, and complex mechanisms.
- Relate the kinetic behavior of macromolecular systems to their functional performance in both industrial and biological applications.

Theory Course Contents: **Credit 3 (45 hours)**

Unit I: **15 hours**

A. Poisson-Boltzmann equation, Derivation of Debye-Hückel model of dilute electrolytic solution, Ionic atmosphere and Debye screening length, Contribution of the Ionic Cloud to the electrostatic potential at central ion and chemical potential change, Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination. Finite ion size correction to model.

B. Derivation of Gouy-Chapman diffuse charge model of the double layer and capacitance. Qualitative discussion of electric double layer.

Unit II: **15 hours**

Macromolecules: Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. 1-D random walk model in detail, Average end-to-end distance. Brownian Dynamics (Qualitative discussion).

Unit III: **15 hours**

A. Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

B. Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

<u>Recommended Texts/References:</u>

1. Bockris, John O'M. and Reddy, A.K. N. Vol 1: Modern Electrochemistry, Ionics, 2nd Edition Springer (1998)
2. Bockris, John O'M., Reddy, A.K. N. and Gamboa-Aldeco, M. Modern Electrochemistry, Vol 2A, Fundamental of Electrodes, 2nd Edition Springer (2000)
3. Atkins, P and Paula, Julio de. Atkin's Physical Chemistry, Oxford University Press, (2002).
4. Laidler, K. J., Chemical Kinetics 3rd Ed., Benjamin Cummings (1997).
5. Billmeyer, F. W., Textbook of Polymer Science, 3rd Ed., Wiley-Interscience: New York (1984).
6. Teraoka, I., Polymer Solutions: An Introduction to Physical Properties, John Wiley & Sons, (2002).

<u>Practical Components</u>: **Credit 1**

1. Conductometric Study of critical micellar concentration (cmc).
2. Calculation of the thermodynamic parameters of micellization of surfactants from (a) conductivity and (b) spectroscopic measurements.
3. Study of the oscillating reaction in redox systems.
4. Determine the dissociation constant of an indicator (phenolphthalein) using calorimetry/spectroscopy.
5. Study the kinetics of the reaction of phenolphthalein with sodium hydroxide.
6. Study the kinetics of the reaction of crystal violet with sodium hydroxide.
7. Determine the molecular weight of macromolecules by the viscosity method.
8. Determine the viscosity-average molecular weight of poly (vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.

<u>Recommended Texts/References:</u>

1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
2. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
3. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
4. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International, 10th Revised edition (4th August 2021).

SKILL ENHANCEMENT COURSES

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SKILL ENHANCEMENT COURSE (SEC)

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 Training of Analytical Instrumentation **CH-SEC-207**	**02**	**01**	—	**01**	U.G. Chemistry	--

Course Objectives:

The course is designed to provide the learning of development of chemistry related models/hands-on training such as sampling for various analytical instruments, which is crucial for higher studies students in materials science, chemistry, and related fields.

Learning Outcomes:

The students will understand the principals of numerous characterization related to their work. Seriousness of safety protocols with various instruments and materials. Components of sample preparation for mentioned techniques: sample quantity, sample form, sample conductivity, sample thinning, sample holder, sample mounting, selection of suitable solvent, crucible selection, reference materials, purge gas selection, interpretation of resulting data etc.

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

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

X-ray diffraction: Brief discussion of principles of X-ray generation, diffraction phenomena and the components of a diffractometer. Sample handling, data analysis techniques like peak indexing, phase identification, and quantitative analysis, including the effects of crystallite size and strain. Applications in materials science, medical, forensic science, mining and mineralogy etc.

Thermogravimetric Analysis and Differential Thermal Analysis: Principles, instrumentation, data interpretation, and applications of both techniques. Theoretical concepts, practical exercises and case studies to provide a thorough understanding of thermal analysis methods.

X-Ray Photoelectron Spectroscopy: Operational fundamentals, components, sample preparation, data acquisition and spectral interpretation.

Auger Electron Spectroscopy: Brief outline of principles, components of an AES system (i.e vacuum system, electron gun, electron energy analyzer etc.), sample handling. Applications in elemental surface analysis, imaging, chemical state analysis etc.

Scanning and Transmission Electron Microscopy: Principles and fundamentals of electron microscopy, its components, and practical applications including sample preparation and image interpretation. Applications in materials science, nanotechnology, biology etc.

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

EXPERIMENTS:

1. Rietveld refinement for crystal structure determination, refinement of crystal structure, stress-strain analysis, use of Bragg's law and all related assignments.

2. Hands on training on Thermogravimetric Analysis and Differential Thermal Analysis.

3. Introduction, experimental setup, instrumentation (electrodes, potentiostat, data acquisition system etc), data analysis and interpretation using Cyclic Voltammetry.

4. Surface area analysis and the procedures for sample preparation, measurement and data analysis using Brunauer-Emmett-Teller (BET) instrument.

5. Electromagnetic spectrum, electronic transitions, function of various components like light sources, monochromators, sample holders, detectors, and recording of spectra using UV-Vis spectrophotometry.

6. Fundamental of instrumentation (light sources, wavelength selection, atomization, beam, signal processing etc.) and interferences, applications in environmental analysis, clinical chemistry, food science, pharmaceutical analysis, quality control etc. using atomic absorption spectrophotometer.

References (Theory):

1. Elements of X-Ray Diffraction, B.D. Cullity, Pearson; 3rd edition (2001), ISBN-13 : 978-0201610918.

2. Thermal Analysis: From Introductory Fundamentals to Advanced Applications, El-Zeiny Ebeid, Mohamed Barakat Zakaria, Elsevier - Health Sciences Division (2021), ISBN-13 : 978-0323901918

3. X-ray Photoelectron Spectroscopy - An Introduction to Principles and Practices, P van der Heide, John Wiley & Sons Inc; 1st edition (2012), ISBN-13 : 978-1118062531.

4. Auger- and X-Ray Photoelectron Spectroscopy in Materials Science: A User-Oriented Guide, Siegfried Hofmann, Springer; 2013th edition (2012), ISBN-13 : 978-3642273803.

5. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM, R.F. Egerton, Springer Cham (2016), ISBN978-3-319-39876-1.

References (Practical):

1. Powder Diffraction: The Rietveld Method and the Two Stage Method to Determine and Refine Crystal Structures from Powder Diffraction Data, Georg Will, Springer Science & Business Media (2006), ISBN: 9783540279860.

2. Electroanalytical Methods, Guide to Experiments and Applications, Fritz Scholz, Springer Berlin, Heidelberg (2002), ISBN: 978-3-662-04757-6.

3. Characterization of Porous Solids and Powders: Surface Area, Pore Size and Density, S. Lowell , Joan E. Shields , Martin A. Thomas , Matthias Thommes, Springer Dordrecht (2004), ISBN: 978-1-4020-2302-6.

4. UV-VIS Spectroscopy and Its Applications, Perkampus Heinz-Helmut, Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, ISBN: 9783540554219.

5. Atomic Absorption Spectrometry: Theory, Design and Applications, S.J. Haswell, Edition: 1, Volume: 5, Elsevier Science (1991), ISBN: 9780444882172

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

SKILL ENHANCEMENT COURSE (CH-SEC-208)

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 Training of Separation Techniques **CH-SEC-208**	**2**	**1**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives

The objectives of this course are as follows:

- To learn about the fundamentals of separation techniques employed in organic synthesis and purification of organic compounds.
- To understand instrumentation (hardware/software) understanding of equipment usually employed in analysis and identification of organic compounds.
- Hands-on training on several sophisticated spectroscopic instruments and separation techniques employed in organic synthesis.

Learning outcomes

After completing the course, the students will:

- Gain experience in various separation techniques typically employed for monitoring reaction progress and purification of pure compounds from mixture.
- Be able to work independently on sophisticated equipment used in organic synthesis, correlating with the principle and the instrumentation part.

SYLLABUS OF CH-SEC-208

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

UNIT 1: **(15 Hours)**

THIN LAYER CHROMATOGRAPHY

Principle of using TLC in monitoring organic reactions, Polarity of Solvents, Retention factor, Principle and application of HP TLC.

COLUMN CHROMATOGRAPHY

Theory of Column Chromatography, Gradient Solvent Systems, Application of Column Chromatography in purification of mixtures.

GAS CHROMATOGRAPHY

Basics and applications of GC, Instrumentation of GC, Applications of GC.

HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

Basics and Instrumentation of HPLC, Normal & Reverse Phase HPLC, Preparative HPLC, Applications of HPLC.

OPTICAL ROTATION

Importance of optical activity, Instrumentation of Polarimeter, Sample preparation, Recording Optical rotation of organic compounds.

PRACTICAL COMPONENT (1 Credit: 30 Hours)

1. (a) To determine the number of organic compounds, present in the given mixture by TLC, and calculate their respective R_f values.
(b) To determine the relative polarities of a set of given organic compounds by comparing their R_f on TLC.

2. (a) To separate a mixture of two or more non-polar organic compounds by column chromatography using gradient solvent system (Hexanes/EtOAc).
(b) To separate a mixture of two or more medium/high polarity organic compounds by column chromatography using gradient solvent system.

3. (a) Hand-on training on running a Gas Chromatography instrument.
(b) To optimize the base peak while running Gas Chromatography.
(c) To separate a mixture of essential oils using Gas Chromatography.

4. (a) Hand-on training on running a HPLC instrument.
(b) To optimize the base peak while running HPLC machine.
(c) To separate a mixture of medium polarity diastereomers with C-18 column using a reverse phase HPLC.
(d) To separate a mixture of enantiomers (e.g. diastereomers) with a chiral column using a reverse phase HPLC.

5. (a) Hand-on training on running a polarimeter and sample preparation.
(b) To measure the optical rotation of a pair of enantiomers.

ESSENTIAL/RECOMMENDED READINGS

- Furniss B. S., Hannford A. J., Smith, P. W. G., Tatcheli, A. R., “Vogel's Textbook of Practical Organic Chemistry” 5th ed., Longman Scientific &Technical.
- Kemp W., 'Organic Spectroscopy', 3rd ed., Palgrave, New York (1991).
- Willard H. H., Merritt Jr. L. L., Dean J. A., Settle F. A. S., “Instrumental Methods of Analysis”, 7th Ed., Wadsworth, 2009, Cengage Learning India Pvt. Ltd. Fifth Indian reprint by CBS Publishers & Distributors Pvt. Ltd.
- Silverstein R. M., and Webster F. X., “Spectrometric Identification of Organic Compounds”, 6th ed., John Wiley & Sons, New York (1998).
- Skoog D. A., Holler F. J., and Crouch S. R., “Principles of Instrumental Analysis”, 6th ed., Thomson Brooks/Cole, Cengage Learning, New Delhi (2007).

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

SKILL ENHANCEMENT COURSE (SEC)

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		
Recent Trends in Advanced Molecules and Materials **CH-SEC-209**	**02**	**01**	-	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives:

- To provide a comprehensive understanding of the synthesis, properties, and applications of advanced nanomaterials and nanoparticles.
- To develop knowledge of polymeric materials, liquid crystals, and their technological applications in modern materials science.
- To equip students with the skills to understand and apply various thin film deposition techniques and Langmuir-Blodgett film fabrication.
- To introduce the fundamentals and applications of optoelectronic materials and luminescent molecules in sensors and lighting technologies.
- To foster the ability to critically analyze material characteristics in relation to synthesis methods and their impact on functional applications in nanotechnology and materials science.

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

- To explain the fundamental concepts of advanced nanomaterials, including quantum dots, quantum confinement, and their applications, along with methods for nanoparticle synthesis and stabilization.
- To describe the properties, types, and applications of polymeric materials, including conducting and ferroelectric polymers, and to understand the mesomorphic behavior and phase transitions in liquid crystals.
- To demonstrate knowledge of various thin film preparation techniques and Langmuir-Blodgett film growth methods and their significance in material science.

- To identify and explain the characteristics and applications of optoelectronic materials, including luminescent phosphors, rare-earth based, semiconducting, and organic molecules used in lighting and sensing.
- To analyze the relationship between material synthesis methods, structure, and functional properties for applications across nanotechnology, polymer science, thin films, and optoelectronics.

Theory Course Contents: **Credit 1 (15 hours)**

Unit I:

A. Advanced Nanomaterials: Quantum dots, band gap, excitons, quantum confinement effect, Bhor's radius. Applications of Quantum dots, Methods of preparation nano particles, Chemical synthesis, Self-assembly processes, stabilization, different reducing agents, stability of nano particles, reactivities and catalytic activities of nanoparticles, different applications. Top down and bottom up approach in nano technology, Green synthesis: clean routes, super critical solvents, ionic liquids, green catalyst, auto exhaust catalyst and clean technology.

B. Polymeric Materials, polymer types and their applications, conducting and ferro-electric polymers; Liquid Crystals, Mesmorphic behavior, thermotrophic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic–nematic transition.

C. Thin film and Langmuir-Blodgett Films: Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) Film, growth techniques.

D. Optoelectronic Materials and molecules: Luminescent phosphor materials including rare-earth based, semiconducting and organic based molecules and materials for lighting/sensor and other applications.

Recommended Texts/References:

1. West, A.R. Solid State Chemistry and its Applications, John Wiley & Sons, 2nd Edition, (2014)
2. Nanomaterials Chemistry: Recent Developments and New Directions by C. N. R. Rao, A. Muller and A. K. Cheetam, Willey- VCH Gmbh & Co (2007).
3. Cao, G. Nanostructures and Nanomaterials: Synthesis, Properties and applications, Imperial College Press, London (2011).
4. Sylvia, L. Nanomaterials (Architecture & Design), Springer Verlag (2008)
5. Brechignac,C. Houdy, P. and Lathmani, M. Nanomaterials and Nanochemistry by, Springer Verlag, Berlin, 1st Edition, 2007.
6. Callister, W. D. Materials Science and Engineering, an Introduction, Willey, 10th Edition, 2018.
7. Thermotropic Liquid Crystals, Ed., G. W. Gray, John Willey (1987).

Practical Contents: **Credit 1**

1. (a) Synthesis of any semiconducting nanomaterials (CdSe, ZnSe, In_2S_3 etc.) and (b) understanding their structural and optical properties like band gap, luminescence, recombination etc. using available laboratory equipments.
2. (a) Preparation of a polymer from their monomer counterpart and (b) their characterization using available equipment and chemicals.

3. (a) Preparation of a liquid crystal using simple soft chemical route in laboratory and (b) their characterization using available equipment and facility.
4. (a) Synthesis of Lanthanide doped nanophosphors using any soft chemical approach and (b) understanding their phosphorescence and other properties.
5. (a) Synthesis of any ionic liquid (for example any imidazolium based ionic liquid) and (b) then confirming its structure by FTIR, ^{1}H NMR studies and other techniques.

Recommended Texts/References:

1. Nanomaterials Chemistry: Recent Developments and New Directions by C. N. R. Rao, A. Muller and A. K. Cheetam, Willey- VCH Gmbh & Co (2007).
2. Gurtu, J.N. Advanced Physical Chemistry Experiments, Pragati Publications, (2008)
3. Khosla, B.D. , Garg, V.C. and Gulati, A. Senior Practical Physical Chemistry by (R. Chand & Co, New Delhi), 18th Edition, 2018
4. Lakowicz, J. R Principles of Fluorescence Spectroscopy, 2nd edition, 1999
5. Banwell, C. N. Fundamentals of Molecular Spectroscopy, 4th Edition, 2017
6. Kemp. W. Organic Spectroscopy, Third Edition, 2002

SKILL ENHANCEMENT COURSE (SEC)

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

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical /Practice		
Concepts and Applications of Artificial Intelligence and Machine Learning in Chemistry **CH-SEC-210**	**02**	**01**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives:

- To understand core concepts and types of AI/ML
- To learn the mathematical foundations of ML
- To explore AI/ML applications in chemistry (e.g., drug discovery, materials design)
- To apply AI/ML to molecular modelling, quantum chemistry, and catalysis
- To gain practical experience with AI/ML tools for chemical problem-solving

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

- Grasp key AI/ML concepts, including data handling, training, and evaluation
- Build and evaluate models (e.g., regression, classification, neural networks) for chemical problems
- Apply AI/ML to property prediction, reaction pathways, and spectroscopy
- Enhance quantum chemistry workflows using AI/ML techniques

Theory Component **Credit: 1 (15 h)**

Unit I: **15 hours**

A. Introduction to AI/ML in Chemistry: Description and overview of Artificial Intelligence (AI) and Machine Learning (ML). Data pre-processing, model selection, training, and evaluation. Types of learning: Supervised and unsupervised learning, Chemistry-specific challenges in applying AI/ML.

Regression and classification models (Linear Regression, SVMs, Decision Trees), Kernel Ridge regression, Neural networks and deep learning. Importance of classical numerical methods in AI/ML Models

B. Qualitative/brief ideas on AI/ML applications across domains of

- Healthcare: AI-assisted diagnosis, treatment planning, and medical image analysis
- Finance: Detection of fraud, algorithmic trading, and risk evaluation
- Transportation: Self-driving vehicles and traffic flow optimization
- Education & Communication: AI-powered chatbots, adaptive learning
- Scientific and Industrial Research: Molecular & Pharmaceutical Chemistry: Drug discovery, reaction pathway modeling, molecular docking, and binding affinity prediction, Spectroscopy & Quantum Chemistry: AI-driven prediction of IR, NMR, Raman spectra; enhancing quantum chemical computations. Emerging trends and future directions in AI.

References:

1) Machine Learning in Chemistry: The Impact of Artificial Intelligence, Hugh M Cartwright (Ed), Royal Society of Chemistry; 1st edition (2020)
2) Machine Learning in Chemistry" by Jon Paul Janet, Heather J. Kulik, American Chemical Society (2020)
3) Applications of Artificial Intelligence in Chemistry, Hugh M. Cartwright, Oxford Chemistry Primers (1994)
4) Quantum Chemistry in the Age of Machine Learning, Pavlo O. Dral, Elsevier - Health Sciences Division (2022)
5) A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
6) Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
7) Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis, *J. Med. Chem.* 2020, 63, 8667−8682

8) Artificial Chemical Intelligence: AI for Chemistry and Chemistry for AI by Prof. Pratyush Tiwary, Link: https://www.youtube.com/watch?v=B3wn3C2ANUw

Lab Components **Credit: 1**

1) Fit a polynomial curve using Excel or spreadsheets (linear, quadratic, cubic, quartic, etc) to find a trendline.
2) Examine interpolation to find the missing data.
3) Examine extrapolation to predict future values or trends.
4) Write a program for data interpolation: from classical methods to machine learning regression models.
5) Write a program for data extrapolation: from classical methods to machine learning regression models.
6) Write a program to implement gradient descent from scratch and apply it to linear regression, highlighting the role of numerical optimization in machine learning model training.
7) Write a program to solve systems of linear equations in ML models.
8) Write a program that demonstrates how numerical methods for solving differential equations can be integrated into ML models
9) Running a simple neural network model in machine learning.
10) Use neural networks for Potential Energy Surface (PES) fitting.
11) Train regression models to predict spectra from structural data.
12) Exploring tools like Jupyter notebooks/Google Colab and libraries like Numpy, scikit-learn, PyTorch etc. for chemistry research, education, and data analysis.

Recommended Texts/References:

1. A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
2. The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
3. Combining Machine Learning and Computational Chemistry for Predictive Insights into Chemical Systems, *Chem. Rev.* 2021, 121, 9816−9872
4. a) https://jupyter.org/ b) https://www.python.org/ c) https://numpy.org/ d) https://scikit-learn.org/stable/ e) https://pytorch.org/

GENERIC ELECTIVE COURSES

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GENRIC ELECTIVE (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		
Introductory Chemistry of The Earth's Atmosphere **CH-GE-211**	**04**	**03**	—	**01**	U.G. Chemistry	--

Course objectives

Atmospheric chemistry encompasses the branch of chemistry which deals with the chemical composition and the reactions happening within the earth's atmosphere. Owing to the current scenario where pollution outstands as a major threat to environment and mankind. For example, the depletion of ozone layer and extending insights into ozone recovery, visibility degradation, acid rain phenomena, smog events, and climate change issues, and other hazards of the chemical reactions taking place in the atmosphere all through advancing scientific knowledge of atmospheric reactivity. This paper will give students the understanding the basic chemistry happening within the earth's atmosphere.

Learning outcomes

On successful completion of the paper the student will have a firm understanding about the chemical composition and its reactivity within the earth's atmosphere. One will learn the impact of trace chemicals and its reactivity, how analytical instrumentation can be used to measure chemical composition of trace chemicals in the earth's atmosphere. Students will also learn the global crisis due to ozone depletion, acid rain, climate change.

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

Unit-1: INTRODUCTION TO THE EARTH'S ATMOSPHERE **(15 Hours)**

(i) Composition & Evolution of the Earth's atmosphere – History of earth's atmosphere in early times - Layers of atmosphere – Proportion of gases in the atmosphere - Pressure and Temperature variations. Types of atmospheric reactions – Photolysis – Bimolecular

(ii) Atmospheric Photochemistry & BioGeoChemical Cycle of Mercury

Photochemistry – Absorption of radiation by atmospheric gases – Absorption by O_2 and O_3 – Photolysis rate as a function of altitude – Photodissociation of O_3, NO_2. GeoChemical cycle of mercury – Mercury oxidation by bromine – mercury deposition in the ocean

(iii) Aerosols and Other Physical Processes:

Aerosols – formation – Size distribution – Chemical composition – Oxidation of SO_2 to sulfate – Sea salt aerosal – aerosol nitrate - thermodynamics of aerosols; Nucleation – Classical theory of homogeneous nucleation – Experimental measurement of nucleation rates – heterogeneous nucleation - Wet and dry deposition. Glyoxal as a source of organic aerosol.

Unit-2: ROLE OF CHEMICAL COMPOUNDS ON OZONE BUDGET (15 Hours)

Chemical composition of the Earth's atmosphere – Compounds containing Sulfur, Nitrogen, Carbon, Halogens – Green House gases – Global climate change and carbon foot print – Major Atmospheric pollutants and its sources - Atmospheric Ozone – Ozone production effciency – Isoprene effect - Ozone loss – role of the chemical compounds – Atmospheric lifetimes – Theories – Determination of the lifetimes – Laser Induced Fluorescence Studies (LIF measurements) – Cavity Ring Down method; Radicals in the Earth's atmosphere – Ozone generation – Global warming – Global Warming Potential (GWP) – Ozone Depletion Potential (ODP)

Unit-3: CHEMISTRY OF TROPOSPHERE AND STRATOSPHERE (15 Hours)

(i) Troposphere – Chemistry of hydroxyl radicals – Photochemical cycles of NO_2, NO and O_3 – Chemistry of NO_x and Methane – Mapping and partitioning NO_x Tropospheric reservoir molecules – H_2O_2, CH_3OOH, HONO, PAN, Role of VOC and NO_x in the ozone formation – Chemistry of VOCs – sulfur compounds – nitrogen compounds;

(ii) Stratosphere – Chapman mechanism – HO_x cycle – HO_x catalysed ozone loss - NO_x catalysed ozone loss - Halogen cycles – Antarctic ozone hole – Polar stratospheric clouds – Heterogeneous stratospheric chemistry – Global sulfur and carbon cycles – Role of H_2O in both troposphere and the stratosphere – Biomass Burning - Acid rain.

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

EXPERIMENTS:

1. Synthesis & Instrumentation: Synthesis of aerosol nanoparticles, AAS and AES Instrumental technique. Qualitative & Quantitative analysis experiments to confirm the presence of Mercury, Cadmium and other inorganic pollutants.
2. Physical characterization methods using FT-IR, UV-Visible experiments
3. Separation Techniques: Fundamentals of GC and hyphenated techniques GC-MS Ex. Identification of key oxidants and breakdown products of Volatile hydrocarbons.
4. Experiments related to DSC and Thermal analysis. Eg. Experiment related to emulsification of dicarboxylic acid.
5. Any other relevant experiment from time to time during the semester.

References (Theory):

2. Atmospheric chemistry and Physics by John H. Seinfeld, Spyros N. Pandis; Second edition, John Wiley, 1997.
3. Introduction to Atmospheric Chemistry by Daniel J. Jacob, Princeton University Press, 1999.
4. Introduction to Atmospheric Chemistry by Peter V. Hobbs, Cambridge University Press, 1st edition, 2000.
5. Chemistry of Atmospheres: An Introduction to the Chemistry of the Atmospheres of Earth, the Planets, and Their Satellites by Richard P. Wayne, Cambridge University Press, 3rd edition, 1991.
6. Atmospheric Chemistry by IstvánLagzi, RóbertMészáros, GyörgyiGelybó, and ÁdámLeelőssy Copyright © 2013 EötvösLoránd University.

References (Practical):

1. Vogel's Qualitative Inorganic Analysis – Arthur. I. Vogel , Imperial College, Longmans, Green And Co, London, New York, Toronto, 1937 or 7th Edition – G. Svehla and B. Ravisankar, Pearson Education 2008.
2. Textbook of quantitative chemical analysis – Arthur. I. Vogel, Longman Publisher, 5th edition 1989.
3. Quantitative Chemical Analysis 7th Edition Daniell C. Harris, Freeman & Company, New York 2007.

4. Principles of Instrumental Analysis – Douglas A. Skoog, F. James Holler & Stanley R. Crouch 7th Edition, Cengage Learning, Australia, 2018

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

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GENERIC ELECTIVE COURSE (CH-GE-212)

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		
Medicines and Therapeutics in Daily Life **CH-GE-212**	**4**	**3**	**0**	**1**	B.Sc. (any stream)	NIL

Course Objectives: The course is designed to study the basic details about various therapeutics of general uses, which are crucial for various diseases. This course also gives the knowledge of active pharmaceutical ingredients in some medicines, their synthesis; therapeutic effects and side effects on human physiology. Therapeutics are essential for a healthy day-to-day life and therefore this course will aware the students about its positive and negative effects.

Learning Outcomes:

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

- Understand the role of different therapeutics on human physiology.
- Gain the knowledge of active pharmaceutical ingredient and their roles in different diseases.
- Learn the proper use of different therapeutics and their effect and side effects.
- Learn the techniques of administering blood group, pulse rate, blood pressure and may other general diagnostic applications.

SYLLABUS OF CH-GE-212

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

UNIT 1: **(15 Hours)**

DIFFERENT CLASSES OF MEDICINES

Introduction- Health, disease, drugs, chemotherapy, classification of drugs and their origin. Structure of active ingredients, uses, dosage, side effects and their natural remedies: *Analgesics and antipyretics*- Aspirin, paracetamol, ibuprofen, morphine, codeine *Antibiotics*- Amoxicillin, norfloxacin, ciprofloxacin; *Antihistamines* or *antiallergics*- Cetrizine and Levocetrizine (role of stereoisomers); *Antiparasitic*- Albendazole; Antidiabetics- Insulin, Glipizide and metformin; *Antihypertensive*–Amlodipine and its natural remedies- Rauwolfia; Diuretic- Lasix; *Antidepressant*- Zoloft and its natural treatment; *Antifungal* – fluconazole, Ketoconazole, Itraconazole; Antacids- Ideal properties of antacids, combinations of antacids, Sodium bicarbonate, ranitidine, milk of magnesia, aluminium hydroxide gel; *Anticoagulants/antiplatelet drugs*- Warfarin, heparin and Ecosprin; *Anaesthetics*- Atracurium, Desflurane. Synthesis of small-molecule drugs like aspirin and paracetamol.

UNIT 2: **(15 Hours)**

VACCINES AND SEDATIVE/ HYPNOTIC DRUGS

Introduction to Vaccines and Their Significance in Immunisation Against Life- threatening diseases. Classification of Vaccines with examples - live attenuated, inactivated, subunit, toxoid, mRNA, and viral vector vaccine.

Sedative and hypnotic drugs and their classification. Structure of active ingredients, uses, dosage, side effects and their natural remedies- Benzodiazepines (e.g. diazepam, alprazolam), Barbiturates (e.g. phenobarbital, secobarbital), Z-drugs (e.g. zolpidem, zaleplon), *Antidepressant*- Zoloft and its natural treatment.

UNIT 3: **(15 Hours)**

MEDICINAL PLANTS

Introduction to medicinal plants, Primary vs. secondary metabolites, Major classes of bioactive compounds: alkaloids, glycosides, flavonoids, terpenoids, tannins, saponins. Active principles, and therapeutic uses of important medicinal plants- *Azadirachta indica* (Neem), *Withania somnifera* (Ashwagandha), *Ocimum sanctum* (Tulsi), *Phyllanthus amarus, Aloe vera, Tinospora cordifolia* (Giloy), *Curcuma longa* (Turmeric), Ginkgo biloba, Tea tree oil. Role of medicinal plants in drug discovery, Examples of plant-derived modern drugs (e.g., morphine, quinine, artemisinin).

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

1. Determination of heart rate and pulse rate, blood pressure and discussion on medicines affecting them.

2. Synthesis of Benzimidazole, precursor for various pharmaceutical agents.
3. Synthesis of Benzocaine, a topical pain reliever.
4. Isolation of paracetamol (API) from a commercial tablet
5. Isolation of aspirin (API) from tablet and recording of melting point (synthesis needs discussion)
6. Estimation of Vitamin C.
7. To perform the ibuprofen/aspirin assay as per I.P. and determine its percentage purity.
8. Extraction of phytochemicals (demonstration of alkaloid or flavonoid extraction).
9. To isolate caffeine from tea leaves using solvent extraction techniques.
10. Visits to herbal gardens, research institutes, or pharmaceutical industries.

ESSENTIAL/RECOMMENDED READINGS

Theory:

1. Patrick, G. L. (2001). Introduction to Medicinal Chemistry, Oxford University Press.
2. Lemke, T. L. & William, D. A. (2002), Foye's Principles of Medicinal Chemistry, 5th Ed., USA.
3. Singh H.; Kapoor V.K. (1996), Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan.
4. Chatwal, G.R. (2010), Pharmaceutical chemistry, inorganic (vol. 1), Himalayan publishing house.
5. Prasad, A. K. (2022) Vaccine Development: From Concept to Clinic, RSC.
6. Beale, Jr., J. M.; Block, J. H. (2023) "Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry", Lippincott Williams & Wilkins.
7. Pengelly, A. (2021) "The Constituents of Medicinal Plants", CAB International.
8. Swamy, M. K.; Patra, J. K.; Rudramurthy, G. R. (2019), Medicinal Plants Chemistry, Pharmacology, and Therapeutic Applications, CRC Press.

Practical:

1. Jeffery, G.H., Bassett, J., Mendham, J., Denney, R.C. (1989), Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons.
2. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
3. Munwar, S., Ammaji, S. (2019), Comprehensive Practical Manual of Pharmaceutical Chemistry, Educreation Publishing.
4. Mondal, P., Mondal, S. (2019), Handbook of Practical Pharmaceutical Organic, Inorganic and Medicinal chemistry, Educreation Publishing.

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

GENRIC ELECTIVE (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		
Modern Materials of Chemistry and Physics, **CH-GE-213**	**04**	**03**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives

- To introduce basic concepts of nanoparticles including quantum confinement effect.
- To provide understanding different facets of liquid crystals.
- To introduce superconductivity and different types of superconductive materials.
- To explore different kinds of optical materials including nonlinearity.
- To explain multiphase materials specially ferrous and non-ferrous alloys

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

- Understand the concept of nanoscience and technology including synthesis using top-down and bottom-up approaches, exciton Bohr radius, quantum confinement etc.
- Understand details and different types of liquid crystals and their transitions etc.
- Understand superconductivity, BCS theory and principles of High Tc superconductors
- Describe the basic principles of optical materials in all three categories i.e, semiconducting, lanthanide doped and organic emitting materials.
- Understand Fe-C phase transformations in ferrous alloys and some other aspect of non-ferrous alloys.

Course Contents (Theory) **Credit: 3 (45 hours)**

Unit I: Nanoparticles and its Chemistry **15 hours**

A. Nanoparticles: Top down and bottom-up approach to prepare different kinds of nanomaterials, Quantum dots, mechanism on the basis of band gap, excitons, quantum confinement effect, Bohr's radius in quantum dots, Different applications

B. Liquid Crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic–nematic transition and clearing temperature-homeotrophic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases

Unit II: Superconductivity and Multiphase Materials **15 hours**

A. 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

B. 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 III: Optical materials: 15 hours

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

Recommended Texts:

1. Nanomaterials Chemistry: Recent Developments and New Directions by C. N. R. Rao, A. Muller and A. K. Cheetam, Willey- VCH Gmbh & Co (2007).
2. Cao, G. Nanostructures and Nanomaterials: Synthesis, Properties and applications, Imperial College Press, London (2011).
3. Callister, W. D. Materials Science and Engineering, an Introduction, Willey, 10th Edition, 2018.
4. Thermotropic Liquid Crystals, Ed., G. W. Gray, John Willey (1987).
5. Ashcroft, N. W. and. Mermin, N. D. Solid State Physics, Saunders College Publishing, (1976)
6. Keer, H. V. Principles of the Solid State, Willey Eastern (1993).
7. Billmeyer Jr, F. W. Textbook of Polymer Sciences, Wiley, 3rd Edition
8. Cowie, J. M. G. Physics and Chemistry of Polymers, Blackie Academic and Professional, 3rd Edition (2007).

Practical Components: Credit 1

1. Preparation of semiconducting CdSe, ZnSe, In_2S_3 (any of one) nanomaterials by any soft chemical approach (emulsion based, co-precipitation etc.).
2. Preparation of any metallic nanoparticle (for example Ag, Cu, Ni-any of one) using standard reducing and capping agent.
3. Preparation of a liquid crystals using soft chemical route.
4. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
5. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).
6. Measurement of photoluminescence properties of semiconducting nanomaterials (at least one) using fluorescence spectroscopy.
7. Measurement of photoluminescence properties of lanthanide doped nanomaterials using fluorescence spectroscopy.

8. 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.

Recommended Texts/References:

1. Nanomaterials Chemistry: Recent Developments and New Directions by C. N. R. Rao, A. Muller and A. K. Cheetam, Willey- VCH Gmbh & Co (2007).
2. Gurtu, J.N. Advanced Physical Chemistry Experiments, Pragati Publications, (2008)
3. Khosla, B.D. , Garg, V.C. and Gulati, A. Senior Practical Physical Chemistry by (R. Chand & Co, New Delhi), 18th Edition, 2018
4. Lakowicz, J. R Principles of Fluorescence Spectroscopy, 2nd edition, (1999)
5. Banwell, C. N. Fundamentals of Molecular Spectroscopy, 4th Edition, (2017)
6. Kemp. W. Organic Spectroscopy, Third Edition, (2002)