# M. Sc. in Chemistry (Total credits: 138)

## Semester-I (36 Credits)

| S. No. | Course Title and course code | Credits | L-T-P-C |
|---|---|---|---|
| 1. | Molecular Spectroscopy | 6 | 3-0-0-6 |
| 2. | Concepts and Mechanisms in Organic Chemistry | 6 | 3-0-0-6 |
| 3. | Symmetry and Group theory | 6 | 3-0-0-6 |
| 4. | Transition Metals and Coordination Chemistry | 6 | 3-0-0-6 |
| 5. | Main group chemistry | 6 | 3-0-0-6 |
| 6. | Chemistry laboratory-I | 3 | 0-0-3-3 |
| 7. | Chemistry laboratory II | 3 | 0-0-3-3 |

## Semester-II (36 Credits)

| S. No. | Course Title and course code | Credits | L-T-P-C |
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| 1. | Instrumental Methods for Structure Determination | 6 | 3-0-0-6 |
| 2. | Organic Reactions and Reagents | 6 | 3-0-0-6 |
| 3. | Organometallic Chemistry and Catalysis | 6 | 3-0-0-6 |
| 4. | Quantum Chemistry | 6 | 3-0-0-6 |
| 5. | Molecular Energetics and Dynamics | 6 | 3-0-0-6 |
| 6. | Chemistry laboratory III | 3 | 0-0-3-3 |
| 7. | Chemistry laboratory IV | 3 | 0-0-3-3 |

## Semester-III (36 Credits)

| S. No. | Course Title and course code | Credits | L-T-P-C |
|---|---|---|---|
| 1. | Bioinorganic and Bioorganic chemistry | 6 | 3-0-0-6 |
| 2. | Concepts in Organic Synthesis | 6 | 3-0-0-6 |
| 3. | Elective-I (Departmental) | 6 | 3-0-0-6 |
| 4. | Elective-II (Departmental) | 6 | 3-0-0-6 |
| 5. | Project-I | 12 | 0-0-0-12 |

## Semester-IV (30 Credits)

| S. No. | Course Title and course code | Credits | L-T-P-C |
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| 1. | Elective-III (Departmental/Institutional) | 6 | 3-0-0-6 |
| 2. | Elective-IV (Departmental/Institutional) | 6 | 3-0-0-6 |
| 3. | Project -II | 18 | 0-0-0-18 |

**List of elective courses:**

1. Statistical mechanics
2. Pericyclic reactions and photochemistry
3. Advanced organic synthesis
4. Supramolecular chemistry and functional inorganic systems
5. Heterocyclic chemistry and natural products
6. Solid state chemistry and its applications
7. Colloids and surface chemistry
8. Chemical biology and medicinal chemistry
9. Material science and polymer chemistry
10. Fundamentals of biophysical chemistry
11. Green and sustainable chemistry
12. Analytical chemistry
13. Principles of biological chemistry
14. Computational chemistry
15. Asymmetric synthesis and catalysis: From basics to frontiers
16. Chemistry of carbohydrates
17. Mathematics for Chemists
18. Radioactivity and Nuclear chemistry
19. Electrochemistry and its applications
20. X-ray crystallography and applications

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| 1 | **Title of the course** (L-T-P-C) | **Molecular Spectroscopy (CH 322)**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Introduction to spectral energy domains and measurement of spectra, Implications of discrete energy levels, Population of States – Boltzmann Distribution, Interaction of radiation with matter, origin of linewidths in molecular spectra, Transition dipole moment and Fermi's Golden Rule, Einstein's Coefficients, Lasers and Masers.<br>Rotational (Microwave) spectroscopy, Molecular vibrations - Infrared spectroscopy, Normal mode analysis, Raman Scattering, Selection Rules from Group Theory, Molecular electronic spectra, Photophysical processes, Non-Linear Spectroscopy, Nuclear Magnetic Resonance, Relaxation times,<br>**1.** FT-NMR, spin-spin coupling, ESR, Nuclear Quadrupolar Resonance. |
| 4 | **Texts/References** | **1.** J. L. McHale, Molecular Spectroscopy, Pearson Education, 2008<br>**2.** M. Hollas, Modern Spectroscopy, Wiley; 4th edition, 2004.<br>**3.** F. A. Cotton, Chemical Applications of Group Theory, An Indian Adaptation, Wiley-Inter science, 2020.<br>**4.** C. M. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition Tata McGraw Hill, 2017<br>**5.** G. M. Barrow, Introduction to Molecular Spectroscopy, Hassle street press, 2021<br>**6.** J. I. Steinfeld, Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy, 2nd edition, Dover, 2012.<br>**7.** J. D. Graybeal, Molecular Spectroscopy, McGraw Hill 2014.<br>**8.** D. A. McQuarrie and J. D. Simon, Physical Chemistry - a molecular approach, Viva Books Pvt. Ltd. 2019. |

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| 1 | **Title of the course** (L-T-P-C) | **Concepts and Mechanisms in Organic Chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Basic mechanistic concepts – kinetic versus thermodynamic control, Hammond's postulate and Curtin-Hammett principle. Methods of determining reaction mechanisms through kinetics, identification of products, intermediates and isotopic labeling. Linear free-energy relationship – Hammett and Taft equations.<br><br>Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, Dia stereoselectivity and asymmetric induction. Geometrical isomerism and optical isomerism. Atropisomerism, and neighboring group participation on reactivity and selectivity.<br><br>Reactive Intermediates: Generation, structure, properties and reactions of carbenes, nitrenes, radicals, carbocations, carbanions and benzynes. Introduction to different reaction types:substitution, elimination, addition, oxidation, reduction, pericyclic<br>and concerted reactions (electrocyclic, cycloaddition and sigma tropic) and molecular rearrangements |
| 4 | **Texts/References** | 1. Jerry March and Michael Smith, "Advanced Organic Chemistry", 7th Ed., Wiley, 2015.<br>2. F. A. Carey and R. J. Sundberg, "Advanced Organic Chemistry, Part A", 5th Ed., Springer, 2008.<br>3. J. Clayden, N. Greeves, and S. Warren, "Organic Chemistry", 2nd Ed., Oxford University Press, 2014.<br>4. W. Carruthers and I. Coldham, "Modern Methods of Organic Synthesis", 4th Ed., Cambridge University Press, 2015.<br>5. P. Bruice, "Organic Chemistry" 7th Ed., Pearson, 2013. |

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| 1 | **Title of the course** (L-T-P-C) | **Symmetry and Group theory**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Introduction to chemical bonding, Symmetry elements and operations, Schön flies notation of point group, Prediction of dipole moment and optical activity from the viewpoint of symmetry, Definition of group, subgroup, class, Matrix representation of a point group Reducible & Irreducible representations, Great Orthogonality Theorem and its corollaries, Construction of character table and meaning of all the term in character table, Mulliken symbol for irreducible representation, Direct product of irreducible representations, Application to spectroscopy, Projection operator and its application to symmetry adapted linear combination (SALC), Application to quantum mechanics, Construction of Molecular Orbital correlation diagram of simple and complex molecule |
| 4 | **Texts/References** | 1. F. A. Cotton, Chemical Applications of Group Theory, An Indian Adaptation, Wiley-Interscience, 2020.<br>2. R. L. Carter, Molecular symmetry & group theory, John Wiley & Sons, 1997<br>3. D. C. Harris, M. D. Bertolucci, Symmetry and Spectroscopy, Dover, 1989.<br>4. Michael Tinkham Group Theory and Quantum Mechanics, Dover publications, 2003. |

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| 1 | **Title of the course** (L-T-P-C) | **Transition Metals and Coordination Chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | 1. Chemistry of transition metals: Introductory survey of transition elements with reference to electronic configuration, oxidation states, complex compounds. Introductory concepts of molecular symmetry. Spectral and magnetic properties.<br>2. Chemistry of titanium, vanadium, chromium, manganese sub-group elements, iron, cobalt, nickel, platinum metals, copper and zinc sub-group elements, group III, IV, V, VI, VII and rare gases with reference to isolation, properties, uses and important compounds.<br>3. Chemistry of Lanthanides and Actinides: Electronic configuration, colour and magnetism, properties of lanthanides and actinides. Synthesis of trans-Uranic elements, chemistry of uranium compounds.<br>4. Introduction to Coordination Compounds: Werner's work, structure, isomerism, thermodynamics of complex formation.<br>5. Bonding in Transition Metal Complexes: Valence bond theory, crystal field theory, ligand field theory, pi- acceptor/donor interactions.<br>6. Electronic Spectra: Energy levels in an atom, coupling of orbital angular momenta, spin angular momenta, and spin-orbit, ground state terms-Hund's rules, microstates, electronic spectra (selection rules), splitting of electronic energy level and spectroscopic stated, Tanabe-Sugano diagrams.<br>7. Reactions and Mechanism: Ligand substitution reactions, base hydrolysis, stereochemistry, isomerization reactions, redox reactions (the inner-sphere mechanism, the outer- sphere mechanism), photochemical reactions. |
| 4 | **Texts/References** | 1. Concise Inorganic Chemistry by J. D. Lee, 5th edition, Blackwell Publishing, 2006.<br>2. Inorganic Chemistry by Gary L. Miessler, Paul J. Fischer, and Donald A. Tarr, 5th edition, 2014.<br>3. Catherine E. Housecroft and Alan G. Sharpe, Inorganic Chemistry, 5th edition., 2018.<br>4. Atkins, P., et al., Shriver and Atkins Inorganic Chemistry, 5th Ed., Oxford UniversityPress, 2010.<br>5. Organometallics by Christoph Elschenbroich, 3rd edition, 2006.<br>6. The Organometallic Chemistry of the Transition Metals by Robert H Crabtree, 2014.<br>7. J. E. Huheey, E. A. Keiter, and R. L. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Ed, Pearson Education, 2006.<br>8. Advanced Inorganic Chemistry by F. A. Cotton, G. Wilkinson C. A. Murillo and M. Bochmann, John Wiley, Chichester, 6th edition, 1999. |

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| 1 | **Title of the course** (L-T-P-C) | **Main group chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | 1. General characteristics of s- and p-block elements, comparative study of second short period elements (B to F) with heavy congeners (Al to Cl), Electron deficient molecules and hyper valency<br>2. Hydrogen and hydrides, the boron and carbon groups, the nitrogen and oxygen groups, the halogens and the noble gases.<br>3. Review of inorganic chains, rings and cages, Inorganic chains, rings, and cages.<br>4. Nuclear magnetic resonance (NMR) and Electron paramagnetic resonance (EPR) spectroscopy of Inorganic System<br>5. Mössbauer spectroscopy<br>6. Vibrational spectroscopy: Fourier transform infrared (FT- IR) and Raman spectroscopy, resonance Raman spectroscopy<br>7. UV-vis, X-ray absorption spectroscopy (XAS) |
| 4 | **Texts/References** | 1. Atkins, P., et al., Shriver and Atkins Inorganic Chemistry, 5th edition, Oxford University Press, 2010.<br>2. Lee, J. D., Concise Inorganic Chemistry, 5th edition, Blackwell Publishing, 2006.<br>3. Douglas, B., McDaniel, D., Alexander, J., Concepts and Models of Inorganic Chemistry, 3rd Ed. Wiley India (P.) Ltd., India, 2010.<br>4. J. E. Huheey, E. A. Keiter, and R. L. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson Education, 2006.<br>5. Chemistry of the Elements, by N.N. Greenwood and A. Earnshaw, Butterworth-Heinmann, London, 1997.<br>6. Advanced Inorganic Chemistry by F. A. Cotton, G. Wilkinson C. A. Murillo and M. Bochmann, John Wiley, Chichester, 1999. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemistry laboratory-I**<br>**0-0-3-3** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Inorganic chemistry: Basic concepts of quantitative analysis, redox, precipitation and complexometric titrations. Solubility product and precipitation, organic precipitants and extractants. A brief survey of separation methods: solvent extraction and chromatography. Volumetric analysis involving redox, precipitation and complexometric titrations.<br><br>Organic chemistry: Determination of physical constants, purification of solids and liquids and methods of checking their purity. Separation of enantiomers and measurements of optical rotation. Studies of electrophilic/nucleophilic substitution reactions, redox reactions<br>Physical chemistry: Ionization constant by spectrophotometry, enzyme kinetics, use of immobilized enzyme electrode, adsorption isotherm |
| 4 | **Texts/References** | 1. G. Svehla and B. Sivasankar, "Vogel's qualitative inorganic analysis, Pearson Education India, 7th Ed, 2023.<br>2. G. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, "Vogel's quantitative chemical analysis" Pearson education India, 6th Ed. 2009.<br>3. A. J. Elias, "A collection of interesting general chemistry experiments"Sangam Books Ltd. First Ed. 2002.<br>4. B. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2010<br>5. A. M. Halpern, and G. C. McBane, Experimental Physical Chemistry: A Laboratory TextBook, 3rd Edition, W. H. Freeman, 2006<br>6. B. S. Furniss, A. J. Hannaford, P.W.G. Smith, A.R. Tatchell, "Vogel's textbook of practical organic chemistry" Pearson education India, 5th Ed. 2003.<br>7. In-house laboratory manual with the experimental procedures and relevant literature. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemistry laboratory II (CH 312)**<br>**0-0-3-3** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Inorganic chemistry: Complex material analyses: minerals/ alloys. Quantitative estimations using conductometry and spectrophotometry.<br><br>Organic chemistry: Qualitative analysis of organic compounds. Chemical separation of binary mixtures and their qualitative analysis, Synthesis of organic compounds and chromatography<br><br>Physical chemistry: Phase equilibria, viscosity and molecular weight of polymers, surface tension, reaction kinetics (rates, order of reaction, influence of ionic strength), use of thermocouples, transition temperature determinations, |
| 4 | **Texts/References** | 1. G. Svehla and B. Sivasankar, "Vogel's qualitative inorganic analysis", Pearson Education India, 7th Ed, 2023.<br>2. G. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, "Vogel's quantitative chemical analysis" Pearson education India, 6th Ed. 2009.<br>3. A. J. Elias, "A collection of interesting general chemistry experiments"Sangam Books Ltd. First Ed. 2002.<br>4. B. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 1st Ed., 2010<br>5. A. M. Halpern, and G. C. McBane, Experimental Physical Chemistry: A Laboratory Textbook, 3rd Edition, W. H. Freeman, 2006 |

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| 1 | **Title of the course** (L-T-P-C) | **Instrumental Methods for Structure Determination (CH 307)**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | **NMR spectroscopy**: Basic principles of $^{1}$H-NMR, instrumentation and interpretation of NMR spectrum, chemical shift: principles, chemical shift values of major organic compound classes, and factors affecting chemical shift, spin-spin coupling, spin systems, coupling with other nuclei, 2D-NMR (COSY, TOCSY), NOE (NOESY), $^{13}$C-NMR-principles and chemical shifts for major organic compound classes, $^{1}$H-$^{13}$C-2D NMR (HSQC, HMBC), DEPT, $^{31}$P and $^{19}$F-NMR, solid state NMR and applications in chemistry.<br>**Mass Spectrometry**: Instrumentation and techniques (ionization techniques, mass analysers, and detection techniques, tandem MS or MS/MS, LC-MS, GC-MS, MALDI-TOF-MS etc.),<br>interpretation of mass spectra, fragmentation patterns of major organic compound classes including rearrangement reactions and applications of mass spectrometry in chemistry and biology.<br>**FTIR and UV-Visible spectroscopy**: Basic concepts and applications in functional group characterization and organic structure elucidation |
| 4 | **Texts/References** | 1. R. Silverstein, F. Webster, D. Kiemle, and D. Bryce "Spectrometric identification of organic compounds", 8th Ed., Wiley, 2015.<br>2. P. Crews, J. Rodriguez, and M. Jaspars, "Organic structure analysis", 2nd Ed., OUP USA, 2009.<br>3. D. Williams and I. Fleming, "Spectroscopic methods in organic chemistry", 6th Ed. McGraw Hill Education, 2011.<br>4. W. Kemp, "Organic spectroscopy", 2nd Ed., Red Globe Press, 2019.<br>5. D. Pavia "Introduction to spectroscopy" Cengage Learning India Private Ltd., 5th Ed., 2015.<br>C. Banwell and E. McCash "Fundamentals of molecular spectroscopy" 4th Ed., McGraw Hill Education, 2017. |

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| 1 | **Title of the course** (L-T-P-C) | **Organic Reactions and Reagents (CH 310)** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Functional group transformations, common named reactions, oxidations, reductions and rearrangements and their applications in organic synthesis. Carbon-Carbon Bond Forming Reactions via enolate, enamine and imine chemistry, Grignard, cuprate and other conjugate reactions, Radical reactions and other classes (via organo silane, borane and tin based reagents, Baylis-Hillman reaction), Selectivity and protecting groups: Illustration of chemoselectivity, regioselectivity and enantioselectivity, stereoselectivity; protecting groups for alcohols, amines, acids, ketones and aldehydes. common catalysts and reagents for reactions (organic, inorganic, organometallic and enzymatic), pericyclic and photochemical reactions in organic synthesis |
| 4 | **Texts/References** | 1. Carey, F. A., Sundberg, R. J. Advanced Organic Chemistry, Part A and B, Springer, 2007.<br>2. Clayden, J., Greeves, N., Warren, S., Wothers, S. Organic Chemistry, Oxford University Press, 2001.<br>3. Carruthers, W., Coldham, I. Some Modern Methods of Organic Synthesis, Cambridge University Press, 2004.<br>4. Smith, M. B. and March, J. Advanced Organic Chemistry, Wiley Interscience, 2007. |

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| 1 | **Title of the course** (L-T-P-C) | **Organometallic Chemistry and Catalysis**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | 1. Organometallic Chemistry: 18-electron rule. Ligands: Carbon monoxide, phosphines, hydrides and dihydrogen complexes, alkyl, -alkenyl, -alkynyl, and -aryl ligands, Alkene and -alkyne ligands, nonconjugated diene and polyene ligands, butadiene, cyclobutadiene, and cyclooctatetraene, benzene and other arenes, the allyl ligand, cyclopentadiene and cycloheptatriene, carbenes, alkanes, agostic hydrogens, dinitrogen and nitrogen monoxide.<br>2. Compounds: d-Block carbonyls, metallocenes, metal–metal bonding and metal clusters.<br>3. Reactions: Ligand substitution, oxidative addition and reductive elimination, s-Bond metathesis, 1,1-migratory insertion reactions 1,2-insertions and b-hydride elimination, $\beta$, ✿-Hydride eliminations and cyclometallations.<br>4. Catalysis: Organometallic catalysts, Terminology in catalysis: Turnover, turnover number (TON), turnover frequency (TOF). |
| 4 | **Texts/References** | 1. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th edition, Oxford University Press, 2014. (South asia edition 2015)<br>2. E. Huheey, E. A. Keiter, R.L. Keiter and O. K. Mehdi, Inorganic Chemistry, Principles of Structure and Reactivity, 4th edition, Pearson, 2006.<br>3. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, 2nd edition, Universities Press (India), 2013.<br>4. Organometallics by Christoph Elschenbroich, 3rd edition, 2006.<br>5. Atkins, P., et al., Shriver and Atkins Inorganic Chemistry, 5th edition, Oxford University Press, 2010.<br>6. The Organometallic Chemistry of the Transition Metals by Robert H Crabtree, 2014. Inorganic Chemistry by Gary L. Miessler, Paul J. Fischer, and Donald A. Tarr, 5th edition, 2014. |

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| 1 | **Title of the course** (L-T-P-C) | **Quantum Chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Introduction: Importance; Historic background; Classical vs Quantum mechanics; Wave particle duality; Uncertainty principle. Postulates of quantum mechanics; Operator algebra; Properties of hermitian operators; Commutators. Schrodinger Equation: Wave function and interpretation; Time dependent and time independent Schrodinger equation; Eigenvalue problem. Quantum mechanics applications to model systems: Free particle; Particle-in-a-box (1D & 3D); harmonic oscillator; Tunneling; Rigid rotor. Hydrogen and hydrogen like atoms. Methods to obtain the approximatesolution of time independent Schrödinger equation: Perturbation theory; variational method; Applications. Many electron atoms: Spin and Pauli exclusion principle; Hund's rule; Slater determinants; Electronic term symbols. |
| 4 | **Texts/References** | 1. D. A. McQuarrie, Quantum Chemistry, Viva Student Edition, 2016<br>2. I. R. Levine, Quantum Chemistry, Pearson publication, 7th Edition 2013. |

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| 1 | **Title of the course** (L-T-P-C) | **Molecular Energetics and Dynamics (CH 320)**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Laws of thermodynamics. Estimations of enthalpy and free energy. Fugacity and activity and their determinations Application to chemical reactions. Overview of rate laws and determining rates and orders of reactions. Complex Reactions. Catalysis Temperature dependence and Arrhenius law. Potential energy surfaces. Kinetic theory of collisions. Transition state theory. RRK and RRKM theories. Reaction cross-section, rate coeffecients, reaction probabilities. Photochemical reactions. |
| 4 | **Texts/References** | 1. P. Atkins and J. de Paula, Atkins' Physical Chemistry, 8th edition, Oxford University Press, 2022.<br>2. G. W. Castellan, Physical Chemistry, Addison - Wesley/Narosa Publishing House, 2004. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemistry laboratory III (CH 313)** **0-0-3-3** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Inorganic chemistry: Determination of composition of complexes in solution. Synthesis and characterization of transition metal complexes (including organometallic compounds) and their study by various methods (spectral, thermal and magnetic etc).<br><br>Organic chemistry: Chemical separation of ternary mixtures and characterization of the components. Simple one or two step preparations involving different techniques, Isolation of natural products, chromatographic analysis of complex mixtures, selectivity in synthesis, enzymatic and chemo-enzymatic synthesis, characterization, Analysis of biomolecules such as DNA and proteins and their spectrophotometric characterization<br><br>Physical chemistry: Determination of the following physical quantities: partial molal volumes, dipole moments, activities by freezing point, quantum yields, heats of vaporization and depressions of freezing points of solutions, velocity constant and activation energy. Electrodes with different substrates for H2 evolution, photoelectrochemical solar cells. Vacuum measurement. IR spectrum of HCl, Use of M.O. theory, solution of Schrodinger equation for polyatomic. |
| 4 | **Texts/References** | 1. G. Svehla and B. Sivasankar, "Vogel's qualitative inorganic analysis", Pearson Education India, 7th Ed, 2023.<br>2. G. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, "Vogel's quantitative chemical analysis" Pearson education India, 6th Ed. 2009.<br>3. A. J. Elias, "A collection of interesting general chemistry experiments" Sangam Books Ltd. First Ed. 2002. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemistry laboratory IV** **0-0-3-3** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Part A: Introduction to computational chemistry and the role of computers in chemistry, molecular simulations and programming, Introduction to applications of artificial intelligence/machine learning (AI/ML) in chemistry<br><br>Part B: Exposure and demonstration of sophisticated instruments such as UV-Vis-NIR spectrophotometer, Fluorimeter, Nuclear Magnetic resonance spectrometer, Infra-red spectrophotometer,<br>mass spectrometer, and various chromatographic techniques (HPLC, GCMS, LCMS), Powder X-ray diffraction, BET etc. |
| 4 | **Texts/References** | 1. Donald A. McQuarrie, Quantum Chemistry, University Science Books, 2nd Edition 2008<br>2. Andrew R. Leach, Molecular modelling principles and applications, Pearson Education Limited 2nd Edition, 2001<br>3. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons., 2017<br>4. In-house laboratory manual with the experimental procedures and relevant literature. |

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| 1 | **Title of the course** (L-T-P-C) | **Bioinorganic and Bioorganic chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Oxygen-activating proteins (cytochrome P450 and cytochrome c oxidase), electron transport proteins (blue copper proteins, Fe–S clusters, and cytochromes), photosystems, and hydrolase enzymes (carbonic anhydrase and peptidase). Metal transport and storage – Ferritin, Hemoglobin and myoglobin, Metals in medicine.<br>Structure, function, properties and chemistry of the biological macromolecules (amino acids, proteins, carbohydrates, nucleic acids, and lipids). Enzymes and cofactors. Introduction to metabolism, Enzyme catalyzed reactions in biological pathways: group transfer, hydrolysis, amination, phosphorylation, reduction, oxidation, oxygenation, substitutions, carboxylation/decarboxylation, isomerization, eliminations, additions, Aldol and Claisen reactions, formylations/methylations, Rearrangements, and pericyclic reactions, Biorthogonal chemistry and chemical biology. |
| 4 | **Texts/References** | 1. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, 2nd edition, Wiley, 2013.<br>2. R. R. Crichton, Biological Inorganic Chemistry - An Introduction, Elsevier, 2008.<br>3. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy Mark Berg, 1994, University Science Publications.<br>4. R. Silverman, "The organic chemistry of enzyme catalyzed reactions" Revised edition, Academic Press, 2002.<br>5. Inorganic Chemistry by Gary L. Miessler, Paul J. Fischer, and Donald A. Tarr, 5th edition, 2014.<br>6. D. Vranken and G.A. Weiss "Introduction to Bioorganic Chemistry and Chemical Biology" 1st edition., Garland Science, 2012.<br>7. McMurry and Begley "The Organic Chemistry of Biological Pathways" 2nd edition., W H Freeman, 2015.<br>8. Nelson and Cox, "Lehninger Principles of Biochemistry", 7th edition., WH Freeman, 2017. |

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| 1 | **Title of the course** (L-T-P-C) | **Concepts in Organic Synthesis (CH 321)**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Synthesis, reactions, mechanisms, and selectivity involving the following- alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids and their derivatives, halides, nitro compounds and amines. Use of compounds of Mg, Li, Cu, B and Si in organic synthesis. Concepts in multistep synthesis- retrosynthetic analysis, disconnections, synthons, synthetic equivalents, linear and convergent synthesis, reactivity umpolung, selectivity, protection and deprotection of functional groups, Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst-controlled reactions; enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic. |
| 4 | **Texts/References** | 1. Clayden, J., Greeves, N., Warren, S., Wothers, S.Organic Chemistry, Oxford University Press, 2001.<br>2. Carruthers, W., Coldham, I. Some Modern Methods of Organic Synthesis, Cambridge University Press, 2004.<br>3. Smith, M. B. and March, J. Advanced Organic Chemistry, Wiley Interscience, 2007.<br>4. Carey, F. A., Sundberg, R. J. Advanced Organic Chemistry, Part A and B, Springer, 2007.<br>5. Smith, M. B. Organic Synthesis, McGraw-Hill, 2001.<br>6. Warren, S.Organic Synthesis: The Disconnection Approach, Wiley, 1983.<br>7. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006. |

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| 1 | **Title of the course** (L-T-P-C) | **Statistical Mechanics** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Ensembles and Averages, equivalence of Ensembles, classical Limit. Monte Carlo and Molecular Dynamics simulations. Distribution functions at equilibrium. Integral equation methods. Perturbation theory. Density functional methods. Molecular fluids. Estimation of thermodynamic functions. Non-equilibrium methods. Linear response theory. Stochastic processes and Brownian motion. Selected applications to problems in chemical dynamics, relaxation processes and neutron diffraction. |
| 4 | **Texts/References** | 1. D. A. McQuarrie, Statistical Mechanics, Viva books publisher, 2018.<br>2. M. P.Allen and D. J. Tildesley, Computer Simulation in Liquids, Oxford University Press, 2017.<br>3. J. P. Hansen and I. R. McDonald, Theory of Simple Liquids, 4th edition, Academic Press,2013.<br>4. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987.<br>5. Mark E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford Graduate Texts, 2nd Edition 2023. |

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| 1 | **Title of the course** (L-T-P-C) | **Pericyclic reactions and Photochemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Conservation of orbital symmetry, Woodward-Hoffmann rules, frontier molecular orbital (FMO) theory, Orbital overlap effects in cycloadditions, electrocyclizations, sigmatropic rearrangements and chelotropic reactions, Paterno-Buchi, Norrish type I and II reactions, Photochemistry of alkenes, carbonyl compounds, and arenes. Photooxidation and photoreduction. Di- π-methane rearrangement, Barton reaction, photocatalysis.<br><br>Cycloaddition reactions: Diels-Alder reaction; hetero-Diels Alder reaction. 1,3-dipolar cycloaddition reactions; [2+2] cycloaddition reactions; Molecular rearrangements; Sigmatropic rearrangements, Cope and oxy- Cope rearrangements; 2,3- sigmatropic rearrangements and ene reaction. |
| 4 | **Texts/References** | 1. F. A. Carey and R. J. Sundburg, "Advanced Organic Chemistry, Part B", Fifth Ed., Plenum Press, 2007.<br>2. J. Clayden, N. Greeves, S. Warren and P. Wothers,"Organic Chemistry", First Ed., Oxford University Press, 2001.<br>3. T. L. Gilchrist and R. C. Storr, "Organic Reactions and Orbital Symmetry", 2nd Edn., Cambridge University Press, Cambridge, 1979.<br>4. K. K. Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.<br>5. I. Fleming, "Pericyclic Reactions", Oxford University Press, Oxford, 1998.<br>6. S. Sankararaman, "Pericyclic Reactions- A Textbook", Wiley- VCH, Weinheim, 2005. |

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| 1 | **Title of the course** (L-T-P-C) | **Advanced Organic Synthesis** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Reaction vs synthetic method; metal atom functionality in organometallic reactions, C-C bond forming reactions, ring forming reactions, organometallics as protecting and stabilizing groups, palladium catalyzed reactions, Heck reaction, cross coupling reactions (Suzuki, Stille, Negishi, Kumada, Hiyama, Sonogashira, Buchwald- Hartwig), Olefin metathesis, NHCs and application to organic synthesis, Role of silicon in organic synthesis, Target and diversity oriented synthesis, Asymmetric synthesis, Chiral and Organocatalytic, Some selected natural and non-natural product total synthesis, Introduction to domino/tandem/cascade reaction concepts. |
| 4 | **Texts/References** | 1. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.<br>2. B. M. Trost and I Fleming, Comprehensive organic synthesis, Pergamon Press, 1992.<br>3. S. Warren, "Designing Organic Syntheses", John Wiley & Sons 2009.<br>4. K. C. Nicolaou, E. J. Sorenson, "Classics in Total Synthesis, I, II and III"<br>5. T.W. Greene, "Protecting Groups in Organic Synthesis" (3rd edition), J. Wiley& Sons, 1999. |

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| 1 | **Title of the course** (L-T-P-C) | **Supramolecular chemistry and functional inorganic systems** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Basic concept and principles; Terminologies and nomenclature in supramolecular chemistry. Chemical interactions leading to supramolecular assemblies (Hydrogen Bonds, Non-covalent interactions), Molecular recognition and host-guest complementarity. Biological supramolecular systems: Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self- assembly. Supramolecular reactivity Biomimetic systems and Artificial receptors (Cation Binding Hosts, Anion binding hosts, Ion Pair Receptors, Hosts for Neutral Receptors). Organic Crystal Structures, Polymorphism, Solvates, Co-Crystals. |
| 4 | **Texts/References** | 1. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1995.<br>2. V. Balzani (Editor), L. De Cola, Supramolecular Chemistry, Wiley Kluwer, Dordrecht, 1992.<br>3. Supramolecular Chemistry by J. W. Steed & J. L. Atwood, 3rd edition John Wiley, 2022.<br>4. Crystal Engineering. The Design of Organic Solids by G.R. Desiraju, Elsevier, 1989. |

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| 1 | **Title of the course** (L-T-P-C) | **Heterocyclic Chemistry and Natural Products**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Significance, structure, preparation, properties, and reactions of three, four, five, and six membered heterocyclic compounds (including furan, pyrrole, thiophene, pyridine, indole, and their derivatives). Aromatic heterocycles, Polyhetero ring systems, modern methods in heterocycle synthesis, Chemistry of natural products: Terpenes, steroids, alkaloids, and pigments: Flavones, xanthones, quinones, pterins, chlorophyll, carotenoids, chemistry of vitamins, carbohydrates, fatty acids, and nucleic acids |
| 4 | **Texts/References** | 1. I. L. Finar, Organic Chemistry, Vol .2, 5th edition, ELBS, 1975.<br>2. K. Nakanishi, T. Goto, S.Ito, S. Najori and S. Nozoe, Natural products Chemistry, Vol. 1 and 2, Academic Press, 1974.<br>3. Topics in Heterocyclic Chemistry. G. W. Gribble. Spinger-Verlag Berlin Heidelberg, 2010.<br>4. Handbook of Heterocyclic Chemistry. Alan R. Katritzky and A. F. Pozharskii, Elservier 2000.<br>5. The Chemistry of Heterocycles. T. Eicher, S. Hauptmann, Wiley-VCH 2003<br>6. R. K. Bansal, Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, Wiley Eastern Ltd., 1990. |

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| 1 | **Title of the course** (L-T-P-C) | **Solid state chemistry and its applications** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Diffraction techniques and the structure of solids; analysis of diffraction data. Crystal defects, non-stoichimetry and solid solutions. Structure of solid electrolytes, zeolites, Solid state transformations and reactions. Electronic structure of solids: Fermi level, Bloch orbitals, energy bands, Brillouin zone. Electric and magnetic properties of solids: insulators, semiconductors, conductors and Fermi surfaces; superconductivity; polarization, refractive index, dielectrics and ferroelectrics; diamagnetism and paramagnetism; ferromagnetism, ferrimagnetism and antiferromagnetism. Molecular metals, phosphors and solid-state lasers. Introduction to nanoscience. |
| 4 | **Texts/References** | 1. C. Kittel, Introduction to Solid State Physics, 8th edition, Wiley, 2012.<br>2. A. R. West, Solid State Chemistry and Its Applications, Wiley, 3rd edition, 2012.<br>3. A. W. Adamson, Physical Chemistry of Surfaces, 6th Edition, Wiley, 1997. |

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| 1 | **Title of the course** (L-T-P-C) | **Colloids and Surface Chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Colloid systems and their properties: Origin of the charges, electro-kinetic phenomena, electrophoresis, electroosmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.<br>Macromolecules: Concepts of mass and number average molecular weights, methods of determining molecular weights (osmometry, viscometry, diffusion and light scattering method), sedimentation, fractional properties of macromolecules, statistical distribution of end to end dimension, calculation of average dimension of various chain structures.<br>Surfactants and Interfacial Phenomena: Classification, micellization, c.m.c. and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emulsions, dispersion and aggregation of solids by surfactants<br>Adsorption on solids and porous materials: Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids. Estimation of specific surface area and pore size<br>distribution. Special problems encountered with very narrow pore size material and adsorption from liquid phase. |
| 4 | **Texts/References** | 1. Hunter, R. J., "Foundation of Colloid Science", 2nd Edition, Oxford Univ. Press. 2000<br>2. Lyklema, J., "Fundamentals of Interface and Colloid Science", Academic Press San Diego. 2005<br>3. Adamson, A.W.,"Physical Chemistry of Surfaces", 6th Ed., John Wiley and Sons, New York. 1997<br>4. Greg, S.J. and Singh, K.S.W., "Adsorption, Surface Area and Porosity", 2nd Ed., Academic Press. U K. 1997<br>5. Flory P. J., "Principles of Polymer Chemistry", Asian books. 2007<br>6. Rubinstein M. and Colby R. C., "Polymer Physics", 1st Ed.,Oxford University Press. 2003. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemical biology and medicinal chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | |
| 3 | **Course content** | Basic introduction to chemical biology and its applications, Role of chemistry in understanding biological systems, Design and synthesis of various chemical probes for investigation of biology<br><br>Basic medicinal chemistry, Chemistry of drug design and drug action, Drug-receptor interactions, Drug targets and drug metabolism, Pharmacokinetics, Enzymes as drug targets, Natural products classes as drug leads, Chemical control of signal transduction, antibiotics, antifungals, antivirals, antidiabetic and anticancer drugs, drug resistance, and drug repurposing |
| 4 | **Texts/References** | 1. R. Silverman, "The organic chemistry of enzyme catalyzed reactions" Revised ed.Academic Press, 2002.<br>2. D. Vranken and G.A. Weiss "Introduction to Bioorganic Chemistry and Chemical Biology" 1st Ed., Garland Science, 2012.<br>3. McMurry and Begley "The Organic Chemistry of Biological Pathways" 2nd ed., WH Freeman, 2015<br>4. Nelson and Cox, "Lehninger Principles of Biochemistry", 7th Ed., WH Freeman, 2017<br>5. Silverman and Holladay "The Organic Chemistry of Drug Design and Drug Action" 3rd Ed., Academic press, 2014<br>6. P. Frey and A. D. Hegeman, "Enzymatic Reaction Mechanisms", 1st Ed., OUP USA, 2007.<br>7. Wiley Encyclopedia of Chemical Biology (Editor: T. Begley), 1st ed., Wiley-Blackwell, 2009 (4 volumes)<br>8. Graham L. Patrick, "An Introduction to Medicinal Chemistry" Oxford Press, 5th edition, 2013. |

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| 1 | **Title of the course** (L-T-P-C) | **Material science and polymer chemistry** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Atomic Bonding, Crystal Structure and Defects, Mechanical and Thermal Behaviour, Metals and alloys, Semiconductors, Ceramics & Glasses, Mechanical properties of inorganic and composite materials.<br>Biomaterials. Basic characteristics of polymers, glass transition temperature, crystallinity, molecular weight and molecular weight distribution. Various types of Polymer Synthesis characterization; Chemical analysis of polymers; Conducting polymers and their applications in optoelectronics and sensors |
| 4 | **Texts/References** | 1. Introduction to Materials Science for Engineers; 8th Edition James F. Shackelford 696 pages; Pearson (April 12, 2014)<br>2. Materials Science and Engineering: An Introduction; 9th Edition William D. Callister Jr. and David G. Rethwisch 984 pages; Wiley (December 4, 2013)<br>3. M. Campbell, Introduction to Synthetic Polymers, 2nd Ed, Oxford University Press, New York (2000)<br>4. Principles of polymerization: G. Odian, 4th Edition, John Wileyinterscience<br>5. Conducting polymers, fundamentals and applications: A practical approach, Prasanna Chandrasekhar, Springer Science+Business media |

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| 1 | **Title of the course** (L-T-P-C) | **Fundamentals of biophysical chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Structure of water, hydrophilic and hydrophobic interactions, Structure and conformations of proteins and nucleic acids, physical techniques for biological structure elucidation, thermodynamics and kinetics of ligand interactions and protein folding, Conformational transitions, Equilibrium across membranes, biophysical techniques |
| 4 | **Texts/References** | 1. R. B. Gregory, ed., Protein-Solvent Interactions, Marcel Dekker,Inc., 1995.<br>2. B.T. Nall and K. A. Dill, ed., Conformations and Forces in Protein Folding, American Association for the Advancement of Science, 1991.<br>3. J. Wyman and S. J. Gill, Binding and Linkage: Functional Chemistry of Biological Macromolecules, University Sciences Books, 1990.<br>4. C. R. Cantor and P. R. Schimmel, Biophysical Chemistry, Part III, W.H.Freeman and Co., 1980. |

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| 1 | **Title of the course** (L-T-P-C) | **Green and sustainable Chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Introduction and metrics of green chemistry, Principles of green chemistry, Designing a sustainable synthesis, Bioremediation, Use of benign solvents in synthesis, Applications of green chemistry in real world, Renewable feedstock, Recycling of materials and chemicals, Toxic chemicals in environment, Green materials synthesis, New Green and sustainable synthetic methods, Society reliant chemicals, Bio catalysis, Green analytical methods, Alternate energy sources, Challenges and Future trends in Green chemistry. |
| 4 | **Texts/References** | 1. Anne E. Marteel-Parrish and Martin A. Abraham, Gre Chemistry and Engineering: A pathway to sustainabilit Wiley, 2014.<br>2. Manahan, S. E. Environmental Chemistry, Eighth Editio CRC Press, 2005.<br>3. Sankar, D; Nayim, S. A textbook of Green Chemistr 2021.<br>4. Anastas, P.T. & Warner, J.K.: Green Chemistry - Theo and Practical, Oxford University Press, 1998.<br>5. Lancaster, M. Green Chemistry: An Introductory Tex Third Edition; RSC Publishing, 2016.<br>6. Matlack, A.S. Introduction to Green Chemistry, Marc Dekker, 2001.<br>7. Ryan, M.A. & Tinnesand, M. Introduction to Gre Chemistry, American Chemical Society, Washingto 2002. |

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| 1 | **Title of the course** (L-T-P-C) | **Analytical Chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Statistics for analytical experimentation: Probability, Regression analysis, Accuracy and propagation of errors, Data analysis and signal enhancement. Covariance and correlation coefficient.<br><br>Advanced chromatographic techniques: Theory of separation methods: HPLC, GC, GC/MS, LC/MS, GPC, and applications<br><br>Electroanalytical techniques: Applications to chemical & biological systems: Potentiometry, Electrogravimetry, Voltammetry, Chronoamperometry, ion-selective electrodes. and Thermoanalytical methods. Quantitative applications of Potentiometry and Voltammetry: Electrochemical sensors<br><br>Spectrometric and Spectroscopic methods: Acid-base equilibria, Methodology in spectrochemical analysis, Spectrophotometry and binding assays. Introduction to electromagnetic radiation, Optical components of a spectrometer, Atomic absorption and emission spectroscopy, Principles and applications of Fluorimetry, Luminescence, Raman Spectroscopy and Dynamic lightscattering. Introduction to spectroscopy in time domain, Time- correlated single photon counting. Physical methods of characterization:<br>Surface Techniques: Principles of Electron<br>spectroscopy for chemical analysis, Scanning Probe Microscopy |
| 4 | **Texts/References** | 1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition, Brooks/Cole Cengage Learning, Belmont, CA, 2007<br>2. H. H. Willard, L. L. Merrln, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, 7th Edition, Belmont., 1989 |

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| 1 | **Title of the course** (L-T-P-C) | **Analytical Chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | 1. F. Rousseac and A. Roessac, Chemical Analysis: Modern Instrumentation Methods and Analysis, 4th Edition, John Wiley & Sons, Ltd., 2000<br>2. J. Wang, Analytical Electrochemistry, 3rd Edition, Wiley – VCH, 2006<br>3. P.T. Kissinger and W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Marcel Dekker Inc., 1996<br>4. B. Voigtlaender, Scanning Probe Microscopy: Atomic Force Microscopy and Scanning Tunneling Microscopy:, Springer - Verlag, Berlin 2015. |
| 4 | **Texts/References** | --- |

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| 1 | **Title of the course** (L-T-P-C) | **Principles of Biological Chemistry**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Structure and function of biomolecules, Biological membranes. Membrane channels and pumps, Signal transduction, Enzymes: classification, kinetics, mechanisms, regulation, and applications, Central Dogma of life, DNA Replication and Repair, Translation, Genetic code, Genome and proteome, RNA chemistry, Recombinant DNA Technology, Primary Metabolism: Glycolysis, Citric acid Cycle, Gluconeogenesis, Oxidative phosphorylation, Pentose phosphate pathway, ß-oxidation, Amino acid transamination and urea cycle, Biosynthesis and secondary metabolism, Bioinformatics |
| 4 | **Texts/References** | 1. Nelson DL and Cox MM; Lehninger principles of Biochemistry, 8th edition, WH Freeman and company, 2021<br>2. Berg JM, Tymoczko JL and Stryer L; Biochemistry, 9th edition, WH Freeman and company, 2019<br>3. Voet D and Voet JG; Biochemistry, Fourth edition, John Wiley and Sons, 2011 |

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| 1 | **Title of the course** (L-T-P-C) | **Computational Chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Potential energy surfaces, Molecular mechanics force- fields, Fitting of force-fields, Electronic structure theory, Hartree-Fock method, Density Functional Theory, Multiscale Methods, Geometry optimization techniques, Normal mode analysis, Locating transition states, Nudged elastic band method, Dimer method Molecular dynamics simulations (Classical and Ab-initio), Molecular dynamics simulations in various ensembles, Modeling chemical reactions, Methods for computing free energy, Umbrella sampling, Metadynamics, Parallel tempering methods |
| 4 | **Texts/References** | 1. Donald A. McQuarrie, Quantum Chemistry, University Science Books, 2nd Edition 2008<br>2. Dominik Marx and Juerg Hutter, Ab-initio molecular dynamics: Basic theory and advanced methods, Cambridge University Press 2009<br>3. Mark E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford University Press 2010<br>4. Andrew R. Leach, Molecular modelling principles and applications, Pearson Education Limited, 2nd Edition 2001<br>5. Daan Frenkel and Berend Smit, Understanding molecular simulation From Algorithms to Applications, Academic Press, 2nd Edition 2002<br>6. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons. 2017 |

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| 1 | **Title of the course** (L-T-P-C) | **Asymmetric Synthesis and Catalysis: From Basics to Frontiers**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | ● Basics of asymmetric catalysis including energetics of reactions.<br>● Lewis acid, Lewis base, Brønsted acid and base catalysis, Phase-transfer catalysis.<br>● Resolution: kinetic, dynamic kinetic and parallel kinetic resolution; desymmetrization reactions.<br>● Mechanistic studies of asymmetric reactions: nonlinear effects, autocatalysis and autoinduction etc.<br>● Bifunctional, dual and multifunctional catalyst systems.<br>● Modern aspects of asymmetric catalysis: counterion- directed catalysis, cooperative, dual and merged, relay catalysis, asymmetric photocatalysis etc.<br>● Application of asymmetric catalysis in the total synthesis of natural products in current literature. |
| 4 | **Texts/References** | 1. Walsh, P. J., Kozlowski, M. C., Fundamentals of Asymmetric Catalysis, 1st Edition, University Science Books, California, 2008.<br>2. Carreira, E. M., Kvaerno, L., Classics in Stereoselective Synthesis, 1st Edition, Wiley-VCH, Weinheim, 2009.<br>3. Corey, E. J., Kürti, L., Enantioselective ChemicalSynthesis, 1st Edition, Direct Book Publishing, Dallas,2010. |

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| 1 | **Title of the course** (L-T-P-C) | **Chemistry of carbohydrates** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Introduction; structure, configuration, and conformation; Stereochemistry, and reaction of monosaccharides, deoxy and amino sugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gan- gliosides and other glycosides. Chemistry of vitamins A,B,C and E. Common protecting groups and protecting group strategies; glycosylation: general concepts, various methods of glycoside bond formation; strategies in oligosaccharide synthesis: carbohydrate-based drug discovery, Carbohydrate biosynthesis and degradation |
| 4 | **Texts/References** | 1. B. G. Davis & A.J. Farbanks, Carbohydrate Chemistry, 1st Edition, Oxford University Press, 2002<br>2. R. V. Stick., Carbohydrates: The Essential Molecules of Life, 2nd Edition, Academic Press, 2009.<br>3. D. E. Levy and P. Fugedi, The Organic Chemistry of Sugars, CRC Press, 2nd ed., 2006. |

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| 1 | **Title of the course** (L-T-P-C) | **Mathematics for Chemists** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Linear algebra: scalar and vector, linear equations, matrix and determinant, diagonalization of matrices, eigenvalue and eigenvectors.<br>Differential Equations: Ordinary differential equations, general solutions, 1st and 2nd order differential equations, Fourier Transforms, statistics, mean, standard deviation, error estimates, Taylor series.<br>Numerical methods: Numerical differentiation and integration, interpolation, matrix eigenvalues, Numerical solution of differential equations. |
| 4 | **Texts/References** | 1. George Arfken, Hans Weber and Harris, Mathematical Methods for Physicists, Elsevier, 7th Edition, 2012<br>2. Donald A. McQuarrie, Mathematical Methods for Scientists and Engineers, University Science Books, 2003<br>3. Erwin Kreyszig, Advanced Engineering Mathematics International Student Version, J. Wiley and Sons, 10th Edition- 2023 |

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| 1 | **Title of the course** (L-T-P-C) | **Radioactivity and Nuclear chemistry** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Radioactivity, Radioactive decay, Nuclear structure and stability, Nuclear models, Nuclear decay, Interaction of radiations with matter, Radiation detectors, Nuclear reactions, Nuclear Fission and fission, Production of radioisotopes, Radiochemical methods, Nuclear analytical techniques, Nuclear probes, Applications of radioisotopes, Actinide concept, Chemistry of actinides, Spectroscopy of actinides, Solution chemistry of actinides, Complexation and separation chemistry of actinides, Trans actinides and Actinide environmental chemistry |
| 4 | **Texts/References** | 1.D.D. Sood, A.V.R. Reddy and N. Ramamoorthy; Fundamentals of Radiochemistry, IANCAS Publication, 2007<br>2.J.J. Katz, L.R. Morss, J.Fuger, and N.M. Edelstein; Chemistry of Actinide and Transactinide Elements, 3rd edition, Springer, Berlin Volume 1-5, 2006.<br>3.J.V. Katz; Nuclear and Radiochemistry: Fundamentals and Applications, WILEY-VCH GmbH, 2021 |

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| 1 | **Title of the course** (L-T-P-C) | **Electrochemistry and its Applications** **3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Ionics: Electrochemistry of solutions, Ion-solvent interactions, ion- ion interactions, ionic migration and diffusion. Phenomenological description of transport processes. Thermodynamics of galvanic cells: Equilibrium electrode potentials, IUPAC convention for electrode potentials, Thermodynamics of electrochemical cells and applications.<br>Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds, Electrocapillary and differential capacitance measurements; Influence of double layer on charge transfer processes.<br><br>Reference electrodes: polarizable and non-polarizable systems. Types of reference and working electrodes<br><br>Electrode kinetics: Current-potential relationship (derivation of Butler-Volmer and Tafel equations). Adsorption isotherms for intermediates formed by charge transfer (Langmuir adsorption and its limitations, relating bulk concentration to surface coverage), Types of overpotentials: origin and minimization; mechanism of electro-organic reactions; hydrogen evolution and oxygen reduction reactions. transition state theory and Gibbs free energy of activation, bulk electrolysis; Quadratic activation –driving force relation –Marcus theory ; outer and inner sphere reactions. Underpotential deposition of metals and applications in catalysis.<br>Corrosion: Different types of corrosion; influence of environment; Evans diagram, Pourbaix diagram; corrosion rate measurements; Stern Geary equation; mixed potential theory and prevention of corrosion |
| 4 | **Texts/References** | 1. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH, 2011<br>2. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley, 2001<br>3. L. I. Antrapov, Theoretical Electrochemistry, Intl Law & Taxation Publications, 2001.<br>4. J. J. O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 1, Springer, 2018.<br>5. P. Atkins and J. de Paula, Atkins' Physical Chemistry, 8th edition, Oxford University Press, 2022.<br>6. Fundamentals of Electrochemistry, 2nd ed, Bagotsky, V.S., Hoboken: Wiley-Interscience 2006. |

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| 1 | **Title of the course** (L-T-P-C) | **X-ray crystallography and applications**<br>**3-0-0-6** |
| 2 | **Pre-requisite courses(s)** | -- |
| 3 | **Course content** | Geometric Crystallography: Lattices, point groups and space groups, and lattice transformations. Processing raw diffraction data: Diffraction data statistics, temperature & scale factor determination, density measurements and calculations, molecular formula and molecular weight determination, space group determination. Structure determination: Heavy atom Patterson methods, direct methods, isomorphous replacement methods. Refinement: isotropic and anisotropic, atom fix and hydrogen fixations, riding models. Interpretation of the structural data: metric parameters, dihedral data, H-bond data, preparation of structure plots including ORTEP and lattice structures including packing diagrams. Practical exercise of structure determination using standard packages: one centro- symmetric and one non-centrosymmetric crystal data. |
| 4 | **Texts/References** | 1. X-ray structure determination: A practical guide, G.H. Stout and L.H. Jensen, Wiley, Second Edition 1989.<br>2. Foundations of Crystallography with Computer Applications, M.M. Julian, CRC Press, 2nd Ed. 2014.<br>3. An Introduction to X-ray Crystallography, M.M. Woolfson, Cambridge University Press; 2nd ed, 1997. |