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, 5^{th} 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

<u>Course Objective:</u>

- 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.

<u>Learning Outcomes:</u> 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.

Recommended Texts/References:

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).

Practical Components: **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.

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).

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

<u>Course Objectives:</u>

- 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.

<u>Learning outcomes</u>: 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)