DISCIPLINE SPECIFIC CORE COURSES

Semester – VII

DSC-I

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical / Practice		
Advanced Inorganic & Organic Spectroscopy, Quantum Chemistry and Molecular Symmetry (DSC-I)	**04**	**03**	—	**01**	Class 12th With Physics, Chemistry, Mathematics	--

Inorganic Chemistry

Learning Objectives

The course is designed to provide the fundamental understanding of the principle of operation and interpretation of spectra of inorganic compounds for their structural characterization relevant to real world application.

Learning Outcomes

The students will learn to:

1. To analyze and interpret experimental data collected of inorganic materials using different spectroscopic techniques
2. To be able to learn and analyze the theory and principle of mass spectroscopy, various ionization techniques involved and different types of detectors used and to implement the theory to interpret the mass spectra.

SYLLABUSOFDSC-1

Unit-1. Spectroscopy for Inorganic Materials

ATR-IR, and Solid state or multinuclear NMR Spectroscopy of inorganic materials: Basics and applications of IR spectra in inorganic materials, total internal reflectance of inorganic materials, diffuse reflectance spectroscopy (DRS), Kubelka-Munk equation. ^{1}H, ^{13}C NMR spectra of metal complexes, dipolar and contact shifts. Basics of Magic angle spinning NMR spectroscopy (MAS NMR).Example of solid-state NMR with ^{10}B, ^{11}B, ^{17}O, ^{19}F, ^{27}Al, ^{29}Si, ^{31}Pnuclei.(10 Lectures)

Unit–2:Basics of Mass Spectrometry

Mass spectrometry: Experimental arrangements, Ion sources, Mass analysers and detectors, Data analysis, Molecular ions, Fragmentation, Ion reactions, combined mass spectrometry methods, Tandem mass spectrometry (MS/MS), Chromatography-coupled mass spectrometry.(05 Lectures)

Practical:

1. Synthesis of substituted ferrocene and its mass-spectrometry analysis.
2. Synthesis of substituted Metal acetylacetonateand its mass-spectrometry analysis.
3. ATR-IR, NMR analysis of metal complexes acetylacetonate complexes of Iron, Manganese and Copper.

Recommended Texts:

1. Banwell, C.N.; McCash, E.M. (2006), Fundamentals of Molecular Spectroscopy, Tata McGraw- Hill.
2. Springsteen, A. (1998), Reflectance Spectroscopy: an overview of classification and techniques. In Applied Spectroscopy; Workman, J., Springsteen, A., Eds.; Academic Press 193–224. DOI: 10.1016/B978-012764070-9/50008-1.
3. Fitzgerald, J.J. and DePaul, S. M. (1999), Solid-State NMR Spectroscopy of Inorganic Materials: An Overview, 2-133, DOI: 10.1021/bk-1999-0717.ch001.
4. Brevard, C. and Granger, P. Handbook of high resolution multinuclear NMR, A Wiley publisher, 1981 and Brevard, C. The multinuclear approach to NMR spectroscopy, Springer Netherlands, 1983.
5. Nielsen, NielsChr, Strassø, Lasse A, and Nielsen, Anders B. Solid state NMR, Springer-Verlag Berlin Heidelberg, 2012.
6. D. W. Rankin, N. Mitzel, and C. Morrison, Structural methods in molecular inorganic chemistry. John Wiley & Sons, 2013.
7. E. A. V. Ebsworth, D. W. Rankin, and S. Cradock, Structural methods in inorganic chemistry. Blackwell Scientific Publications, Oxford, 1987.
8. William Henderson and J. Scott McIndoe, Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools – Techniques – Tips, John Wiley and Sons, Ltd, 2005, ISBN 0-470-85015-9
9. J.M. Modern spectroscopy, Hollas, 4th edition John Wiley and sons Ltd., 2004.

Organic Chemistry

Objectives: Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.

Course Outcomes: The students will acquire knowledge of solving structural problems based on UV-VIS, IR, ^{1}HNMR, ^{13}CNMR, and Mass spectral data.

Course/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.

Theory Course Content: ***Credit 1 (15Lectures)***

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and ^{1}HNMR)**(2 Lectures)**

13-CNMR and 2D NMR Spectroscopy: Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling, noise decoupling, broadband decoupling; Deuterium, fluorine, and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and general introduction about 2D NMR.(**5 Lectures)**

MASS: Theory, Fourier transform mass spectrometry instrumentation (FTMS); Unit mass and molecular ions; Important terms singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity; Recognition of M^{+} ion peak; Nitrogen rule; Rule of 13; Ionization methods (EI and ESI). General fragmentation rules: McLafferty rearrangement, ortho effect. **(4 Lectures)**

ESR: Basic Principles and applications for organic Compounds **(2 Lectures)**

Structure elucidation of organic compounds using UV, IR, NMR, and Mass Spectra.
(2 Lectures)

Recommended Reference and Textbooks:

1. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (**1991**).
2. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds. John Wiley & Sons (**1981**).
3. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy. Cengage Learning (**2014**).
4. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., **2007**

PRACTICALS

Course Outcome: The students will acquire knowledge of:

1. Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. Synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.

List of Practical's	***Credit 1/3***

(Spectra to be provided wherever required)

1. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
2. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/*p*-nitrobenzaldehyde) and active methylene compounds (malononitrile/ethylcyanoacetate/diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
3. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.
4. Determination of the effect of pH on absorbance maximum (UV-Vis spectra) of the organic compounds. (Aniline, Benzoic acid, phenol etc.)
5. Demonstration of the separation of the mixture of *p*-nitrophenol and *o*-nitrophenol by columnchromatography and their characterization bymelting point and spectroscopic techniques.

Recommended Reference and Textbooks:

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. Morrill, L. A., Kammeyer, J. K., & Garg, N. K. (**2017**). Spectroscopy 101: A practical introduction to spectroscopy and analysis for undergraduate organic chemistry laboratories.*J. Chem. Educ.*94(10), 1584-1586.

Physical Chemistry

Course Objectives:

- To introduce fundamental concepts of quantum mechanics, including vector spaces, operator algebra, angular momentum, spin, and the application of these concepts to atomic and molecular systems.
- To develop a quantitative understanding of Dirac notation, commutation relations, the Heisenberg Uncertainty Principle, and spin eigenfunctions.
- To provide a foundational understanding of molecular symmetry through symmetry elements, point groups, and character tables.
- To apply group theory to interpret spectroscopic data, derive selection rules, and understand molecular vibrations in infrared and Raman spectroscopy.

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

- Understand the basic concepts and quantitative aspects of chemical phenomena, which require knowledge of both quantum chemistry and mathematics.
- Apply relevant mathematical methods essential for solving problems in quantum chemistry.
- Interpret symmetry elements and operations in molecules using the principles of group theory.
- Predict spectroscopic transitions using symmetry considerations and selection rules.
- Demonstrate an integrated understanding of how quantum chemistry and group theory together contribute to the interpretation of molecular spectroscopy.

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

Unit I: Quantum Chemistry (7 lectures)

Introduction to vector spaces (Particle in 1-D box), Dirac's Bra-ket notation, Turn-over rule, Commutation of operators Heisenberg's Uncertainty principle (derivation and physical significance), Angular momentum: definitions, creation and annihilation operators; spherical harmonics, Spin operators and eigenfunctions; two-electron systems (qualitative).

Unit II: Molecular Symmetry (8 lectures)

Symmetry elements and operations; Point groups (BF_3, NH_3, H_2O), Classes,reducible and irreducible representations, Similarity transformation, Character table&Great Orthogonality Theorem (without proof)), Transition moment integrals, Selection Rules, IR and Raman activity: Group theoretical approach, examples predicting vibrational activity using character tables.

Recommended Texts/References:

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. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. &Friedman, R.S.,Molecular Quantum Mechanics 3rd Ed., Oxford University Press (2004).

6. Kakkar R., *Atomic and Molecular Spectroscopy*, Cambridge University Press, (2015).
7. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
8. Bakhshi, A. K., and Thakral P., Quantum Chemistry Simplified, Vidyavani Foundation, New Delhi, ISBN: 9788196225107 (2023).
9. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
10. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973)

Supplementary readings

11. Quantum Chemistry and Group Theory, MCH-018, IGNOU Self Learning Material, egyankosh, Indira Gandhi National Open University (2025) https://egyankosh.ac.in/handle/123456789/107771
12. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)
13. Rakshit, S. C.; Atomic & Molecular Symmetry Groups and Chemistry, CRC Press, Taylor and Francis Group.

Laboratory Exercises (Practical) (atleast four): **Credit 1/3**

1. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the Initial Rate Method.
2. Titrate a moderately strong acid (Salicylic/Mandelic acid) by the (a) salt-line method (b) double alkali method.
3. Titrate a tribasic acid (phosphoric acid) against NaOH potentiometrically.
4. Plotting of atomic orbitals (Spherical Harmonics S(θ) versus θ using polar graph paper. Student will be provided with the *p*-, *d*- and *f*- functions.
5. Plotting of $\psi_n(x)$, and $|\psi_n(x)|^2$ for wavefunctions of 1D harmonic oscillator in different energy levels within the domain of x, $-\infty < x < +\infty$.
6. Calculate the bond length of conjugated dye molecules (i.e., cyanine/β-carotene) using particle in 1D box model.
7. Simulated IR Spectra: assign bands using symmetry and selection rules.

Recommended Texts/References:

1. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
2. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
3. Kapoor, K.L., A Textbook of Physical Chemistry, Vol. IV, fifth Edition, McGraw Hill Education.
4. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).

Semester – VIII

DSC-II

Course title &Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisiteof the course (if any)
		Lecture	Tutorial	Practical / Practice		
Advanced Bioinorganic Chemistry, Application of Reagents in Organic Synthesis, Statistical Thermodynamics and Applications	**04**	**03**	—	**01**	Class 12th With Physics, Chemistry, Mathematics	--

Inorganic Chemistry

Unit I: Metals in Biological System

Biominerals and biomineralization, Detailed study of biocatalyst in the metabolism of Hydrogen, carbon, and sulfur, Biological actions of manganese, cobalt and nickel ions, Metal ions in brain and medicine, Homeostasis of Metals, Potassium-Dependent Molecules, Inorganic Nanoparticles in Wound Healing and Drug Delivery (5 Lectures)

Unit II: Inorganic Materials for Biomedical Applications

Natural Bone Structure and Composition, Calcium Phosphate Ceramics (e.g., hydroxyapatite, tricalcium phosphate), Metal Implants (e.g., titanium, stainless steel), Natural Tooth Structure and Composition (enamel, dentin), Dental Ceramics (e.g., zirconia, alumina), 3D Bioprinting.
(10 Lectures)

Course Objective:

This course delves into the fascinating intersection of bio-inorganic metals and their crucial roles in living systems. The detailed investigation of bio-inorganic chemistry of essential elements towards biomedical applications.

Course Outcome:

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

Understand the advance application of bio-inorganic metals.
Explore the structure and properties of inorganic materials used in biomedical applications.
Investigate the biocompatibility and bioactivity of inorganic biomaterials.
Discuss current research and future directions of bio-inorganic chemistry.

Practical Components:

1. Synthesis and characterization of calcium phosphate ceramics spectrophotometrically /any other method.
2. Analyzing the composition of Bio materials(Stainless steel, hydroxyapatite)
3. Fabrication of a simple Bio-hydrogel (Polyvinyl alcoholhydrogel, polysaccharide hydrogel, cellulose,starch)
4. Preparation of Zirconia(ZrO_2).
5. Preparation and characterisation of transition metal complexes of riboflavin using commercially available Vitamin B2 supplements

References:

1. Bio-coordination Chemistry, D E Fenton, OUP, 2002
2. Principles of Bioinorganic Chemistry, S J Lippard and, J M Berg, USB, California, 1994
3. Biological Inorganic Chemistry, R.R Crichton, Elsevier, 2012
4. Y. Bar-Cohen, Biomimetics: Biologically Inspired Technologies, Taylor & Francis CRC Press, Boca Raton, FL, 2006.
5. R.L. Reis, S. Weiner, Learning from Nature How to Design New Implantable Biomaterials, Kluwer Academic Publishers, New York, 2005.
6. P. Behrens, E. Bäuerlein, Handbook of Biomineralization: Biomimetic and Bioinspired Chemistry, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
7. H. Lowenstam, S. Weiner, On Biomineralization, Oxford University Press, New York, 1989.
8. S. Mann, Biomineralization: Principles and Concepts in Bioinorganic Materials Chemistry, Oxford University Press, Oxford, New York, 2001.
9. E. Bäuerlein, Biomineralization: Progress in Biology, Molecular Biology and Application, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
10. E. Bäuerlein, Handbook of Biomineralization: Biological Aspects and Structure Formation, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
    F.E. Round, R.M. Crawford, D.G. Mann, The Diatoms: Biology and Morphology of the Genera, Cambridge University Press, Cambridge, 1990.

Organic Chemistry

Objectives:Tofacilitate chemical transformations by providing the necessary conditions and catalysis.

Course Outcome:At the completion of this course, the students should be able to:

i) Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.

ii) Understand the conversion of specific functional groups without affecting othersand maximize yields and selectivity for the desired products.

Theory Course Content ***1 Credit (15 lectures)***

i. Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents. **(3 Lectures)**

ii. ***Reagents in Organic Synthesis***: Triacetoxyborohydride, Lead Acetate, Phenyliodine (III) diacetate (PIDA), DCC, Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification &Swern Oxidation); Oxidation of organic compounds using thallium nitrate, selenium dioxide, phase transfer catalyst, crown ethers, $KMnO_4$, PCC, OsO_4, CrO_3, $K_2Cr_2O_7$. **(10 Lectures)**

ii. Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN. **(2 Lectures)**

Recommended Reference and Textbooks:

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. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (**2000**)

PRACTICALS

Course Outcome: The students will acquire knowledge of:

1. Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. Characterization by physical and spectroscopic techniques.

List of Practical's ***Credit: 1/3***

Identification of the product based on Melting point and spectroscopic techniques (IR, ^{1}HNMR, and ^{13}C NMR spectroscopy, data to be provided).

1. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
2. Reduction of *p*-nitrobenzaldehyde using suitable reagents. ($NaBH_4$/Sn-HCl)
3. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
4. Oxidation of Aryl Aldehydes into Ester by I_2 and Alcohols.

Recommended Reference and Textbooks:

1. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.

2. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
3. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
4. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

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Physical Chemistry

Course Objectives:

- To provide a brief foundational understanding of the core principles of classical and quantum statistical mechanics.
- To explore the connection between macroscopic thermodynamics and microscopic quantum mechanics using various statistical ensembles.
- To introduce the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics with a brief, qualitative understanding and focus on their applications.
- To enable students to apply statistical concepts in key areas such as the standard model for macromolecular systems, chemical kinetics, and chemical equilibrium.

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

- Understand the fundamental principles of statistical mechanics, including how they link microscopic behaviour to macroscopic properties of systems.
- Apply the Boltzmann distribution, Bose-Einstein statistics, and Fermi-Dirac statistics to various physical and chemical systems.
- Utilize partition functions to analyze and solve problems related to the thermodynamic properties of systems.
- Explore the application of statistical mechanics to key areas such as chemical kinetics, chemical equilibrium, and random walk models in macromolecular systems.

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

Unit I- Statistical Thermodynamics (8 lectures)
Microstates, Configurations, coin tosses, rolling of dices, spin systems (in the absence of magnetic field),Thermodynamic probability, Stirling's approximation, Concepts of ensembles (Microcanonical and Canonical), Characteristic thermodynamic functions, Translational partition function (quantitative), Rotational and vibrational partition functions (qualitative), Maxwell-Boltzmann distribution, Bose-Einstein, and Fermi-Dirac Statistics (Qualitative).

Unit II-Applications (7 lectures)
Conventional transition state theory derived from partition functions, Equilibrium constants in terms of partition function: gas-phase reactions (K_p),isotope effects.
1-D random walk model, Number and weight average molecular weight, polydispersity index.

Recommended Texts/References:

1. McQuarrie, D. A. *Statistical Mechanics,* Viva Books Pvt. Ltd.: New Delhi (2003).
2. L. D. Landau and E. M. Lifshitz, Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed. (2005).
3. Bagchi B. *Statistical Mechanics for Chemistry and Material Science,* CRC Press (2018).
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. Pathria, R.K.; and Beale, P. D.;Statistical Mechanics, Fourth Edition, Elsevier, Academic press.
7. Huang, K., Statistical Mechanics, 2nd Ed., John Wley& Sons, New York (2000)

Laboratory Exercises (Practical) (atleast four): Credit 1/3

1. Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.
2. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
3. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
4. Statistical Treatment of Error Analysis (Null Hypothesis, T-test, F-test, Q-test (criteria for reject of hypothesis) Statistical analysis of laboratory data.
5. Determination of standard deviation, mean and maximum absolute errors, root-mean-square deviation (error) and Correlation coefficient of linear straight-line plot.

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 2 Revised ed edition (1 February 1988).

DISCIPLINE SPECIFIC ELECTIVE COURSES

SEMESTER – VII

INORGANIC CHEMISTRY

DISCIPLINESPECIFICELECTIVECOURSE-1(DSE-1):Inorganic Main Group Clusters-Basics and Applications

CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

Coursetitle & Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite ofthecourse (if any)
		Lecture	Tutorial	Practical/ Practice		
Main Group Clusters-Basics and Applications (DSE-1)	**04**	**02**	**--**	**02**	Class12th with Physics, Chemistry	**--**

Objectives:
To introduce the basic concepts of clusters.To gather a good understanding of the chemistry and various aspects of main group cluster compounds with respect to synthesis, structure and properties.

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

1. Ensures the students understand the concepts and the properties of clusters.
2. Acquire knowledge of cluster compounds and explain structure-property, electron counts, and surface analogies of cluster compounds.
3. Identify the structure and bonding aspects of main group clusters.
4. Identify the different types of main group cluster reactions and apply the above concepts to explain reactivity of the clusters.

SYLLABUSOFDSE-1

Introduction to molecular clusters - Clusters in elemental states, cluster classification, skeletal electron (Elm) counting.
Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the *closo-, nido-, arachno-hypho-, klado-,*borane structural paradigm, Wade-Mingos and Jemmis electron counting rules,Lipscomb topological diagrams, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.Heteroboranes,boron-carbides and metal-borides.Illustrative examples from recent literature.(30 Lectures)

Keywords: Clusters, skeletal electron count, boranes, synthesis, reactivity.

Teaching Learning Process:
Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

Assessment Methods:
● Presentations by Individual Student/ Group of Students
● Class Tests at Periodic Intervals.
● Written assignment(s)
● End semester University Theory Examination

Practical

1. Determination of Boron colorimetrically.
2. Preparation of borax/ boric acid.
3. Synthesis of zinc borate from zinc oxide and boric acid and their analysis using various instrumentation techniques: IR, UV, TGA, and DSC. Thermal decomposition of borax and its structural characteristics using XRD, FTIR.
4. Qualitative analysis of cobalt, nickel, copper etc. using borax (borax bead test).
5. Other new novel synthesis reported in literature from time to time
6. Syntheses and characterisation of zinc(II)acetylacetonate and tin(II)acetylacetonate complexes

Text Books:--

1. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.
2. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth-Heinemann, 1997.
3. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid-state Chemistry, Cambridge University press, 2007.
4. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
5. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press, 1998.
6. C. E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press, 1996.

Reference Books:
1. F. Holleman and E. Wifrg, Inorganic Chemistry, Academic Press, New York, 1995.
2. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.

3. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt Ltd, New Delhi, 2001.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver & Atkins Inorganic Chemistry,
4th Edn, Oxford, 2006.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorgnic Chemistry: Principles of Structures and Reactivity, 4th Edn, Pearson, New Delhi, 2006.
7. R. Xu, W. Pang and Q. Huo (Eds), Modern Inorganic Synthetic Chemistry, Elsevier, New York, 2011.
8. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
9. J. R. Anderson and M. Boudart (Eds), Catalysis: Science and Technology, Springer, London, 2012.
10. P. Powell, Principles of Organometallic Chemistry, 2nd Edn, Chapman and Hall, London, 1988.
11. G. O. Spessard and G. L. Miessler, Organometallic Chemistry, International 2nd Edn, Oxford University Press, Oxford, 2010.
12. D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), The Chemistry of Metal Cluster Complexes, VCH, New York, 1990.
13. K. J. Klabunde, Free Atoms, Clusters and Nanoscale Particles, Academic Press, New York, 1994.
14. D. M. P. Mingos (Ed.), Structural and Electronic Paradigms in Cluster Chemistry, Springer, Berlin, 1997.
15. P. Braunstein, L. A. Oro and P. R. Raithby (Eds), Metal Clusters in Chemistry, Wiley-VCH, Weinheim, 1999.
16. M. Driess and H. Noth (Eds), Molecular Clusters of the Main Group Elements, Wiley-VCH, Weinheim, 2004.
17. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.
18. F. Wells, Structural Inorganic Chemistry, 5th Edn, Oxford University Press, Oxford, 1984.

DISCIPLINESPECIFICELECTIVECOURSE-2(DSE-2):

Advanced Coordination Chemistry

CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

Coursetitle & Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite ofthecourse (if any)
		Lecture	Tutorial	Practical/ Practice		
Advanced Coordination Chemistry (DSE-2)	**04**	**02**	**--**	**02**	Class12th with Physics, Chemistry, Mathematics	**--**

Objectives:

- To introduce the basic concepts of coordination polymers and porous and cavity containing structures.
- To gather a good understanding of the chemistry, principles, design and synthesis of coordination polymers like metal-organic frameworks, coordination clustersalong with exploring their structures, properties and applications.

Learning Outcomes:

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

- Have a strong foundation in understanding the basic concepts and properties of coordination polymers and porous and cavity containing systems.
- Gain an understanding of the different types of structures (single metal-noded, metal cluster-noded, pillared layer nets) of coordination polymers.
- Acquire knowledge on synthesis methods and how reaction conditions in synthesis can be used to design targeted coordination polymers.
- Acquire knowledge on the different types of structures of coordination polymers, e.g. MOFs, coordination clusters, etc and applications in catalysis and hydrogen storage.
- Learn about the design and morphology of self-assembling coordination compounds using suitable examples.

SYLLABUSOFDSE-2

Coordination polymers, assembly, single metal-noded nets, metal cluster-noded nets, pillared layer nets, and structural modulation by reaction conditions, including in situ metal/ligand reactions.

Coordination Polymers: Metal-Organic Frameworks and Other Terminology , 0D Coordination Clusters , 1D, 2D and 3D Structures , Magnetism , Negative Thermal Expansion , Interpenetrated Structures , Porous and Cavity-Containing Structures, Catalysis by MOFs , Hydrogen Storage by MOFs,

Self-Assembling Coordination Compounds: Design and Notation, Supramolecular Cube, Molecular Squares and Boxes, Self-Assembly of Metal Arrays (30 Lectures)

Keywords:
Coordination polymers, metal-organic frameworks, self-assembly, catalysis, hydrogen storage

Teaching Learning Process:
Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of the teaching learning process.

Assessment Methods:
● Presentations by Individual Student/ Group of Students
● Class Tests at Periodic Intervals.
● Written assignment(s)
● End semester University Theory Examination

Practical:

1. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using prepared zeolite A.
2. Estimation of MnO_2 in pyrolusite.
3. Preparation and characterization of following the following complexes/organometallic compound including their structural elucidation by the available physical methods. (Element analysis, molecular weight determination, conductance and magnetic measurement and special studies):
    - Synthesizing a nickel-citric acid coordination polymer using nickel nitrate, citric acid, and dimethylformamide (DMF) under solvothermal conditions.
    - Synthesizing Cu(II) coordination Polymers with 4,4-bipyridine.
    - Synthesis of *cis* and *trans* isomers of bis(glycinato) copper(II) monohydratye.
    - Synthesis of Cu acetate complex
4. Solid State synthesis-
    - Preparation of oxides and mixed oxides (Mn_2O_3, NiO, Cu_2O, Fe_3O_4, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuMn_2O_4$ and $NiFe_2O_4$).
    - Preparation of Silica and Alumina by sol-Gel technique.
5. To study the electrical conductivity of ferrites, Magnetites, doped oxides and pure samples and determine band gap.

Books for practical:

1. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Experiments, J. DerckWoollins, VCH.
3. Practical Inorganic Chemistry, G. Marrand, B. W. Rockett, Van Nostrand.
4. A Text Book of Quantitative Inorganic Analysis, A. I.Vogel, Longoman.
5. EDTA Titrations. F. Laschka
6. Instrumental Methods of Analysis, Willard, Merit and Dean (CBS, Delhi).
7. Inorganic Synthesis, Jolly
8. Instrumental Methods of Chemical Analysis, YelriLalikov
9. Fundamental of Analytical Chemistry, Skoog D.A. and West D.M Holt Rinehart and Winston Inc.
10. Experimental Inorganic Chemistry, W. G. Palmer, Cambridge.
11. Solid state Chemistry, N. B. Hanney
12. Introduction to Thermal Analysis, Techniques and Applications, M.E.Brown, Springer
13. Preparation and Properties of solid state Materials, Wilcox, Vol.IandII, Dekker
14. The Structure and Properties of Materials Vol.IV, JohnWulff, Wiley Eastern.

References:

1. S.R. Batten, S.M. Neville, D.R. Turner, Coordination Polymers: Design, Analysis and Application, the Royal Society of Chemistry, Cambridge, UK, 2009.
   a. A.F. Wells, Three-Dimensional Nets and Polyhedra, Wiley-Interscience, New York, 1977.
   b. A.F. Wells, Further Studies of Three-dimensional Nets, ACA Monograph No.8, American Crystallographic Association, Knoxville, TN, 1979.
   c. A. F. Wells, Structural Inorganic Chemistry, fifteenth ed., Oxford University Press, Oxford, 1984.
2. J. Weitkamp, L. Puppe, Catalysis and Zeolites: Fundamentals and Applications, Springer, 1999.
3. D.W. Breck, Zeolite Molecular Sieves: Structure, Chemistry, and Use, Wiley, New York, 1973.
4. J.W. Steed, J. L. Atwood, Supramolecular Chemistry Chapters 9 and 10. pp. 561-583 and 620-637, John Wiley & Sons Ltd, Second Edition (2e, 2009) ISBN: 9781119582519
5. R.M. Barrer, Hydrothermal Chemistry of Zeolites, Academic Press, London, 1982.
6. J. Cejka, H. van Bekkum, A. Corma, et al., Introduction to Zeolite Molecular Sieves third ed. (Studies in Surface Science and Catalysis, Vol. 168), Elsevier, 2007.
7. S.M. Auerbach, K.A. Carrado, P.K. Dutta, Handbook of Zeolite Science and Technology, CRC, 2003.
8. C.J. Brinker, G.W. Scherer, Sol-Gel Science, Academic Press, New York, 1990.

9. R. Szostak, Molecular Sieves: Principles of Synthesis and Identification, Blackie Academic & Professional, London, 1998.

ORGANIC CHEMISTRY

DISCIPLINE-SPECIFIC ELECTIVECOURSE-I (DSE-I)

Title: Advanced Stereochemistry (DSE-I, 30 Lectures)

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

Coursetitle &Code	Credits	Credit distribution			Eligibility criteria	Pre-requisite (if any)
		Lecture	Tutorial	Practical/ Practice		
AdvancedStereochemistry (DSE-I, 30 Lectures)	04	02	---	02	Class 12thwith Physics,Chemistry, Mathematics	

Objectives:To provide a comprehensive understanding of molecular symmetry, isomerism, and chirality, including their applications in organic reactions.

Course Outcomes:

1. Students will be expected to gain knowledge of the basic concept of chirality in molecules due to their spatial arrangement of atoms that leads to chiroptical properties.
2. The three-dimensional arrangement of atoms in a molecule can lead to distinct physical and chemical properties, particularly for stereoisomers.Understanding stereochemistry is crucial for designing effective drugs, predicting reaction outcomes, and developing new materials.
3. Stereochemistrysignificantly impacts drug action, biological processes, and chemical reactions, influencing factors like drug efficacy, selectivity, and even the rate of chemical reactions.

Theory Course Content: ***Credit 2 (30Lectures)***

Stereoisomerism: Chiral (stereogenic) centre, principle of axial and planar chirality; Stereochemistry and configurations of biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes, allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes and helicity. **(15 Lectures)**

***Topicity and prostereoisomerism*:**Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.
(5 Lectures)

Asymmetric induction: Cram's, Prelog's, and Felkin-Ahn model. **(3 Lectures)**

***Cyclostereoisomerism*:** Configurations, conformations and stability of cyclohexanes (di-, and tri-substituted), cyclohexenes, cyclohexanones, decalin. **(5 Lectures)**

Applications of ORD and CD to Stereochemical Problems (**2 Lectures**)

Reference and Textbooks:

1. Eliel, E. L. (2000), Stereochemistry of Carbon Compounds, Tata McGraw-Hill.

2. Nasipuri, D.(2018), Stereochemistry of Organic Compounds: Principles and Applications, 4th Edition, New Age International.

PRACTICALS

Course Outcome:

1. Understand the spatial arrangement and naming conventions of**E/Z and cis-trans stereoisomers**
2. Visualise chiral centres and identify enantiomers/diastereomers
3. Understand photo-induced isomerization
4. Resolution of enantiomers by formation of diastereomeric adducts

List of Experiments ***2 Credit***

(Any 10 practicals may be done depending upon the availability of resources.)

1. E/Z and Cis-Trans Isomerism of 2,3-dimethyl-2-butene by ball and stick models
2. Identification of ChiralCentres and Diastereomers by ball and stick models
3. Bromination of cis and trans stilbene
4. Addition of Bromine to trans-Cinnamic Acid
5. Photoinduced isomerization of *cis*-Stilbene to *trans*-Stilbene and *vice versa*
6. Photocatalytic/ thermal isomerization of maleic acid to fumaric acid.[3]
7. Preparation of stilbene dibromide by bromination of *trans*-stilbene.
8. Determination of optical rotation of sucrose, glucose, and fructose using polarimetry and determiningtheir concentration.
9. Two-step synthesis of acetonide from benzil and analysis of its stereochemistry using NMR and IR spectroscopy
10. Determination of specific rotation of(R)-limonene and (S)-limonene using Polarimeter.
11. Preparation of hydroxybenzoin by pinacol coupling reaction: Investigating the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: Affording *meso*- and dl-Hydrobenzoin.[4]
12. Proline-catalyzed aldol reaction of cyclohexanone with nitro-substituted benzaldehydes.[5]

Recommended Reference and Textbooks:

1. Microscale Organic Laboratory (Multistep and Multiscale Syntheses). By Dana W. Mayo, Ronald M. Pike, David C. Forbes.**2011**

2. Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments, Kenneth M. Doxsee, James E. Hutchison. Thomson-Brooks/Cole, **2004**

3. The photochemical isomerization of maleic to fumaric acid: an undergraduate organic chemistry experiment. Albert J. Castro, Suzanne R. Ellenberger, and James P. Sluka. *J. Chem. Edu.***1983**,*60* (6), 521 (DOI: 10.1021/ed060p52)

4. Using ^{1}H NMR Spectroscopy to Investigate the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: An Undergraduate Lab Experiment Involving a Green Carbon–Carbon Bond-Forming Reaction Affording *meso*- and dl-Hydrobenzoins. Shahrokh Saba**;** Isabella Fante; James A. Cordero Jr.*J. Chem. Educ.* 2025, 102, 2, 847–851) doi.org/10.1021/acs.jchemed.4c01379

5. Proline-catalyzed asymmetric reactions. List, Benjamin. *Tetrahedron*. **2002**, 58 (28): 5573–5590. doi:10.1016/S0040-4020(02)00516-1

DISCIPLINE-SPECIFIC ELECTIVE COURSE-II (DSE-II)

Title: Reactive Intermediates of Organic Chemistry (DSE-II, 30 Lectures)

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

Coursetitle &Code	Credits	Credit distribution			Eligibility criteria	Pre-requisite (if any)
		Lecture	Tutorial	Practical/ Practice		
ReactiveIntermediates of Organic Chemistry (DSE-II, 30 Lectures)	04	02	---	02	Class 12thwith Physics,Chemistry, Mathematics	

Objectives:To learn and understand the involvement of intermediates,their role in reaction mechanisms, predict their behavior, and apply this knowledge to organic synthesis. Also, to learn and understand the orbital interactions (Woodward-Hoffmann rules) in concerted reactions.

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

i. Understandthe structure-reactivity pattern of reactive intermediates involved in organic reactions.

iiWrite themechanism of organic reactions involving reactive intermediates and apply these reactions in organic synthesis

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Theory Course Content ***2 credit (30 Lectures)***

Carbocations:Difference between classical and non-classical carbocations.Introduction of neighboring group participation (NGP), ion-pairs, molecular rearrangements in acyclic, monocyclic, and bicyclic systems, stability and reactivity of bridgehead carbocations.

(8 Lectures)

Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications. **(3 Lectures)**

Carbenes: Structure of carbenes, generation of carbenes, addition and insertion reactions,rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylid by carbenoid decomposition. Examples of inter/intramolecular insertions.

(7 Lectures)

Nitrenes:Structure of nitrene, generation and reactions of nitrene and related electron-deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement reactions.

(5 Lectures)

Ylides:Chemistry of Phosphorus and Sulfur ylids – Wittig and related reactions, Peterson olefination. **(2 Lectures)**

Radicals: Generation of radical intermediates and their addition to: i) on alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin's rules.ii) fragmentation and rearrangements. Name reactions involving radical intermediates, such as Barton deoxygenation and decarboxylation, McMurry coupling. **(5 Lectures)**

Recommended Reference and Textbooks:

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. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, **2007**.

PRACTICALS

Course Outcome: The students will acquire knowledge of:

1. Starting materials, functional groups, mechanism, and typical reaction conditions.

2. Characterisation by physical and spectroscopic techniques.

List of Experiments	***2 Credit***

1. Separation, purification, and identification of binary mixtures of organic compounds (neutral and acidic; neutral and basic) using chemical methodsand preparation of a suitable crystalline derivative for both the components. (Examples: (i) Benzoic acid/Any dicarboxylic acid and Naphthalene (ii)*p*-toludine/*p*-anisidine and Naphthalene)

2. **Two-step synthesis**

2.1 ***Synthesis of triacetoxybenzene***

*Step 1:*Synthesis of *p*-benzoquinone from hydroquinone using $KBrO_3$ and

*Step 2:*Synthesis of Triacetoxybenzene from *p*-benzoquinone.

2.2 ***Synthesis of p-acetamido benzene sulphonamide***

*Step 1:*Synthesis of *p*-Acetamido benzene sulfonyl chloride from acetanilide and

Step 2: Synthesis of *p*-Acetamido benzene sulphonamide from *p*-Acetamido benzene sulfonyl chloride.

2.3 ***Synthesis of benzopinacolone***

*Step 1:*Synthesis of benzopinacol from benzophenone

Step 2: Synthesis of benzopinacolone from benzopinacol *via* pinacol-pinacolone rearrangement.

Recommended Reference and Textbooks:

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
6. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

PHYSICAL CHEMISTRY

DISCIPLINE SPECIFIC ELECTIVE COURSE-I (DSE-I):

Title: Advanced Molecular Spectroscopy and Applications (DSE-I, Semester-VII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Advanced Molecular Spectroscopy and Applications (DSE-I, Semester-VII, 30 Lectures)	**04**	**02**	**---**	**02**	**Class 12th with Physics, Chemistry, Mathematics**	**---**

Course Objectives:

- Introduce the principles of molecular spectroscopy across electronic, vibrational, rotational, and nuclear domains.
- Apply quantum mechanical concepts such as the Born–Oppenheimer approximation, Heisenberg's Uncertainty Principle, and time-dependent perturbation theory to spectroscopic transitions.
- Use symmetry and operator-based formalisms to derive selection rules.
- Analyze UV-Vis, fluorescence, Raman, Mössbauer, and CD spectroscopy.
- Explore applications in structure elucidation, dynamics, and single-molecule detection.

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

- Understand the principles of electromagnetic radiation and molecular transitions.
- Interpret selection rules using quantum and symmetry considerations.

- Analyze vibrational fine structure and electronic transitions using the Franck–Condon principle.
- Describe the principles and applications of fluorescence, phosphorescence, and circular dichroism.
- Apply advanced tools such as Mössbauer spectroscopy, and single-molecule spectroscopy.

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

Unit 1: Fundamentals & Quantum Background (6 lectures)

Electromagnetic radiation and spectral regions. Born–Oppenheimer approximation and Uncertainty Principle. Time-dependent perturbation theory (TDPT) and transition moments. Einstein coefficients and derivation of Beer–Lambert law. Selection rules (qualitative) using symmetry and operator formalism.

Unit 2: Electronic Spectroscopy (8 lectures)

Electronic transitions in diatomic molecules (π–π^*, n–π^*, n–σ^*, etc.). Selection rules (qualitative). Breakdown of selection rules. Franck–Condon principle and vibrational fine structure. P, Q, R branches in rovibrational spectra. Dissociation energies (e.g. iodine spectrum).

Polyatomic molecules: Chromophores and auxochromes: structure–property relationships. Solvent effects: polarity, hydrogen bonding and solvent shifts, vibronic coupling, Charge transfer (CT) transitions and their spectral features. Qualitative interpretation of UV-Vis spectra of polyatomic organics (e.g. ethene, formaldehyde, cis- and trans-butadiene) using symmetry principles.

Unit 3: Photophysical Processes in Molecules (6 lectures)

Jablonski diagram, Fluorescence and phosphorescence: mechanisms and applications. Deactivation pathways, internal conversion, intersystem crossing. Mirror-image symmetry and polarization effects in emission spectroscopy.

Unit 4: Mössbauer Spectroscopy (4 lectures)

Mössbauer spectroscopy: Isomer shifts, quadrupole and Zeeman splitting. Applications to oxidation state and bonding.

Unit 5: Advanced Applications (6 lectures)

Fluorescence quenching (static/dynamic) and lifetime measurements. Single molecule spectroscopy and fluorescence correlation spectroscopy (FCS). Circular Dichroism (CD):

principle and biological examples. Mirror-image symmetry and its breakdown. Selection rules and polarization effects.

Forward look: qualitative overview of emerging methods (e.g. AI-assisted spectra interpretation)-non-evaluative.

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

1. J. Michael Hollas, Modern Spectroscopy, 4th Ed.
2. Rita Kakkar, Atomic and Molecular Spectroscopy, Cambridge University Press
3. C. N. Banwell & E. M. McCash, Fundamentals of Molecular Spectroscopy
4. Satyanarayana, D. N., Handbook of Molecular Spectroscopy, I.K. International
5. P. Atkins & R. Friedman, Molecular Quantum Mechanics
6. Jeanne L. McHale, *Molecular Spectroscopy*
7. **J. Chem. Rev. 2021, 121, 9816–9872 –** *ML + Computational Chemistry*

<u>Laboratory Exercises (Practical) (atleast 10)</u>: **Credits: 2**

1. Analyse UV-Vis absorption spectra of conjugated systems (e.g., β-carotene) and determine the HOMO-LUMO gap.
2. Use UV-Vis spectra of a pH-sensitive dye (e.g., phenolphthalein) to determine its pK_a.
3. Study the effect of structure on the UV spectra of organic compounds.
4. Study the spectra of mesityl oxide/benzophenone in different solvents and classify the observed transitions in terms of $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transitions. Discuss the shift in transitions relative to those in acetone.
5. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron (III) by Job's method of continuous variation.
6. (a) Record the UV spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the ground state.

   (b) Record the fluorescence spectra of a weak acid (α-naphthol) at different pH and determine the dissociation constant in the excited state.

   Comment on the difference in the two values using MO theory.

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

7. Record and compare IR spectra of alcohols in pure form and diluted in non-polar solvents to understand the effect of hydrogen bonding on O-H stretching frequency.
8. Create calibration curve and use it to determine the concentration of a fluorophore (quinine, riboflavin) in unknown samples.

9. Study UV-Vis spectra of d^0 transition metal complexes (e.g., Ti^{3+}) and assign electronic transitions using computational or experimental techniques.
10. Measure absorbance vs. time data to study the kinetics of fast photochemical reactions (using Time-Resolved Absorption Spectroscopy for Reaction Kinetics).
11. Resolve and assign vibrational fine structure in the UV-Vis spectrum of iodine vapour.
12. UV spectra comparison of substituted benzenes (π–π* vs n–π*)
13. Fluorescence quenching and lifetime (model system, Rhodamine or naphthol)
14. CD analysis of protein model (experimental or literature spectra)

15. Simulation and analysis of Franck–Condon transitions using potential energy diagrams for diatomic molecules.

16. Interpret Mössbauer isomer shift and quadrupole splitting data from literature spectra of iron complexes.

Recommended Texts/References:

1. Rita Kakkar, Atomic and Molecular Spectroscopy, Cambridge University Press.
2. B. D. Khosla, V. C. Garg, A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi.
3. Donald A. McQuarrie & John D. Simon, Physical Chemistry: A Molecular Approach.
4. J. Michael Hollas, Modern Spectroscopy.
5. Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis.
6. Jeanne L. McHale, Molecular Spectroscopy.

DISCIPLINE SPECIFIC ELECTIVE COURSE-II (DSE-II):

Title: Interfaces, Macromolecules and Biophysical Chemistry (DSE-II, Semester-VII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the Course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Interfaces, Macromolecules and Biophysical Chemistry (DSE-II, Semester-VII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives:

- To understand fundamental surface and interfacial phenomena including adsorption, wetting, and catalysis.
- To introduce classification and characterization of polymers, polymerization mechanisms, and molecular weight determination.
- To apply thermodynamics and kinetics to protein folding, ligand binding, and enzyme catalysis.
- To familiarize students with analytical and optical tools used to study biomolecular structure and interactions.
- To bridge molecular understanding with biological function through biophysical chemistry.

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

- Explain micellization, surface tension, adsorption isotherms, and thin film properties.
- Describe polymer synthesis, types, and methods for determining molecular weights.
- Analyze biological macromolecules using thermodynamic, kinetic, and statistical models.
- Use key spectroscopic and separation techniques to investigate biomolecular properties.
- Connect experimental methods with structural and functional insights in biophysical chemistry.

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

Unit-I: Surface and Interface Chemistry (8 lectures)

Surface-active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature.
Packing parameters, thermodynamics of micellization, solubilization, reverse micelles. Electrokinetic phenomena, Young-Laplace and Kelvin equations.
Adsorption: - Gibbs adsorption isotherm, Langmuir and BET isotherms, surface area measurements.
Thin films and Langmuir-Blodgett films.
Catalytic activity at surfaces (overview).

Unit II: Polymer Structure and Characterization (8 lectures)

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

Unit III: Biophysical Chemistry of Macromolecules (8 lectures)

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

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

Unit IV: Spectroscopic and Analytical techniques(3 lectures)

Basic principles and applications of analytical and optical techniques in biological systems: Absorption and fluorescence spectroscopy (overview only), Isothermal Titration Calorimetry

(ITC), Linear and Circular Dichroism (CD), Single and multidimensional NMR spectroscopy. Single molecule spectroscopy.

Unit V: Separation techniques (3 lectures)

Methods for the separation of biomolecules: General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

Recommended Texts/References:

1. Adamson, A. W. & Gast, A. P., Physical Chemistry of Surfaces, 6th Ed., Wiley
2. Somorjai, G. A. & Li, Y., Surface Chemistry and Catalysis
3. Israelachvili, J. N., Intermolecular and Surface Forces
4. Carraher, C. E., Introduction to Polymer Chemistry
5. Odian, G., Principles of Polymerization
6. Cantor, C. R. & Schimmel, P. R., Biophysical Chemistry (3 vols)
7. Wilson, K. & Walker, J., Principles and Techniques of Biochemistry and Molecular Biology
8. Dill, K. A. & Bromberg, S., Molecular Driving Forces
9. Hiemenz, P. C. & Lodge, T. P., Polymer Chemistry
10. Hiemenz, P. C. & Rajagopalan, R., Principles of Colloid and Surface Chemistry
11. Van Holde, Principles of Physical Biochemistry

Laboratory Exercises (Practical) (atleast 10): **Credit: 2**

1. Study of adsorption of Acetic Acid on Charcoal.
2. Conductometric Study of Critical Micellar Concentration.
3. Calculation of the thermodynamic parameters of micellization of SDS surfactant from conductivity/spectroscopic measurements.
4. Determination of pK_a values and the isoelectric point of an amino acid (both acidic and basic) using pH titration against acid and base.
5. Determination of surface area of a surfactant molecule using Gibbs adsorption isotherm.
6. Study of the catalytic efficiency of a non-specific enzyme by measuring the rate of the enzyme-catalysed reaction.
7. Separation of serum proteins using paper electrophoresis/ Ammonium Sulphate fractionation.
8. Molecular docking study for binding interaction of Fluconazole with 14a-demethylase enzyme (lanosterol) of prominent fungal pathogens Candida albicans using protein structure from protein data bank (PDB ID: CYP51) and Open-source software i.e. AutoDock Vina/ Swiss Dock, etc.

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

9. Instruction mode transaction of working principle of CD spectroscopy and demonstrating experimental protocol for determining protein folding and the percent helix, sheet, turns, and random structure change in protein (Bovine Serum Albumin) upon binding with a suitable ligand i.e. Rhodamine B.
10. Instruction mode transaction of working principle of MALDI-TOF instrumentation technique and its application to identify serum proteins (i.e. Bovine Serum Albumin) and their post translational modifications.
11. Instruction mode transaction of working principle of fluorescence spectroscopy and demonstrating experimental protocol for designing fluorescence/phosphorescence-based chemo sensors for detection of amino acid arginine.
12. Experimental Demonstration of the thermodynamics of urea induced denaturation of a protein, bovine serum albumin, by using fluorimetry.

Recommended Texts/References:

1. Voet, D.; Voet, J. G.; Pratt, C. W. Fundamentals of Biochemistry (Fifth Edition), John Wiley & Sons, Inc.
2. Lakowicz, J. R.; Principles of Fluorescence Spectroscopy, Springer Nature; 3rd edition (4 August 2006).
3. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
4. Hiemenz, P. C.; Rajagopalan, R. Principles of Colloid and Surface Chemistry (3^{rd} Edition) MarceldEkkerin, C.
5. Adamson, A. W.; Gast, A. P.; Physical Chemistry of Surfaces, Sixth Editions, John Wiley & Sons, Inc.

DISCIPINE SPECIFIC ELECTIVES-IV (DSE-III)

Title: Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the Course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Mathematical Methods in Chemistry (DSE -III, Semester-VII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives:

- To build a working knowledge of essential mathematical tools used in physical chemistry.
- To develop confidence in applying calculus, algebra, and probability in thermodynamics, kinetics, and spectroscopy.
- To illustrate concepts with examples relevant to chemical phenomena.

Learning outcomes: After completing the course, the student will be able to:

- Use vector and matrix operations to solve chemical problems (e.g., molecular orbitals, symmetry).
- Understand and apply vector calculus to thermodynamic and electrostatic systems.
- Solve differential and integral problems relevant to kinetics and quantum chemistry.
- Apply probability and curve-fitting concepts to experimental data analysis.
- Understand the role of eigenvalues and coordinate transformations in physical chemistry models.

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

Unit I: Vectors and Matrix Algebra (10 lectures)

Vectors: Dot, cross, and triple products

Vector calculus: Gradient, divergence,and curl.

Integral theorems: Gauss' and Stokes' theorem (physical interpretation only).

Matrices:Types (square, diagonal, identity), operations (addition, multiplication, transpose), Inverse and adjoint.

Special matrices: Symmetric, skew–symmetric, Hermitian, skew- Hermitian, unitary-properties and physical relevance (e.g., Hermitian in quantum mechanics).

Determinants: Evaluation (2x2, 3x3 only), properties, Cramer's rule.

Eigenvalues and eigenvectors: Definition and physical meaning, Diagonalization with examples from Hückel theory and moment of inertia tensor.

Second-rank tensors (conceptual only): Brief mention of how second-rank tensors like polarizability and magnetic susceptibility help describe molecular properties.

Unit II: Differential and Integral Calculus (8 lectures)

Functions, continuity and differentiability, rules for differentiation. Exact and inexact differentials with their applications to thermodynamic properties.

Differentiation and chemical applications, including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution, etc).

Partial differentiation, coordinate transformations (for example,cartesian to spherical polar).

Basic rules for integration, integration by parts, substitution, partial fractions and substitution, reduction formulae. Applications of integral calculus.

Curve sketching and thermodynamic functions.

Unit III: Differential Equations (7 lectures)

First order differential equations: separable, linear, exact.

Applications to rate laws and chemical equilibrium.

Second-order differential equations: harmonic oscillator, Legendre equation (qualitative)

Introduction to Fourier series and boundary value problems (qualitative).

Examples from quantum chemistry (H-atom, angular momentum)

Unit IV: Probability, Statistics, and Curve Fitting (5 lectures)

Permutations and combinations

Probability distributions, RMS, mean, most probable values (Maxwell-Boltzmann distribution).

Error analysis in chemical experiments (standard deviation, RMS error)

Least squares fitting, polynomial trendlines (chemical data)

Recommended Texts/References:

1. Martin C. R. Cockett and Graham Doggett, Math for Chemist: Volume 1&2, Royal Society of Chemistry, Thomas Graham House, Cambridge, UK, 2003.
2. Robert G. Mortimer, Mathematics for Physical Chemistry, Elsevier

Supplementary Reading

1. McQuarrie, D. A., Mathematical methods for scientists and engineers, University Science Books, 2003.
2. Arfken, G., Weber, H., and Harris, F., Mathematical methods for physicists, Academic Press, 7th Ed., 2012.
3. Boas, M. L., Mathematical methods for the physical sciences, Kaye Pace, 3rd Ed., 2006.

Laboratory Exercises (Practical)/Tutorials: Credit: 2

1. Least-squares fit: Linear regression for absorbance vs. concentration data.
2. Matrix multiplication: Three-matrix multiplication, Group theory example.
3. Diagonalization: Secular determinant from Hückel Theory
4. Error analysis: Calculate SD, RMS error, correlation from experimental data.
5. Differential calculus: Maxima/minima problems (e.g., Boltzmann populations).
6. Integral calculus: Evaluation of thermodynamic integrals (e.g., partition functions).
7. Differential Solve and interpret rate equations, harmonic oscillator.
8. Curve fitting: Polynomial fit using spreadsheet or Python (optional).

Recommended Texts/References:

1. Cockett & Doggett, *Maths for Chemists*, Vols 1 & 2 (Royal Society of Chemistry)
2. Robert G. Mortimer, *Mathematics for Physical Chemistry*
3. McQuarrie & Simon, *Physical Chemistry: A Molecular Approach* (selected examples)
4. Excel or Google Sheets for plotting; Python (optional)

SEMESTER – VIII

DISCIPLINESPECIFICELECTIVECOURSE-3(DSE-3):

Transition Metal Clusters-Introduction and Applications

CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

Coursetitle & Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite ofthecourse (if any)
		Lecture	Tutorial	Practical / Practice		
Transition Metal Clusters-Introduction and Applications (DSE-3)	**04**	**02**	**--**	**02**	Class12th with Physics, Chemistry, Mathematics,	**--**

Objectives:

To introduce the basic concepts of transition metal clusters. To gather a good understanding of the chemistry and various aspects of metal-carbonyl clusters, carboranes, metalloboranes and heteroboranes, metallocarboranes with respect to synthesis, structure and properties.

Learning Outcomes:

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

- Ensures the students understand the concepts and the properties of transition metal clusters.
- Acquire knowledge of transition metal clusters cluster compounds and explain structure-property, electron counts, and surface analogies of cluster compounds.
- Identify the structure and bonding aspects of transition metal clusters.
- Identify the different types of transition metal clusters reactions and apply the above concepts to explain reactivity of the clusters.
- To study the application of molecular clusters in catalysis.

SYLLABUSOFDSE-3

Transition-metal clusters: Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms, polyhedral skeletal electron pair theory

(PSEPT), metalloboranes, metallocarboranes. Structure, synthesis, bonding aspects and reactivity. Capping rules, metal-ligand complexes vs heteronuclear cluster.

Main-group-Transition-metal clusters: Isolobalanalogs of p-block and d-block clusters, limitations and exceptions.

Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Chevrel compounds, infinite metal chains, multidecker molecules-cluster surface analogy.

Molecular clusters in catalysis, clusters to materials.Illustrative examples from recent literature.(30 Lectures)

Keywords: Transition Metal Clusters, metal-carbonyl clusters, carboranes, metalloboranes, heteroboranes, metallocarboranes, Capping rules, Isolobal relationship, interstitial main group elements, cubane clusters and naked or Zintl clusters, Chevrel compounds, catalysis, clusters to materials, boron-carbides, metal-borides, Synthesis, Reactivity.

Teaching Learning Process:

Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

Assessment Methods:

● Presentations by Individual Student/ Group of Students

● Class Tests at Periodic Intervals.

● Written assignment(s)

● End semester University Theory Examination

Practicals

1. Synthesis of ferrocene and its characterisation using IR, ^{1}H NMR and UV-Visible spectroscopy
2. Synthesis of acetylferrocene and its characterisation using IR, ^{1}H NMR and UV-Visible spectroscopy
3. Synthesis of $[Fe(\eta\text{-}C_5H_5)(\eta\text{-}C_6H_6)]PF_6$ using ligand exchange reaction. Characterisation of the product using IR, ^{1}H NMR and UV-Visible spectrum
4. Estimation of metal ions in the mixture solution- Mg^{2+}- Zn^{2+}, Ca^{2+}- Mg^{2+}, Cu^{2+} - Zn^{2+}titrimetrically.
5. Analysis of given transition metal cluster(metal carbonyls) using various spectroscopic techniques - IR, UV-Visible and mass spectrometry.

Text Books:

1. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.

2. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth-Heinemann, 1997.
3. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid-state Chemistry, Cambridge University press, 2007.
4. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
5. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press, 1998.
6. C.E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press, 1996.

Reference Books:

1. F. Holleman and E. Wifrg, Inorganic Chemistry, Academic Press, New York, 1995.
2. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
3. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt Ltd, New Delhi, 2001.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver & Atkins Inorganic Chemistry, 4th Edn, Oxford, 2006.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Inorgnic Chemistry: Principles of Structures and Reactivity, 4th Edn, Pearson, New Delhi, 2006.
7. R. Xu, W. Pang and Q. Huo (Eds), Modern Inorganic Synthetic Chemistry, Elsevier, New York, 2011.
8. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
9. J. R. Anderson and M. Boudart (Eds), Catalysis: Science and Technology, Springer, London, 2012.
10. P. Powell, Principles of Organometallic Chemistry, 2nd Edn, Chapman and Hall, London, 1988.
11. G. O. Spessard and G. L. Miessler, Organometallic Chemistry, International 2nd Edn, Oxford University Press, Oxford, 2010.
12. D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), The Chemistry of Metal Cluster Complexes, VCH, New York, 1990.
13. K. J. Klabunde, Free Atoms, Clusters and Nanoscale Particles, Academic Press, New York, 1994.
14. D. M. P. Mingos (Ed.), Structural and Electronic Paradigms in Cluster Chemistry, Springer, Berlin, 1997.
15. P. Braunstein, L. A. Oro and P. R. Raithby (Eds), Metal Clusters in Chemistry, Wiley-VCH, Weinheim, 1999.
16. M. Driess and H. Noth (Eds), Molecular Clusters of the Main Group Elements, Wiley-VCH, Weinheim, 2004.

17. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.
18. F. Wells, Structural Inorganic Chemistry, 5th Edn, Oxford University Press, Oxford, 1984.

DISCIPLINESPECIFICELECTIVECOURSE-4(DSE-4):

Advanced Analytical Techniques for Inorganic Compounds

CREDITDISTRIBUTION,ELIGIBILITYANDPRE-REQUISITESOFTHE COURSE

Coursetitle & Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite ofthecourse (if any)
		Lecture	Tutorial	Practical /Practice		
Advanced Analytical Techniques for Inorganic Compounds (DSE-4)	**04**	**02**	**--**	**02**	Class12th with Physics, Chemistry, Mathematics,	**--**

Learning Objectives

This course is to equip students in handling advanced analytical instruments and techniques important for analysing inorganic compounds.

Learning outcomes

- By the end of the course, the students will be able to:
- To apply the fundamentals of various types of spectroscopic techniques like UV, IR, EPR and Mossbauer spectroscopy and applications of these techniques to interpret data.
- To describe the advancement in spectroscopic methods like IR, UV, EPR and Mossbauer and can recognize necessity of these techniques in the field of analytical science.
- To perform quantitative and qualitative measurements of samples by IR, UV.
- To use different techniques like liquid-liquid extraction, counter current extraction, digestion and solid phase extraction for sample preparation
- To be able to identify, recognize and compare principle, instrumentations and application of Atomic Absorption Spectroscopy (AAS), inductively coupled plasma atomic emission spectroscopy (ICP-AES),

SYLLABUSOFDSE-4

Unit 01- Purification and drying of solvent. Reagents used in undergraduate laboratory: preparation, purification and handling. (04 Lectures)

Unit 02 – Introduction, Physical and Chemical Principles, Spectrometers, Detection, Calculation, and Output, Analytical Information: Qualitative and Quantitative, Applications

Instrumental techniques in laboratory: Infrared spectrophotometer, UV-Visible spectrophotometer. Column chromatography and metal ions separation through ion exchange chromatography.(10 Lectures)

Unit 03- Atomic Absorption and Emission Spectrometry

Introduction, hollow cathode lamp as a source and its working, premix chamber burner and total consumption burner, Flame atomizer - principle and working mechanism of electrothermal atomizers, line width, different interferences observed in AAS. Inductively Coupled Plasma Atomic Emission Spectroscopy.(10 Lectures)

Unit 04: Introduction to EPR and Mossbauer spectroscopy andtheir Applications

(06 Lectures)

Keywords: Solvent, Reagents Infrared spectrophotometer, UV-Visible spectrophotometer. Column chromatography, Ion exchange chromatography, AAS, ICP-AES, EPR and Mossbauer spectroscopy

Teaching Learning Process:

Lectures, ICT enabled teaching, presentations by students, group discussion and quiz will be the part of teaching learning process.

Assessment Methods:

● Presentations by Individual Student/ Group of Students
● Class Tests at Periodic Intervals.
● Written assignment(s)
● End semester University Theory Examination

<u>Practical:</u>

1. Preparation of VO $(acac)_2$ and its characterisation by determining magnetic moment, UV-Visible and IR spectroscopy.
2. Separation of Ni^{2+} and Zn^{2+} in the given mixture through column chromatography.
3. Preparation of $[Co(en)_3]Cl_3$, *cis*- and *trans*- $[Co(en)_2Cl_2]Cl$by oxidation of $Co^{2+}$and measurement of their optical activity.
4. Spectrophotometric estimation of Cr^{3+} in the given solution by 1,5-diphenylcarbazide
5. Estimation of Cu^{2+}-Fe^{3+}/Cu^{2+}-Bi^{3+} in the mixture solution with EDTA spectrophotometrically.
6. Synthesis of any ligand of choice (for example- carboxylate, ester, Schiff base, amides, amines etc.).

7. Synthesis of a transition metal complex using above ligand
8. Characterisation of above complex using suitable analytical technique
9. To determine the solubility and solubility product of a sparingly soluble electrolyte conductometrically.

References for both theory and practical

1. Fundamentals of Analytical Chemistry by Crouch, West and Skoog,9th edition , Brooks/Cole(2013)
2. Analytical Chemistry, Gary D. Christian, 6th Edition, John Wiley and Sons Inc. New Jersey,2007.
3. Instrumental Methods of Chemical Analysis, by Galen W. Ewing, 4thEdition, International Student Edition, 1969.
4. Instrumental methods of analysis, 7th Ed, Willard, Merritt, Dean, SettleCBS Publishers & Distributors 2004.
5. Advanced practical inorganic chemistry, D.M. Adams, J.B. Raynor John Wiley & Sons Ltd 1965
6. Advanced practical organic chemistry, 2nd Ed. Leonard, Lygo, Procter.CRC Press; 3rd edition 2013
7. Inorganic experiments, J.D. Woollins, Wiley VCH 2009
8. General Chemistry Experiments. Anil J. Elias, universities press,2016.
9. Fundamentals of Analytical Chemistry, Skoog and West's, 9th Edition, Cengage Learning Publisher, 2014.
10. Analytical Chemistry-An Indian Adaption,Gary D Christian, Purnendu K Dasgupta, Kevin A Schug , Wiley India Pvt.Ltd,2020.
11. Specrochemical Analysis by Atomic Absorption and Emission, Lajunen L H J, Cambridge, UK: The Royal Society of Chemistry, 1992.
12. Advances in Atomic Spectroscopy, Sneddon J, CT: JAI Press, Greenwich, 1992.
13. CRC Handbook of Inductively Coupled Plasma Atomic Emission Spectrometry, Varma A, FL: CRC Press, Boca Raton, 1991.

GE (2+2) Credit

The existing pool of GE papers of Chemistry can be extended to VII and VIII semesters.

DISCIPLINE-SPECIFIC ELECTIVE COURSE-III (DSE-III)

Title: Fundamentals of Natural Products (DSE-III, Semester-VIII, 30 Lectures)

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

Coursetitle &Code	Credits	Credit distribution of theCourse			Eligibility criteria	Pre-requisite (if any)
		Lecture	Tutorial	Practical/ Practice		
Fundamentals of Natural Products (DSE-III, 30 Lectures)	04	02	---	02	Class 12thwith Physics,Chemistry, Mathematics	

Objectives:The primary objective of this course is to provide students with a comprehensive understanding of natural product chemistry, including its historical development, modern applications, classification, biosynthesis, and methods for isolation and purification.

Outcomes:By the end of this course, students will understand the scope and significance of natural product chemistry in both historical and modern contexts, particularly its role in drug discovery. Students will classify major natural product groups-such as alkaloids, terpenoids, flavonoids, phenolics, peptides, glycosides, polyketides, steroids, and hormones-and understand their structures and functions.

Theory Course Content ***2 Credit (30 lectures)***

Introduction:Definition and scope of natural product chemistry, historical significance and modern relevance, Primary vs secondary metabolites, Sources of natural products: terrestrial and marine origin, importance in drug discovery and development.**(4 Lectures)**

Classification of Natural Products:Alkaloids, Terpenoids, Flavonoids, Phenolics, Peptides and Proteins, Glycosides, Polyketides, Steroids and Hormones (structure and function only).Isoprene rule, mevalonate and non-mevalonate pathways, Shikimic acid pathway. **(7 Lectures)**

Isolation and Purification Techniques:Extraction methods (solvent extraction, Soxhlet, maceration, etc.), Chromatographic techniques (TLC, Column, HPLC, GC-MS), Crystallization and distillation techniques, Bioassay-guided fractionation.**(4 Lectures)**

Total Synthesis of Natural Products: Artemisinin (Antimalarial);Berberine (anti-inflammatory); Lysergic Acid Diethylamide(Psychedelic drug).

(10 Lectures)

Biosynthesis of Natural Products:Artemisinin, Berberine, and Lysergic Acid Diethylamide (LSD). **(5 Lectures)**

Recommended Reference and Textbooks:

1. Mann, J.; Davidson, R. S. & Hobbs, J. B.,**Natural Products: Their Chemistry and Biological Significance, Longman Scientific & Technical (1994)**
2. Mann, J. Secondary Metabolites, Oxford University Press, Oxford, UK, (**1980**)
3. Hanson, J. R., **Natural Products:The Secondary Metabolites, The Royal Society of Chemistry, Cambridge, UK (2003)**
4. Chatwal, G.,**Organic Chemistry of Natural Products, Himalaya Publishing House (1994)**

PRACTICALS

***Course Outcome*:** The students will acquire knowledge of:

1. To isolate natural alkaloids using solvent extraction.
2. Characterization by physical and spectroscopic techniques.

List of Practical's	*2 Credit*

1. Isolation of natural products: Isolation of β-carotene from carrots.
2. Isolation of natural products: Isolation of caffeine from tea leaves.
3. Isolation of natural products: Isolation of piperene from black pepper.
4. Isolation of natural products: Isolation of eugenol from cloves.
5. Synthesis of 7-hydroxy-4-methylcoumarin
6. Synthesis of a simple dipeptide(gly-gly)by DCC coupling using N-protected amino acids.
7. Synthesis of simple amino acids

Recommended Reference and Textbooks:

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
6. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

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DISCIPLINE-SPECIFIC ELECTIVE COURSE-IV (DSE-IV)

Title: Fundamentals of Medicinal Chemistry (DSE-IV, 30 Lectures)

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

Coursetitle &Code	Credits	Credit distribution			Eligibility criteria	Pre-requisite (if any)
		Lecture	Tutorial	Practical/ Practice		
Fundamentals of Medicinal Chemistry (DSE-III, 30 Lectures)	04	02	---	02	Class 12thwith Physics,Chemistry, Mathematics	

Objectives: This course aims to introduce students to the foundational concepts of medicinal chemistry, highlighting its historical development and the significance of natural products as drug sources. Additionally, the course examines the structure, synthesis, therapeutic use, and basic SAR of key drugs like Ibuprofen, Paracetamol, Aspirin, and Penicillin.

Outcome: By the end of the course, students will be able to explain the development and role of medicinal chemistry, understand the stages of drug discovery, and evaluate drug screening and clinical processes. They will interpret how stereochemical and physicochemical properties influence drug behavior and efficacy.

Theory Course Content ***2 Credit (30 Lectures)***

Introduction: History and development of medicinal Chemistry. Sources of drugs, including natural products with examples, Stages of drug discovery, Stereochemical aspects, Physicochemical properties: solubility, acid-base, partition coefficient. (**7 Lectures**)

Drug discovery: Target identification and validation, Screening of drugs, High throughput screening (HTS), Random and Systematic screening. Structure activity relationship (SAR), Hit identification, and Lead optimization. ` (**8 Lectures**)

Pharmacokinetics (ADME): Drug administration/absorption, drug distribution, drug metabolism - Phase 1 and Phase 2, drug excretion, Half-Life of drugs, and Clinical trials. (**5 Lectures**)

Representative Synthetic Drugs:Structure, Synthesis, and Therapeutic Valueof Representative Drugs:Fluconazole (antifungal), Penicillin (antibiotic), Isoniazid (antibiotic),and Azidothymidine (AZT; anti-HIV). (**7 Lectures**)

Bioinformatics:Use of computational tools for drug design.(**3 Lectures**)

Recommended Texts:

1. Patrick, G. L. *Introduction to Medicinal Chemistry*, Oxford University Press (2001)

2. Lemke, T. L. & William, *D. A., Foye's Principles of Medicinal Chemistry*, 5th Ed., USA (2002)
3. Dunlap, N. K. &Huryn, D. M., *Medicinal Chemistry*, Garland Science, New York (2018)
4. Mark W. Holladay, Richard B. Silverman.*The Organic Chemistry of Drug Design and Drug Action,* 3rd Ed. Academic Press (**2014**)

PRACTICALS

Course Outcome: The students will acquire knowledge of:

1. Synthesis and isolation of active ingredients and biologically active compounds/drugs.
2. Characterizationof active ingredients by physical and spectroscopic techniques.
3. Basic drug designing using computational methods

List of Practical's	***2 Credit***

1. Isolation and estimation of aspirin from commercial tablets
2. Synthesis of paracetamol from *p*-aminophenol
3. Synthesis of benzotriazole/benzimidazole.
4. Synthesis of 5,5'-Diphenylhydantoin.
5. Synthesis of dihydropyridine (DHP)/dihydropyrimidine (DHPM).
6. Study of physicochemical properties of pharmaceutically active compounds using computational methods.

Recommended Reference and Textbooks:

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
6. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
7. Pasricha, S., Chaudhary, A. (**2021**), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi

DISCIPLINE SPECIFIC ELECTIVE COURSE-IV (DSE-IV):

Title: Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Interfacial Electrochemistry (DSE-IV, Semester-VIII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives:

- To introduce the structure and thermodynamics of electrochemical interfaces including models of the electric double layer.
- To explain electrode kinetics with emphasis on Butler-Volmer kinetics, Tafel plots, and cyclic voltammetry.
- To introduce Marcus theory and concepts of electrocatalysis and corrosion with real-world relevance.
- To explain transport in electrolyte solutions using laws of diffusion laws, Debye-Hückel theory, and transport numbers.
- To explore adsorption thermodynamics and applications of electrochemical principles in energy storage and conversion devices.

Learning Outcomes:

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

- Explain and compare models of electric double layer and relate them to interfacial properties.

- Apply the Butler-Volmer equation and cyclic voltammetry to interpret reaction mechanisms.
- Describe Marcus theory and the role of parameters in HER, OER and corrosion control.
- Interpret adsorption isotherms and thermodynamic data related to interface processes.
- Evaluate electrochemical energy devices like fuel cells, batteries and supercapacitors.

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

Unit I: Structure and Thermodynamics of Electrochemical Interface (5 lectures)

Overview of interfaces and electrochemical systems.Electric Double Layer: Models: Helmholtz Model, Gouy-Chapman Model (derivation), Stern Model, Graham-Devanathan-Mott-Watts model, Tobin, Bockris-Devanathan model, Thermodynamics of the EDL

Electrocapillary phenomena

Unit II: Electrode Kinetics and Cyclic Voltammetry (6 lectures)

Standard, formal and equilibrium potentials, Overpotentials and their types, Butler-Volmer equation: Derivation and its physical implications, Exchange current density and transfer coefficient, Tafel equation and graphical interpretation, Cyclic voltammetry: Theory and experimental design. Distinguishing reversible, quasi-reversible, irreversible, and capacitive processes.

Unit III: Electron Transfer and Electrocatalysis (4 lectures)

Marcus theory (qualitative description only): activationless region, reorganization energy

Introduction to electrocatalysis, Parameters influencing HER, OER, and oxygen reduction reaction (ORR), Role of electrode materials.

Unit IV: Transport in Electrolytes (5 lectures)

Ionic mobility and transport number, Fick's laws of diffusion, Einstein equation for diffusion

Debye–Hückel–Onsager limiting law, Electrophoretic and relaxation effects, time of relaxation

Dependence of transport number on concentration

Unit V: Adsorption and Surface Thermodynamics (3 lectures)

Adsorption of ions and molecules at interfaces, Thermodynamic treatment of adsorption

Adsorption isotherms:Langmuir, Frumkin, Temkin, Determination of surface excess and charge

Unit VI: Corrosion and its Control (3 lectures)

Types of corrosion: uniform, galvanic, pitting, crevice, etc., Thermodynamics and kinetic aspects.Monitoring methods: electrochemical noise, impedance, Inhibition and protective coatings.

Unit VII: Electrochemical Energy Conversion and Storage (4 lectures)

Fuel cells: PEMFC, Alkaline, Methanol, Batteries: Lithium-ion, Redox flow

Supercapacitors: EDLC and pseudocapacitors. Comparative performance and limitations

Recommended Texts/References:

1. Bard, A. J. Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley & Sons: New York, 2002.
2. Oldham, K. B., Myland, J. C. and Bond, A. M. Electrochemical Science and Technology: Fundamental and Applications, John Wiley & Sons, Ltd. (2012).
3. Bagotsky, V.S., Fundamentals of electrochemistry 2nd Ed. Wiley – Interscience, (2006)

Supplementary References

1. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 1: Ionics 2nd Ed., Springer (1998).
2. Bockris, J. O' M. & Reddy, A. K. N. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science 2nd Ed., Springer (2001).
3. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. Modern Electrochemistry 2A: Fundamentals of Electrodics 2nd Ed., Springer (2001).
4. Brett, C. M. A. & Brett, A. M. O. Electrochemistry, Oxford University Press (1993).
5. Koryta, J., Dvorak, J. & Kavan, L. Principles of Electrochemistry John Wiley & Sons: NY (1993).
6. Hamann, Carl H., Hamneff, Andrew &Vielstich, Wolf., Electrochemistry, 2nd Ed. (2007)

Laboratory Exercises (Practical) (atleast 10: **Credit: 2**

1. Conductometric Titration of a Charge Transfer System, the formation of charge transfer complex between an electron donor and acceptor is studied and the stoichiometry of the complex is determined by following the variation of conductance of the solution with concentration of the donor and acceptor.
2. Study of the oscillating reaction using the Ce^{3+}/Ce^{4+} system; and the dependence of the oscillation period on the metal ion concentration.
3. Intercalation of sodium into vanadium oxide and potentiometric estimation of extent of intercalation.
4. Effect of ionic strength on reaction rate (persulfate-iodine reaction).
5. Potentiometric determination of solubility and solubility product of AgCl(s) in water.

6. Potentiometric determination of mean ionic activity coefficient of HCl at different concentrations.
7. Potentiometric titration of Phosphoric acid vs NaOH.
8. Determination of dissociation constant of acetic acid from its potentiometric titration curve.

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

9. Record cyclic voltammogram for the electrochemical capacitors (electric double layer) response with varying scan rates,

i) plot anodic and cathodic plateau currents vs scan rates.

(Use aqueous solution of 1.5 M $NaNO_3$)

10. Record cyclic voltammogram for a reversible heterogeneous electron transfer system with varying scan rates,

(i) Determine anodic and cathodic peak current ratio.

(ii) Determine anodic and cathodic peak potential difference.

(iii) Plot peak current vs square root of scan rates.

(Use aqueous solution of 10 mM $K_4Fe(CN)_6$ + $K_3Fe(CN)_6$ + 1.5 M $NaNO_3$)

11. Record cyclic voltammogram for a quasi-reversible heterogeneous electron transfer system with varying scan rates,

(i) Determine anodic and cathodic peak current ratio.

(ii) Determine anodic and cathodic peak potential difference.

(iii) Plot peak current vs square root of scan rates.

(Use aqueous solution of 10mM $Fe(NH_4)_2$ $(SO_4)_2$ + $Fe(NH_4)(SO_4)_2$ + 1 M $HClO_4$)

12. Record the CV of aqueous solution of sulphuric acid (0.5 M) at Pt electrode as working electrode and counter electrode.

(i) Interpret and explain various peaks and region of the CV and their significance.

Determine the area and roughness factor of the electrode by Pt oxide region.

Recommended Texts/References:

1. Elgrishi, N.; Rountree, K. J.; McCarthy, B. D.; Rountree, E. S.; Eisenhart, T. T.; Dempsey, J. L. A Practical Beginner's Guide to Cyclic Voltammetry, *J. Chem. Educ.***2018**, *95*, *2*, 197–206.

2. B. D. Khosla, V. C. Garg, A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
3. Field, R. J.; Schneider, F. W. Oscillating Chemical Reactions and Nonlinear Dynamics, *J. Chem. Educ.* **1989**, *66*, *3*, 195–204.

DISCIPLINE SPECIFIC ELECTIVE COURSE-V (DSE-V):

Title: Fundamentals of Solid-State and Materials Chemistry (DSE-V, Semester-VIII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the Course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Fundamentals of Solid-State and Materials Chemistry (DSE-V, Semester-VIII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives:

- To introduce solid-state and wet chemical synthesis methods, and basics of nanomaterials.
- To explain electronic properties of solids using band theory.
- To understand crystal structures, symmetry, and structure determination via diffraction techniques.
- To use thermal and spectroscopic techniques to characterize materials.
- To explore magnetic properties and structure via electron and atomic force microscopy.

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

- Apply solid-state and chemical synthesis methods to create nanomaterials.
- Interpret band structures and explain properties of metals, insulators, and semiconductors.
- Analyze crystallographic data using symmetry concepts and X-ray/electron diffraction.
- Characterize materials using TGA, DSC, UV-Vis, FTIR, PL, and NMR.
- Evaluate magnetic ordering and interpret SEM, TEM, and AFM data.

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

Unit I: Materials Synthesis and Nanochemistry (6 lectures)

Solid state reaction and wet chemical synthetic routes, Top down and bottom-up approach to prepare different kinds of nanomaterials, Fundamental concept of nanoscience including quantum confinement effect, Examples: ZnO, TiO_2, Ag nanoparticles.

Init II: Structure and Bonding in Solids (6 lectures)

Fundamentals of lattice including Bravais Lattices, crystal's direction and planes, symmetry operations and symmetry elements, point group, space group and crystal structures, Miller indices, Types of closed packed structures, Factors which influence crystal structures,Introduction to band theory. Metals, insulators and semiconductors, Electronic structure, k-space and Brillouin zones (qualitative).

Unit III: Structure Determination by Diffraction (6 lectures)

Bragg condition and Bragg method, Laue method, PXRD: principles and instrumentation, Crystallite size (Scherrer) and Williamson-Hall method to determine lattice strains from diffraction patterns, Basics of Single Crystal X-ray diffractometer (SCXRD), electron and neutron diffraction.

Unit IV- Spectroscopy and Thermal Analysis (6 lectures)

UV-Visible, FTIR, Photoluminescence (PL) and NMR techniques to understand materials properties, Thermogravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), principles and interpretation, Examples: thermal decomposition, phase changes.

Unit V: Advanced Characterization and Magnetic Properties (6 lectures)

Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Atomic Force Microscope (AFM): working principles and applications, Magnetic behaviour: Curie and Curie-Weiss laws, magnetic ordering, exchange interactions, Hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism.

Recommended Texts/References:

1. H. V. Keer, Principles of the Solid State, Wiley Eastern.

2. W. D. Callister, Materials Science and Engineering, Wiley.
3. C. N. R. Rao, Nanomaterials Chemistry: Recent Developments and New Directions, Wiley-VCH.
4. R. S. Drago, Physical Methods in Chemistry, Saunders College.
5. Ray Egerton, Physical Principles of Electron Microscopy, Springer.
6. Principles of Fluorescence Spectroscopy by Joseph R Lakowicz
7. Fundamentals of Molecular Spectroscopy by C. N. Banwell
8. Introduction to Molecular Spectroscopy, G. M. Borrow, McGraw Hill.

Supplementary reading

1. Ashcroft & Mermin, Solid State Physics, Saunders College

Laboratory Exercises (Practical)(atleast 10): Credit: 2

Hands-on experiment

1. Synthesis of oxide nanomaterials (e.g., ZnO, TiO_2) using solid-state or sol-gel methods.
2. Preparation of semiconducting CdSe, ZnSe, In_2S_3 (any of one) nanomaterials by any soft chemical approach (emulsion based, co-precipitation etc.).
3. Preparation of metal nanoparticles (e.g., Ag, Cu, or Ni) using standard reduction and capping agents.
4. Studying photocatalytic degradation of environmentally pollutant dye (Crystal Violet, Rhodamine B, methyl orange etc.) by any semiconducting (In_2S_3, CdSe, ZnO- any one) or metallic nanoparticles under visible light irradiation and using UV-Visible spectrophotometer.
5. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
6. Determination of glass transition temperature of a given salt (e.g. $CaCl_2$) conductometrically.
7. Understanding the differences of functional groups by FTIR analysis of different organic compounds (For example, acids, carbonyls, esters, phenolic OH groups etc.).
8. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
9. Determination of band gap of a semiconducting nanoparticle (in solid) using UV-visible spectrophotometer (DRS mode).

Analysis of Compounds/Sample with pre-recorded spectra/diffraction patterns and images subject to availability of instruments

1. Measurement and interpretation of different spectra from UV-Vis, IR and NMR using organic, inorganic compounds and molecules. [At least 6 spectra (two from each category) to be provided to students for analysis].
2. Analysis of diffraction pattern obtained from Powder X-ray diffractometer etc (calculation of crystallite size using Scherer equation and lattice strain calculation using Williamson-Hall equation etc). [At least two diffraction patterns of known sample can be provided to students for analysis]
3. Thermogravimetric analysis of compound, molecules etc.
4. Structural analysis using SEM images, EDX analysis of known samples. Students can be provided SEM images and others for analysis.
5. Calculation of particle sizes, aspect ratio from low magnification TEM images of known samples and lattice plane/d spacing calculations from HRTEM images.
6. Facility (PXRD, SCXRD, TEM, SEM and NMR) visits of the students.

Recommended Texts/References:

1. B.D. Khosla, V.C. Garg and Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand & Co.
2. J.N. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan.
3. G.N. Mukherjee, University Handbook of Undergraduate Chemistry Experiments, Univ. of Calcutta.
4. Ian M. Watt, The Principles and Practice of Electron Microscopy.
5. Ray F. Egerton, Physical Principles of Electron Microscopy – An Introduction to SEM, TEM and AFM.
6. Yoshio Waseda et al., X-ray Diffraction Crystallography: Introduction, Examples and Solved Problems.
7. Journal articles and datasets from ACS, RSC, Elsevier, as applicable (Ind. Eng. Chem. Res. 2014, 53, 3131−3139; ChemSusChem 2011, 4, 1796−1804; ACS Appl. Mater. Interfaces 2017, 9, 11651−11661; Journal of Luminescence 2007, 124, 327–332)

DISCIPLINE SPECIFIC ELECTIVE COURSE-VI (DSE-VI):

Title: Machine Learning and Artificial Intelligence in Chemistry (DSE-VI, Semester-VIII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Machine Learning and Artificial Intelligence in Chemistry(DSE-VI, Semester-VIII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives

- To develop a fundamental understanding of ML/AI, including their basic concepts and different types of learning
- To become familiar with the basic mathematical foundations of ML
- To understand the principles of ML/AI as applied to chemistry.
- To explore the applications of ML/AI in molecular modeling, drug discovery, quantum-mechanical calculations, catalysis, materials design, etc.
- To gain hands-on experience in implementing ML/AI algorithms and tools in solving chemical problems.

Learning Outcome

After completion of this course, learners will be able to-

- Understand core ML/AI principles, including data preprocessing, model training, evaluation, and types of learning.
- Implement and assess ML/AI models (regression, classification, neural networks) for chemistry problems.
- Apply ML/AI to chemical tasks like property prediction, reaction mechanisms, and spectroscopy.
- Integrate ML/AI with quantum chemistry to improve computational efficiency.

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

Unit I: Introduction to ML/AI in Chemistry(6 lectures)

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

Unit II: Mathematics for ML/AI(6 lectures)

Linear Algebra: Vector and Matrix Dot Product, Probability Theory: Random Variables, Bayes Theorem, Conditional Probability, Optimisation: Gradient Descent, First/Second Order Condition.

Unit III: Machine Learning Models and Techniques(8 lectures)

Regression and classification models (Linear Regression, SVMs, Decision Trees), Kernel Ridge regression, Neural networks and deep learning, Backpropagation(qualitative), Unsupervised methods: Clustering.

Unit IV: Applications of ML/AI in Chemistry(10 lectures)

Application of ML/AI for the discovery of Molecular Design, Materials Sciences and Computational Chemistry; Predicting molecular properties. Prediction of reaction mechanisms and pathways. Binding affinity prediction and molecular docking. QSAR modelling in drug discovery, ML/AI in the design of functional materialsand pharmaceutical chemistry. Predicting spectroscopic properties (IR, NMR, Raman). Accelerating quantum chemistry with ML/AI (e.g., approximating post-HF methods, PES fitting).

Recommended Texts/References:

1) Hugh M Cartwright (Ed), Machine Learning in Chemistry: The Impact of Artificial Intelligence, Royal Society of Chemistry; 1st edition (2020)
2) Jon Paul Janet, Heather J. Kulik,Machine Learning in Chemistry, American Chemical Society (2020)
3) Hugh M. Cartwright Applications of Artificial Intelligence in Chemistry, Oxford Chemistry Primers (1994)
4) Pavlo O. Dral,Quantum Chemistry in the Age of Machine Learning, Elsevier - Health Sciences Division (2022)
5) Artificial Intelligence in Chemistry: Current Trends and Future Directions, *J. Chem. Inf. Model.* 2021, 61, 3197−3212
6) A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modelling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
7) The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
8) Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
9) Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis, *J. Med. Chem.* 2020, 63, 8667−8682
10) Artificial Chemical Intelligence: AI for Chemistry and Chemistry for AI by Prof. Pratyush Tiwary, Link: https://www.youtube.com/watch?v=B3wn3C2ANUw

Laboratory Exercises (at least 10 practical) **Credit: 2**

1) Fit a polynomial curve using Excel/spreadsheets/colab (linear, quadratic, cubic, quartic, etc) to find a trendline.
2) Perform interpolation and extrapolation on chemical datasets and also find the missing data.
3) Examine extrapolation to predict future values or trends.

4) Build and train a neural network model for molecular property prediction.
5) Running a simple neural network model in machine learning.
6) Fit potential energy surfaces (PES) using neural networks.
7) Use regression models on open-source chemical data (e.g., QM9).
8) Train regression models to predict spectra from structural data.
9) ML pipeline creation in scikit-learn using simple property prediction.
10) Use standard ML python pipelines to train models.
11) Visualization & analysis using tools like Jupyter notebooks/Google Colab.
12) Explore tools and libraries like Numpy, scikit-learn, PyTorch etc. for chemistry research, education, and data analysis.
13) Optional: Explore AI-driven retrosynthesis using IBM RXN or similar platforms (demo only).

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. McQuarrie & Simon,*Physical Chemistry: A Molecular Approach* (for PES concept)
5. a) https://jupyter.org/ b) https://colab.research.google.com/ c) https://www.python.org/ d) https://numpy.org/ e) https://scikit-learn.org/stable/ f) https://pytorch.org/

List of Instruments/Software required for Fourth year for each College

1. UV- Vis Spectrophotometer
2. Digital Photo Fluorometer
3. Polarimeter
4. Table top IR Spectrophotometer
5. ChemDraw
6. HyperChem
7. Access to NMR Spectrophotometer in Department of Chemistry/USIC
8. Rota Evaporator