SYLLABI FOR CORE CHEMISTRY COURSES

BS@CHEMISTRY, IIT MADRAS

SEMESTER I

Course title	**Basic Concepts of Inorganic Chemistry**									Course No	**CY 1011**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3	1			6	10			3	1	0	4
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to apply basic concepts of inorganic chemistry to identify the structure, bonding, and reactivity of inorganic compounds

Course Contents:

Atomic Structure and Periodicity- Elementary aspects of the quantum mechanical model of hydrogen-like atoms, quantum numbers, radial and angular wave functions, symmetry and energies of orbitals, Pauli exclusion principle, Aufbau principle, Hund's rule.
General trends in properties of *s*, *p*, *d*, and *f*-block elements: atomic radii, ionic radii, shielding, ionization energy, electron affinity, and electronegativity.

Chemical Bonding- Types of bonds, ionic bond, size effects, radius ratio, packing and crystal lattice, lattice energy, Born-Haber cycle, Fajan's rule, hydrogen bond.
Covalent bond, molecular orbital theory, symmetry and overlap, bonding in homo- and hetero-nuclear diatomic molecules, triatomic molecules/ions, van der Waal's radii, Walsh diagram, Lewis structures, resonance, formal charge, hybridization, VSEPR theory, Bent's Rule.

Molecular Symmetry- Symmetry elements, symmetry operations, determination of point groups of inorganic/organic molecular species, and coordination complexes.

Acid Base Chemistry- Lewis acid-base model, Brønsted-Lowry definition, Lux-Flood definition, acid-base strength, pH scale, solvation effects and related anomalies, HSAB concept, applications in real life.

Aqueous and Nonaqueous Solvents- Protic and aprotic solvents, molten salts, solutions of metals in ammonia, electrode potentials and electromotive forces.

Text Books:

1. J. E. Huheey, E. A. Keiter, and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity,* 4th Edition, Pearson, 1993.

2. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, 7th Edition, Oxford University Press, 2018.

3. C. E. Housecroft, and A. G. Sharpe, *Inorganic Chemistry*, 5th Edition, Pearson, 2018.

4. S. Zumdahl, S. Zumdahl, and D. J. DeCoste, *Chemistry*, 11th Edition, Cengage, 2023.

Course title	**Mathematics-I**									Course No	**CY 1013**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3	1			6	10			3	1	0	4
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to solve conceptual problems in chemistry using principles of Calculus and Linear algebra

Course Contents:

Limits, Continuity, And Differentiation: Introduction, The Mean-Value Theorem and L'hospital's Rule, Logarithmic Differentiation, Derivatives of Functions in Parametric Forms, Higher Order Derivatives, The Extrema of a Function and its Critical Points, Taylor's Series, Binomial expansion, Functions of Several Variables, Chain Rule, Exact and Inexact Differentials.

Integrals: Integration as an Inverse Process of Differentiation, Methods of Integration: Integration by Substitution, By Partial Fractions, By Parts, Definite Integral, Fundamental Theorem of Calculus, Area Under Simple Curves, The Gaussian and its Moments.

Differential Equations: Definition, Order And Degree, General And Particular Solutions of a Differential Equation, Methods of Solving First Order Differential Equations, Separation of Variables, Integration Factor for Linear First Order Differential Equations, Homogeneous and Nonhomogeneous Linear Differential Equations with Constant Coefficients, Examples of Classical Harmonic Oscillator and Damped Oscillator.

Vectors: Vector Addition, Scalar Product, Vector Product, Triple Products, Differentiation of Vectors, Scalar and Vector Fields, Gradient, Divergence, Curl, Laplacian, Line and Surface Integrals, Vector Space, Subspaces, Linear Dependence and Independence of Vectors, Linear Span, Basis, and Dimension of a Vector Space, Gram-Schmidt Orthogonalization.

Text Books:

1. George Turrell, Mathematics for Chemistry and Physics, Academic Press, 2002.

2. D. A. McQuarrie, Mathematics for Physical Chemistry: Opening Doors, University Science Books, 2008.

3. Robert G. Mortimer, Mathematics for Physical Chemistry, Academic Press, 4th Edition, 2013.

4. D. A. McQuarrie, Mathematical methods for scientists and engineers, University Science Books, 2003.

Reference Books:

1. M. L. Boas, Mathematical methods for the physical sciences, Kaye Pace, 3rd Ed., 2006.

2. G. Arfken, H. Weber, and F. Harris, Mathematical methods for physicists, Academic Press, 7th Ed., 2012.

3. P. W. Atkins, J. De Paula, & J. Keeler, Atkins' physical chemistry. Oxford University Press, 2023.

SEMESTER II

<table>
<tr><td>Course title</td><td colspan="9">Basic Organic Chemistry</td><td>Course No</td><td colspan="4">CY 1020</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

Learners should be able to comprehend the structure, bonding and conformation of organic molecules and analyze their reactivity.

Course Contents:

Structure, bonding and IUPAC nomenclature of organic molecules; electron delocalization; resonance, inductive, hyperconjugation, and steric effects; tautomerism; dipole moment; structure and stability of carbocation, carbanion, and carbon radical; acidity, basicity, pK_a and structural effects.

Basic stereochemistry, geometrical isomerism, *cis* & *trans*, and *E* & *Z*; optical isomerism, point and axial chirality;
D & L, *R* & *S*, and *P* & *M* nomenclature; *erythro* and *threo*; configuration vs conformation, conformation of acyclic and cyclic compounds; nomenclature of bicyclic systems.

Reactions and mechanisms: arrow-pushing formalism, addition (*syn*/*anti*), substitution (S_N1, S_N2, S_N2' and S_Ni), elimination (E1, E2, E1cB) reactions (*syn*/*anti*), conformation and reactivity.

Syntheses and reactions of alcohols, ethers, epoxides, amines, thiols, and thioethers.

Introduction to aromaticity, Hückel rule (aromatic, anti-aromatic and non-aromatic), Möbius aromaticity; aromatic electrophilic and nucleophilic substitution reactions, including mechanisms; application of Sanger's method and aryl diazonium salts (Sandmeyer reaction).

Textbooks:

1. J. E. McMurry, Organic Chemistry, CENGAGE learning, 10th Ed., 2023.
2. P. Y. Bruice, Organic Chemistry, Pearson, 8th Ed., 2020.
3. R. T. Morrison, R. N. Boyd, and S. K. Bhattacharjee, Organic Chemistry, Pearson, 7th Ed., 2012 .
4. T. W. G. Solomons, C. B. Fryhle, and S. A. Snyder, Solomon's Organic Chemistry, WILEY, Global Edition, 2024.

Course title	Mathematics-II									Course No	CY 1022			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3	1			6	10			3	1	0	4
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to solve conceptual problems in chemistry using principles of Linear Algebra and Calculus

Course Contents:

Complex Numbers: Introduction, Algebra of Complex Numbers, The Modulus and the Conjugate of a Complex Number, Argand Plane, Functions of a complex variable, Euler's formula and Polar Representation, Roots of a complex number, Trigonometry and hyperbolic functions. (Cauchy's) Residue theorem.

Sequence & Series: Convergence of a Sequence, Convergence and Divergence of Infinite Series, Tests of Convergence, Power series and Maclaurin Series.

Series Solutions of Differential Equations: Power Series method, Ordinary Points and Singular Points of a Differential Equation, Series Solutions near an Ordinary Point: Legendre's Equation, Solutions Near Regular Singular Point.

Functions defined as Integrals: The Gamma Function, The Error Function, The Dirac Delta Function.

Laplace and Fourier Transforms: Laplace transforms, Inverse Laplace transforms, Convolution theorem, Applications to Ordinary differential equations. Fourier transforms, Inverse Fourier transform, Fourier sine and cosine transforms and their inversion, Properties of Fourier transforms, Convolution, Applications to partial differential equations.

Curvilinear Coordinates: Plane polar coordinates, vectors in plane polar coordinates, cylindrical coordinates, spherical coordinates, Curvilinear coordinates.

Operators, Matrices, And Determinants: Introduction, The Algebra of Operators, Commutators, Hermitian Operators, Operations on Matrices, Transpose of a Matrix, Diagonal, Symmetric, Skew Symmetric, Orthogonal, and Unitary Matrices, Determinants, Area of a Triangle, Minors and Cofactors, Adjoint and Inverse of a Matrix, Solution of System of Linear Equations using Inverse of a Matrix, Gauss-Jordan Elimination, Cramer's rule, Eigenvalue Problem, Matrix Eigenvalues and Eigenvectors, Jacobian, Trace of a Matrix and its Properties, Linear Transformations.

Text Books:

1. George Turrell, Mathematics for Chemistry and Physics, Academic Press, 2002.

2. D. A. McQuarrie, Mathematics for Physical Chemistry: Opening Doors, University Science Books, 2008.

3. Robert G. Mortimer (2013). Mathematics for Physical Chemistry, 4th Edition, Academic Press.

4. D. A. McQuarrie, Mathematical methods for scientists and engineers, University Science Books, 2003.

Reference Books:

1. M. L. Boas, Mathematical methods for the physical sciences, Kaye Pace, 3rd Ed., 2006.

2. G. Arfken, H. Weber, and F. Harris, Mathematical methods for physicists, Academic Press, 7th Ed., 2012.

3. P. W. Atkins, J. De Paula, & J. Keeler, Atkins' physical chemistry. Oxford University Press, 2023.

<table>
<tr><td>Course title</td><td colspan="9">Biochemistry</td><td>Course No</td><td colspan="4">CY1024</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The learners will be able to:
Describe the structure and properties of major biomolecules (proteins, nucleic acids, lipids and carbohydrates)
Explain the principles of enzymatic catalysis and regulation
Explain metabolic pathways and their role in cellular function

Course Contents:

Structure and function of nucleic acids: Nucleotides and nucleic acids; DNA- Single and Double-stranded DNA; RNA; DNA replication, Transcription, and translation; Genetic code, DNA sequencing (Sanger Method)

Structure and function of Proteins: Amino acids: structure, properties, and classification; Protein structure and folding, Protein dynamics and proteins in action (associated functions and diseases).

Enzyme structure, catalytic mechanisms and regulation; factors affecting enzyme activity; Temperature, pH, substrate concentration, and inhibitors; role of cofactors in enzymatic activity

Structure and function of carbohydrates: Monosaccharides, Oligosaccharides, and Polysaccharides; Polysaccharides in cell wall

Types of lipids; Structure and function of biological membranes

Text Books:

1. Donald Voet, Judith G. Voet, Biochemistry, Wiley Publication, 4th Edition, 2010

2. Albert Lehninger, David L. Nelson, Michael M. Cox, Lehninger Principles of Biochemistry, Worth Publishers, 5th Edition, 2008

3. Jeremy M. Berg, John L. Tymoczko, Lubert Stryer, Biochemistry, W. H. Freeman Publication, 6th Edition, 2006

<table>
<tr><td>Course title</td><td colspan="9">Organic Laboratory I</td><td>Course No</td><td colspan="4">CY1026</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes:

Learners should be able to acquire hands-on practice and skills involved in the laboratory techniques of synthetic organic chemistry. Use the skills for synthesis, purification and analysis of organic compounds

Course Contents:

The lab course aims at imparting experience on techniques used for separation and purification of organic compounds at the basic/introductory level. The experience gained through the techniques will be applied to the experiments that will be related to the theory taught in the classroom lectures. The following are the illustrative set of experiments.

1. Soxhlet extraction of curcumin from turmeric power
2. Fractional distillation of toluene and *p*-xylene mixture
3. Separation of binary/ternary mixtures and preparation of derivatives
4. Friedel–Crafts acylation of ferrocene to acetylferrocene and diacetylferrocene
5. Preparation of 2,4-dinitrophenylthiocyanate
6. Addition of bromine to *cis*-/*trans*-cinnamic acid
7. Determining the optical purity of an unknown sample (tartaric acid, menthol, and camphor)
8. Synthesis of phthalic anhydride from phthalic acid via sublimation, and preparation of fluorescein
9. Preparation of aspirin/paracetamol/phenytoin
10. Preparation of dicinnamalacetone
11. Reduction of *m*-dinitrobenzene to *m*-nitroaniline

Textbooks:

1. Vogel's Textbook of Practical Organic Chemistry, John Wiley and Sons, 5th Ed., 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, and R. G. Engel, Microscale Approach to Organic Laboratory Techniques, CENGAGE Learning, 5th Ed., 2013.
3. C. A. M. Afonso, N. R. Candeias, D. P. Simão, and A. F. Trindade, J. A. S. Coelho, B. Tan, and R. Franzén, Comprehensive Organic Chemistry Experiments for the Laboratory Classroom, The Royal Society of Chemistry, 2017

SEMESTER III

<table>
<tr><td>Course title</td><td colspan="9">Coordination and Bioinorganic Chemistry of Transition Metals</td><td>Course No</td><td colspan="4">CY 2011</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to apply various bonding theories to explain the properties of transition metal complexes

Course Contents:

The structure, bonding and properties of coordination compounds - basic concepts, recapitulation of periodic trends of metal ions, ligands and types, coordination numbers, geometries, nomenclature, isomerism and types, Bailar twist and Ray-Dutt mechanisms, stability constants and chelate effect.

Bonding theories - valence bond theory, its basic principles and limitations; crystal field theory – its applications and limitations applicable to octahedral, tetrahedral, square planar geometries, other coordination geometries, spectrochemical series and ligand field strength; crystal field stabilization energy (CFSE), pairing energy, and its implications on the electronic, magnetic (spin only) and colors of complexes; selection rules.

Angular overlap model (octahedral, tetrahedral and square planar geometries)

Bioinorganic Chemistry - Essential and trace transition elements in biology, the role of metal ions in different biological processes, the structure and functions of selected metalloproteins and metalloenzymes, the structure, electronic and magnetic properties of oxy (including oxygen binding behaviour) forms of hemoglobin, myoglobin, hemerythrin, and hemocyanin.

Text Books:

1. J. E. Huheey, E. A. Keiter, and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity,* Pearson, 4th Edition, 1993.

2. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 7th Edition, 2018.

3. C. E. Housecroft, and A. G. Sharpe, *Inorganic Chemistry*, Pearson, 5th Edition, 2018.

4. G. L. Miessler, P. J. Fischer, and D. A. Tarr, *Inorganic Chemistry*, Pearson Education Limited, 5th Edition, 2013

5. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry,* University Science Books, 1994.

<table>
<tr><td>Course title</td><td colspan="9">Organic Chemistry of Multiple Bonds</td><td>Course No</td><td colspan="4">CY 2013</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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Course Learning Outcomes:

Learners should be able to comprehend the synthesis and reactions of alkenes, alkynes and carbonyl compounds. Analyze and predict their reactivity through reactions and mechanisms.

Course Contents:

Formation of alkenes: from alcohol, carbonyl and alkyne; elimination and fragmentation reactions. Reaction of alkenes: halogenation, hydrohalogenation, hydration, hydrogenation, ozonolysis, dihydroxylation, aminohydroxylation, halolactonization, oxymercuration-demercuration, hydroboration, epoxidation, aziridination.

Formation of alkynes by elimination reactions. Reactions of alkynes: hydrogenation, reduction by alkali metal, DIBAL-H and $LiAlH_4$, hydrohalogenation, hydration, hydroboration; substitution reactions of terminal alkynes.

Reactions of carbonyls: with water, alcohols, thiols, amines, HCN, hydrides ($NaBH_4$, $LiAlH_4$); MPV reduction, and Cannizzaro reaction. Reactions with solvated electrons (pinacols and acyloin condensation); reaction with organolithium, organomagnesium (Grignard reagent), and Reformatsky reaction; extension to conjugate addition; aldol reaction, Henry reaction, Perkin reaction, Stobbe reaction, Knoevenagel and Claisen ester condensation, Dieckmann reaction, Darzens reaction, benzilic acid rearrangement, and Seyferth–Gilbert homologation. Reaction with ammonia, NH_2OH, and $PhNHNH_2$; Beckmann rearrangement; applications in the synthesis of aromatic heterocycles like furan, thiophene, pyridine, indole, quinoline and isoquinoline.

Reversal of polarity (umpolung): Benzoin condensation and extension to Stetter reaction.

Stereoselective addition to carbonyls: Cram, Felkin-Anh and Cram-chelate models.

Textbooks:

1. R. T. Morrison, R. N. Boyd, and S. K. Bhattacharjee, Organic Chemistry, Pearson, 7th Ed., 2012.
2. T. W. G. Solomons, C. B. Fryhle, and S. A. Snyder, Solomon's Organic Chemistry, Wiley, Global Edition, 2024.
3. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, Pearson, 6th Ed., 2009.
4. J. L. Clayden, N. Greeves, and S. Warren, Organic Chemistry, Oxford, 2nd Ed., 2012.

<table>
<tr><td>Course title</td><td colspan="9">Thermodynamics</td><td>Course No</td><td colspan="4">CY2015</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes: The learners will be able to Apply and Analyze the concepts in equilibrium Thermodynamics

Chemical Thermodynamics:

Concepts of temperature (zeroth law), Exact and Inexact differentials, First law of thermodynamics, Reversible and irreversible processes, concept of entropy (II law of TD), Clausius inequality, entropy change accompanying specific processes, Free energy and criteria for spontaneity. Fundamental equations of Thermodynamics, Gibbs Helmholtz equation, Maxwell's relations, Chemical potential, partial molar properties, Gibbs-Duhem equation, van't Hoff equation

Chemical and Phase equilibria:

Chemical equilibrium, interrelations between Kp, Kc and Kx, the effect of temperature and pressure on equilibrium constant, Le Chatelier's principle, Raoult's law: Ideal and non-ideal solutions, Gibbs phase rule, Clausius-Clapeyron equation, one component phase diagram of CO_2 and water. Ehrenfest classification of phase transitions. Two-component phase diagrams- vapour pressure diagrams, temperature- composition diagrams, Liquid-liquid solutions, liquid-solid solutions, Activity and activity coefficients, colligative properties

Concepts on Thermo and Electro Chemistry:

Activity of electrolytes, Ionic mobility and conductivity, Kohlrausch law, Debye-Hückel limiting law. Debye-Hückel-Onsager equation. Standard electrode potentials and electrochemical cells. EMF and Nernst Equation, relationship between Electrode potential and thermodynamic quantities, Basic process at electrode and electrode-electrolyte interface

Text Books:

1. Silbey, Alberty and Bawandi, Physical Chemistry, John Wiley and Sons, 4th Edn, 2004.
2. P. W. Atkins and J. de Paula, Physical Chemistry, Oxford University Press, 10th Eds., 2014.
3. D. A. McQuarrie and J. Simon, Physical Chemistry, A molecular approach, University Science Books, California, 1997.

<table>
<tr><td>Course title</td><td colspan="9">Quantum Mechanics and Spectroscopy</td><td>Course No</td><td colspan="4">CY2017</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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Course Learning Outcomes: The students will be able to learn the basic principles of quantum mechanics and spectroscopy.

Course contents:
Black-body radiation, photoelectric and Compton effects, line spectra of atoms, Bohr model of the hydrogen atom, Young's double slit experiment, and Wave-particle duality.

Time-dependent and time-independent Schrödinger equations (TISE), Hamiltonian, Solve TISE for a particle in a 1D box as an example and its applications, Energy quantization, Wave function and probabilities, observables and measurements, expectation value, stationary states.

Operators, eigenvalues and eigenfunctions, commutation relations, Heisenberg uncertainty principle.

A free particle, Particle in a finite square well, tunneling, particle in a two- and three-dimensional box, the origin of degeneracy.

Harmonic oscillator, power series solution.

Angular momentum (orbital & spin), commutation relations, the solution to the particle on a ring, rigid rotor problem, matrix representation, unitary transformation, and change of basis.

Rotational Spectroscopy: Rigid rotor energy level, pure rotational spectra of diatomic rigid rotors - rotational transitions, intensities & selection rules, calculation of molecular parameters (bond lengths, bond angles, and dipole moments).

Vibrational Spectroscopy (IR and Raman): Harmonic and anharmonic oscillators, vibration of diatomic molecules, vibrational-rotational couplings in diatomic molecules, application of IR spectroscopy in structure elucidation. Raman scattering, vibrational Raman lines & selection rules, vibrational Raman spectra of diatomic molecules, and some applications.

Text Books:

1. I. Levine, Quantum Chemistry, Pearson Press, 6th ed., 2009.
2. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2nd ed, 2008.
3. N. Zettili, Quantum Mechanics: Concepts and Applications, John Wiley & Sons, 2009.
4. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994,
5. P. W. Atkins, Molecular Quantum Mechanics, 4^{th} ed, Oxford University Press, 2005.
6. C. N. Banwell, Fundamentals of molecular spectroscopy, 4^{th} ed, 2017.

<table>
<tr><td>Course title</td><td colspan="9">Inorganic Chemistry Laboratory I</td><td>Course No</td><td colspan="4">CY2019</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
<tr><td></td><td colspan="2"></td><td colspan="7"></td><td colspan="5"></td></tr>
</table>

Course Learning Outcomes: The students will be able to conduct quantitative analysis and prepare inorganic complexes

Course Contents:

1. Qualitative semi-microanalysis of inorganic salts containing 4 cations and 4 anions. (3 lab classes)
2. Gravimetric estimation of nickel(II) by dimethylglyoxime
3. Estimation of copper in brass by colorimetry
4. Determination of the percentage of iron in haematite ore
5. Preparation of copper(I) thiourea complex and estimation of copper
6. Determination of calcium in milk powder by EDTA complexometry
7. Preparation of *cis*- and *trans*-$[Co(en)_2Cl_2]Cl$ complexes and analysis by UV-Visible and IR spectroscopy
8. Preparation of $Hg[Co(\underline{N}CS)_4]$ and determination of magnetic susceptibility of the complex

Text Books:

1. Jeffery, Bassett, Mendham, Denney, *Textbook of Quantitative Chemical Analysis,* 5^{th} Ed., 1989.

2. A. J. Elias, *General Chemistry Experiments,* Universities Press, 2007.

SEMESTER IV

Course title	**Organometallic Chemistry of Transition Metals**									Course No	**CY2020**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to identify the structure, bonding, and reactivity in organometallic compounds

Course Contents:

Introduction to organometallic compounds: ligand types (σ,π-donor and π-acceptor), hapticity, 18 and 16 electron rules, counting of electrons and determining metal-metal bonds, validation and verification of the rule with different transition metal carbonyls and related complexes.

Metal Carbonyls: Molecular orbital diagram of CO; Structure, bonding, and properties of metal carbonyls, Synthesis and reactions of metal carbonyls, metal carbonyl hydrides and metal carbonylates, Infrared spectroscopy of metal carbonyls, alkenes and derivatives.

Synthesis, structure, properties of metallocenes, organometallic compounds containing nitrosyls, alkyls, alkenes, allyl, dienyl, trienyl, alkynes, cyclopentadienyl and arenes. Cyclopentadienyl containing metal carbonyls, nitrosyls and hydrides complexes.

Organometallic Complexes with Metal-Carbon Double Bonds: Synthesis, bonding and reactivities of Fischer and Schrock carbene complexes. Neutral spectator ligands: phosphines and N-heterocyclic carbenes.

Metal-Metal Bonds and Clusters: Di-, tri-, tetra- and higher-nuclearity clusters, electron counting rules: polyhedral skeletal electron pair theory/Mingo's rules, Wades Rules, The isolobal analogy.

Types of organometallic reactions: Substitution, oxidative addition, reductive elimination, insertion and de-insertion reactions.

Organometallic catalysis of industrial relevance: Hydrogenation, hydroformylation, Monsanto and related processes, Wacker process, Ziegler-Natta polymerization.

Text Books:

1. J. E. Huheey, E. A. Keiter, and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity,* Pearson, 4th Edition, 1993.
2. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 7th Edition, 2018.
3. C. E. Housecroft, and A. G. Sharpe, *Inorganic Chemistry*, Pearson, 5th Edition, 2018.

5. G. L. Miessler, P. J. Fischer, and D. A. Tarr, *Inorganic Chemistry*, Pearson Education Limited, 5th Edition, 2013.

6. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry,* University Science Books, 1994.

<table>
<tr><td>Course title</td><td colspan="9">Reactive Intermediates in Organic Chemistry</td><td>Course No</td><td colspan="4">CY2022</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:
Learners should be able to comprehend and apply the knowledge of reactive intermediates in organic reactions.

Course Contents:

Carbanions: Chemistry of enolates and enamines, kinetic and thermodynamic enolates, alkylation and acylation of enolates, diastereoselective aldol reactions with lithium and boron enolates; Michael reactions with enolates and cuprates, phosphorus and sulfur ylides; Julia, Peterson and Zweifel olefinations, and Shapiro reaction.

Carbocation: Classical and non-classical carbocations, neighboring group participation, rearrangements including Wagner-Meerwein, Pinacol-pinacolone, and semi-pinacol rearrangement.

Carbon radicals: Generation and reactions, addition to alkenes & alkynes (inter and intramolecular), fragmentation and rearrangements. Name reactions involving radical intermediates; Barton deoxygenation, decarboxylation, and McMurry coupling. Radical reactions with SmI_2 and $Mn(OAc)_3$.
Baldwin's rules and modes of cyclization.

Carbenes: Structure and generation, addition and insertion reactions, rearrangement reactions of carbenes; Wolff rearrangement, and Arndt-Eistert homologation; generation and reactions of metal carbene (including ylides).

Nitrenes: Structure, generation and reactions, and related electron-deficient nitrogen intermediates; Curtius, Hoffmann, Schmidt, and Beckmann rearrangements.

Textbooks:

1. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, 5th Ed., 2007.
2. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, Springer, 5th Ed., 2007.
3. W. Carruthers, and I. Coldham, Modern Methods of Organic Synthesis, Cambridge, 4th Ed., 2004.
4. G. S. Zweifel, M. H. Nantz and P. Somfai, Modern Organic Synthesis – An Introduction, Wiley, 2nd Ed., 2017.

<table>
<tr><td>Course title</td><td colspan="9">Chemical Kinetics and Dynamics</td><td>Course No</td><td colspan="4">CY2024</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcome: The learners will be able to identify the basic principles in chemical kinetics and use them to find the mechanisms of chemical reactions

Course Contents:

Basics: Introductory chemical kinetics, types of reactions, steady state approximation, Arrhenius equation, activated complex theory

Reaction Rate Theories: Potential energy surfaces, transition state theory, Eyring equation, estimation of rate constants, Lindemann-Hinshelwood mechanism, Rice-Ramsperger-Kassel-Marcus (RRKM) theory for unimolecular reactions

Experimental Approach: Study of fast reactions by flow method, relaxation method, flash photolysis, pulsed radiolysis, dynamics of unimolecular reactions, laser, and molecular beam methods.

Kinetics at Surfaces: Physical and chemical adsorption, adsorption isotherms, Langmuir, Tempkin, and BET. Determination of surface area of adsorbate; temperature dependence of adsorption isotherms.

Kinetics in the excited state: Kinetics in the excited electronic states, Jablonski diagram, photophysical and photochemical processes, photoisomerization, excimers, exciplexes, sensitization, quantum yields, static and dynamic quenching, Stern-Volmer equation, resonance energy transfer, light-induced electron transfer, and Marcus theory

Electrode Kinetics: Metal/solution interface, electrochemical reaction rate dependency on overpotential-current density for single and multi-step process; influence of electrical double layer on rate constants

Enzyme Kinetics: Michaelis-Menten Kinetics, graphical methods to analyze enzyme kinetics

Text Books:

1. K. J. Laidler, Chemical Kinetics, Pearson, 3rd Ed., 2003
2. M. R. Wright, An Introduction to Chemical Kinetics, John Wiley, 2004
3. P. Atkins, J. de Paula and J. Keeler, Atkins' Physical Chemistry, Oxford University Press, 11th Ed., 2018.
4. N. J. Turrro, V. Ramamurthy and J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, Viva Student Edition, Viva, 2017
5. J. I. Steinfeld, J.S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 2nd Ed., 1999
6. W. J. Alberty, Electrode Kinetics, Clarendon Press, Oxford, 1975

<table>
<tr><td>Course title</td><td colspan="9">Solid State Chemistry</td><td>Course No</td><td colspan="4">CY2026</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcome: The learners will be able to explain various crystal structures, defects, and methods of thermal analysis; predict the crystal structure, type of bonding in solids, and properties

Course Contents:

Crystal Structure: Kinds of solids - crystalline, amorphous, and molecular solids; ionic crystals, metallic crystals, covalent network solids, close packing, crystal lattices, symmetry in crystals, space lattices and unit cells, one and two-dimensional lattices, crystal systems, Bravais lattices, crystallographic direction, lattice planes, Miller indices, interplanar spacings, crystallographic axes, α-Po, fcc, bcc and hcp metals and their packing efficiency, structure types of ionic solids: CsCl, NaCl, ZnS, CaF_2, CdI_2, TiO_2, spinel and inverse-spinel structure, AB_2O_4, perovskite ABO_3 ($CaTiO_3$), $YBa_2Cu_3O_7$, spinel and olivine, C_{60}, quasicrystals and 5-fold symmetry, ionic radii, cubic, octahedral, and tetrahedral holes, radius ratios rules; lattice energy, Born-Haber cycle

Crystal defects and non-stoichiometry in solids: perfect and imperfect crystals, point, line, defects; Intrinsic Defects - Frenkel and Schottky defects, vacancies; Extrinsic Defects - colour centers, interstitial defects, dislocations, non-stoichiometry in FeO.

Probing the structure of solids: X-ray crystallography, Generation of X-rays, diffraction of X-rays by crystals, Bragg's law, powder diffraction and indexing XRD patterns (for the simple systems NaCl), interplanar spacing for a cubic system, systematic absences, Structure factor, determination of lattice type, unit cell parameter and density for α-Po, fcc, bcc and hcp metals, NaCl, ZnS, diamond.

Bonding in solids and electronic properties: Band theory of solids – metals, insulators and semiconductors (extrinsic and intrinsic), doping, ionic conductivity, Hall effect; thermoelectric effects (Thomson, Peltier and Seebeck); insulators – dielectric, ferroelectric, pyroelectric and piezoelectric properties, multiferroics.
Superconductivity: Basics, discovery and high Tc materials, e.g. $YBa_2Cu_3O_7$.

Magnetic properties: Basic properties of magnetic materials; select magnetic materials such as spinels, garnets and perovskites, hexaferrites and lanthanide-transition metal compounds; magnetoresistance.

Thermal analysis of solids: Thermogravimetric analysis (TGA) and Differential Thermal Aanalysis (DTA)

Text Books:

1. Anthony R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984. (Reprint Edition)
2. Lesley Smart and Elaine Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012.
3. H.V. Keer, Principles of the Solid State, New Age International, 2nd Edition, 2017.
4. Weller, T. Overton, J. Rourke, and F. Armstrong, Inorganic Chemistry, Oxford University Press, , 6th Edition, 2014. (South Asia Edition 2015)
5. Glen E. Rodgers, Inorganic and Solid-State Chemistry, India Edition, 2002.
6. T. P. Radhakrishnan, Core Concepts for a Course on Materials Chemistry, RSC, 2023

Course title	**Organic Laboratory II**										Course No	**CY 2028**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH		Old Credits	L	T	P	C
			0	0	0	5	0	5				0	0	5	5
Offered for	BS										Status				
Faculty	**CY Faculty**										Type	CORE			
Pre-requisite skills	Nil										To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC								Date of approval by Senate				

Course Learning Outcomes:

Learners should be able to gain first-hand experience in implementing synthetic schemes, purification of synthesized compounds, and characterization by spectroscopic/analytical methods.

Course Contents:

The lab course aims at advanced organic chemistry experiments utilizing techniques and skills gained in the earlier lab class. The lab course will have experiments related to the theory taught in the classroom lectures in organic chemistry-related courses. The following is the illustrative set of experiments.

1. Estimation of ^{n}BuLi concentration and heteroatom-directed lithiation.
2. Formylation of aromatic compound (anisole)
3. Coupling reaction (Cu-catalyzed reaction)
4. Wittig salt preparation and reaction
5. Reduction of benzil
6. Quinoline *N*-oxide to 2-quinolone
7. Diels-Alder reaction
8. Resolution of racemic acid/base
9. Protection and deprotection (Cbz of amines)
10. Rearrangement (Beckmann)

Textbooks:

1. Vogel's Textbook of Practical Organic Chemistry, John Wiley and Sons, 5th Ed., 1989.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, and R. G. Engel, Microscale Approach to Organic Laboratory Techniques, CENGAGE Learning, 5th Ed., 2013.
3. C. A. M. Afonso, N. R. Candeias, D. P. Simão, and A. F. Trindade, J. A. S. Coelho, B. Tan, and R. Franzén, Comprehensive Organic Chemistry Experiments for the Laboratory Classroom, The Royal Society of Chemistry, 2017.

SEMESTER V

<table>
<tr><td>Course title</td><td colspan="9">Chemistry of Main Group Elements</td><td>Course No</td><td colspan="4">CY3011</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td></td><td></td><td></td><td>6</td><td>9</td><td></td><td>3</td><td></td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to identify the properties of the main group elements

Course Contents:

Importance of main group elements in chemistry: historical perspective, relevance to biology, material science, and industry. Effect of size, electro-negativity/positivity on their chemical bonding and chemical reactivity, diagonal relationship. Hypervalency.

Boron group: Structure and bonding of boron hydrides, polyhedral boranes and carboranes. styx notation and Wade's rule: electron count in polyhedral boranes. Synthesis of various boranes and polyhedral boranes. Isolobal analogy; boron halides; phosphine-boranes; boron oxides and boron-nitrogen compounds. Hydrides and halides of Al and Ga. Organyls of Al, Ga, In and Tl.

Carbon group: Carbenes, graphenes, silanes, silicon halides, silicates, silanols, Organyls of germanium, tin and lead.

Nitrogen group: Hydrides, oxides, halides, acids and oxyacids. Phosphides, phosphines and related compounds. Phosphazenes, and NS based hetero-cycles.

Oxygen group: Sulphur halides, oxo acids of sulphur. Structural features and reactivity of S-N heterocycles. Chemistry of selenium and tellurium

Halogen group: Atomic properties and uses. Reactions with oxygen, and metals. Interhalogen compounds.

Rare gases: Properties and applications of noble gases, Synthesis and structures of Xe compounds

Chemistry of Alkali and alkaline earth elements: Binding with crown ethers, cryptands and calixarenes, organometallic compounds.

Text Books:

1. A. J. Elias, The *Chemistry of the p-Block Elements: Syntheses, Reactions and Applications, 1st Edition,* Universities Press, 2019.

2. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edition, Elsevier, 1997.

3. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, 7th Edition, Oxford University Press, 2018.
4. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, Wiley, 2007.

<table>
<tr><td>Course title</td><td colspan="9">Physical Organic Chemistry and Concerted Reactions</td><td>Course No</td><td colspan="4">CY 3013</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

Learners should be able to connect to the physical aspects of organic reactions and catalytic processes. Correlate both the ground and excited state reactivities of organic molecules to product formation.

Course Contents:

Kinetics and thermodynamics: Potential energy surface for substitution and elimination reactions, the rate limiting step, Hammond postulate, the principle of microscopic reversibility, Curtin-Hammett principle, the principle of least motion, kinetic and thermodynamic control of products.
Correlation of structure with reactivity, linear free-energy relationships, Hammett equation, interpretation of substituent and reaction constants, polar and steric substituent constants, the Taft model, deviation from Hammett equation; acidity functions, determination of solvent polarity and solvent polarity scales.

Catalysis: Specific and general acid/base catalysis, Brønsted catalysis law, interpretation of Brønsted coefficient, nucleophilic and electrophilic catalysis, mechanisms of acid-base catalyzed reactions in carbonyl and olefin chemistry.

Pericyclic Reactions: Electrocyclic, cycloaddition, sigmatropic, ene, and cheletropic reactions; Woodward-Hoffmann rules, Frontier Molecular Orbital (FMO) approach and stereochemical aspects; Diels-Alder reactions, dipolar cycloadditions, Cope and Claisen rearrangements.

Photochemistry: Introduction, laws and principles, singlet and triplet states - reactivity, free radical reactions, photoreactions of carbonyl compounds (Norrish and Paternò-Büchi reactions) and alkene isomerization.

Photoredox catalysis: HAT and ZAT reactions, SET processes and energy transfer reactions.

Textbooks:

1. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, 5th Ed., 2007.
2. H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry, Harper & Row, 2nd Ed., 1981.
3. S. Sankararaman, Pericyclic Reactions - A Textbook, Wiley, 2005.
4. I. Fleming, Pericyclic Reactions, Oxford Chemistry Primers, 1998.
5. S. Kumar, V. Kumar, and S. P. Singh, Pericyclic Reactions: Mechanistic and Problem-Solving Approach, Elsevier, 2016.
6. E. V. Anslyn and D. A. Dougherty, Modern Physical Organic Chemistry, University Science, 2nd Ed., 2006.

Course title	**Chemical Bonding and Spectroscopy**									Course No	**CY 3015**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: In continuation with **CY2017: Quantum Mechanics and Spectroscopy-I,** Students will further learn principles of quantum mechanics and will be able to apply them to understand Chemical Bonding.

Schrödinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals, and Hydrogen-like atoms.

Helium atom, many-electron systems, Approximate methods, Time-independent perturbation and variation methods, Pauli Exclusion & Aufbau Principles, Slater Determinants

Origin of Chemical Bonding, Introduction to Valance-Bond & Molecular Orbital Theories, linear combination of atomic orbitals (LCAO), Application to H_2 Molecule, Concept of Overlap, Coulomb and Resonance Integrals.

Molecular Symmetry: symmetry elements/operations, Groups, Representations & Character tables, Projection Operator, Symmetry Adapted Linear Combination (SALC), Formation of MOs in terms of symmetry Adapted Linear Combination (SALC), Illustration with simple examples for sigma and pi-bonding in molecules, Spectroscopic Selection rules

Orbital and Spin Angular Momenta, Addition of Angular Momenta, Atomic & Molecular Term Symbols & their Significance

Electronic spectra of diatomic molecules, vibrational and rotational fine structure, selection rules, Jablonski diagram, Frank-Condon principle and its consequences, Fluorescence and Phosphorescence and dissociation/pre-dissociation of excited molecules, Applications.

Nuclear/Electronic spin resonance spectroscopy

Text Books:

1. D. A. McQuarrie, Quantum Chemistry, 2nd ed, University Science Books, 2008.
2. N. Zettili, Quantum Mechanics: Concepts and Applications, John Wiley & Sons, 2009.
3. P. W. Atkins, Molecular Quantum Mechanics, 4^{th} ed, Oxford University Press, 2005.
4. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994,
5. M. S. Gopinathan, Group Theory and Molecular Spectroscopy, Vishal Publishing Co., 2022
6. C. N. Banwell, E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata-McGraw Hill, 2007.
7. E. D. Becker, *High Resolution NMR: Theory and Applications*, Academic Press, 1991.

<table>
<tr><td>Course title</td><td colspan="9">Physical Chemistry Laboratory I</td><td>Course No</td><td colspan="4">CY 3017</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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</table>

Course Learning Outcomes: The students will be able to conduct experiments by applying the basic principles in thermodynamics

Course Contents:

1. Phase Rule: Two-component systems
2. Phase Rule: Three-component systems
3. Azeotropic mixtures: Two-component liquid-liquid systems
4. Differential scanning calorimetry
5. a) Polarimetry-Inversion of sucrose

   b) CST: Phenol-water system
6. a) Dissociation constant of KI_2 by distribution method

   b) Ideal solubility

Text Books:

1. Shailendra K Sinha, Physical Chemistry: A Laboratory Manual, Narosa Publications, 2014
2. A. O. Thomas, Practical Chemistry, , Scientific Book Centre, Kannur, 7th Edn., 1999
3. W. G. Palmer, Experimental Physical Chemistry, Cambridge University Press, 2009

SEMESTER VI

Course title	**Advanced Coordination Chemistry**									Course No	**CY 3020**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to analyse the structure-property relations of coordination compounds

Course Contents:

Ligand field theory of coordination compounds – Ligand group orbitals, construction of MO diagrams of selected octahedral, square planar, and tetrahedral complexes containing σ-donor, π-donor and π-acceptor ligands; interpretation of electronic spectra and magnetic properties; spin-only and spin-orbit coupling. Interpretation of absorption spectra of selected octahedral and tetrahedral metal complexes - term symbols, Orgel diagram and Tanabe-Sugano diagram of both high spin and low spin complexes, prediction of the number of spin-allowed and spin-forbidden transitions, their relative energies, and relative intensities, calculation of the octahedral splitting energy and Racah parameter.

Reaction mechanisms of coordination compounds - substitution reactions in octahedral and square planar complexes, *trans*-effect and its applications, ligand exchange, associative and dissociative mechanisms, electron transfer processes- the inner-sphere and outer-sphere mechanisms.

Lanthanides and actinides - the effects of lanthanide contraction, difference between them in the structure, bonding, magnetic and spectral properties, materials and medicinal applications.

Textbooks:

1. J. E. Huheey, E. A. Keiter, and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity,* 4th Edition, Pearson, 1993.
2. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, 7th Edition, Oxford University Press, 2018.
3. C. E. Housecroft, and A. G. Sharpe, *Inorganic Chemistry*, 5th Edition, Pearson, 2018.
5. G. L. Miessler, P. J. Fischer, and D. A. Tarr, *Inorganic Chemistry*, 5th Edition, Pearson Education Limited, 2013.
6. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry,* University Science Books, 1994.

<table>
<tr><td>Course title</td><td colspan="9">Modern Methods and Strategies in Organic Synthesis</td><td>Course No</td><td colspan="4">CY 3022</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

Learners should be able to use the various reagents and reactions in organic synthesis. Comprehend the retrosynthetic methods and logically apply to dissect complex organic molecules and devise synthetic approaches.

Course Contents

Oxidation: Metal-based and non-metal-based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine); peracid oxidation of alkenes and carbonyls; alkenes to diols (manganese and osmium), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead); Wacker oxidation, Fleming-Tamao oxidation, and selenium-based allylic oxidation; Sharpless asymmetric epoxidation and dihydroxylation.

Reduction: Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst; metal-based reductions: Li/Na in liquid ammonia, sodium, magnesium, zinc, titanium, and samarium; hydride transfer reagents: $NaBH_4$, L-selectride, K-selectride, $LiAlH_4$, DIBAL-H, Red-Al, Trialkylsilanes, and Trialkylstannane, and Luche reduction; enantioselective reductions: chiral boranes, Corey-Bakshi-Shibata, and Noyori asymmetric hydrogenation.

Modern Synthetic Methods: Baylis-Hillman reaction, Kulinkovich reaction, Sakurai reaction, Brook rearrangement, Tebbe olefination, and Dötz reaction; metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi Sonogashira, Nozaki-Hiyama-Takai-Kishi, Takai, Buchwald-Hartwig, and Ullmann coupling; directed *ortho*-metalation; stereoselective synthesis of tri- and tetra-substituted olefins; synthetic applications of Claisen rearrangement, and ene reaction (metallo-ene, and Conia ene).

Construction of Ring Systems: Different approaches towards synthesizing three, four, five, and six-membered rings; Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization, and radical-olefin cyclization, interconversion of ring systems (contraction and expansion); construction of macrocyclic rings and ring-closing metathesis.
Illustration of multi-component and cascade reactions with examples.

Retrosynthetic Analysis: Basic principles, terminology - retron, synthon, synthetic equivalent, strategic bond, etc.; one group and two groups disconnections of C-C and C-X bonds, functional group interconversion (FGI) and transposition; strategies for 1,n-difunctionalized (n = 3-6) molecules, illustration with small bioactive molecules.

Protecting groups: Protection and deprotection of hydroxyl, amino, carbonyl, and carboxyl groups, and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration in organic synthesis.

Textbooks:

1. I. Coldham, and W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 4th Ed., 2004.
2. J. L. Clayden, N. Geeves, and S. Warren, Organic Chemistry, Oxford University Press, 2nd Ed. 2012.
3. F. A. Carey, and R. J. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis Springer, 5th Ed., 2007.
4. S. Warren, and P. Wyatt, Organic Synthesis - The Disconnection Approach, Wiley, 2nd Ed., 2008.
5. T. W. Greene, and P. G. M. Wuts, Protective Groups in Organic Synthesis, Wiley, 4th Ed., 2006.

<table>
<tr><td>Course title</td><td colspan="9">Modern Methods in Analytical Chemistry</td><td>Course No</td><td colspan="4">CY 3024</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcome: The learners will be able to identify the basic principles involved in the analytical methods for chemical analysis

Course Contents:

Statistical approaches in analytical experimentation: probability, regression analysis, accuracy & precision, error propagation in experiments, data analysis

Separation Methods: Normal and reversed phase liquid chromatography (NP- & RP-LC); Gas Chromatography (GC); GC-MS; High Performance Liquid Chromatography (HPLC)**;** Size-Exclusion Chromatography (SEC); Ion Chromatography (IC).

Spectroscopic Techniques: Spectrophotometry and binding assays, using fluorimetry and light scattering techniques for analyzing samples, excited state lifetime-based studies: time-correlated single photon counting

Surface Techniques: Principles and applications of electron spectroscopy for chemical analysis (ESCA) and Scanning Probe Microscopy, Atomic Force Microscopy

Electroanalytical techniques: Applications to chemical & biological systems: Principles of Potentiometry, Electrogravimetry, Voltammetry, Stripping methods, Chronoamperometry, Quantitative applications of Potentiometry and Voltammetry: Electrochemical sensors, ISFETs, CHEMFETs

Text Books:

1. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, Brooks/Cole Cengage Learning, Belmont, CA, 6th Edition, 2007.
2. H. Willard, L. L. Merrln, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, Belmont., 7th Edition,1989.
3. Rousseac and A. Roessac, Chemical Analysis: Modern Instrumentation Methods and Analysis, John Wiley & Sons, Ltd., 4th Edition, 2000.
4. Wang, Analytical Electrochemistry, Wiley – VCH, 3rd Edition, 2006.
5. T. Kissinger and W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, Marcel Dekker Inc., 2nd Edition, 1996.
6. Voigtlaender, Scanning Probe Microscopy: Atomic Force Microscopy and Scanning Tunneling Microscopy:, Springer – Verlag, Berlin 2015.

<table>
<tr><td>Course title</td><td colspan="9">Inorganic Chemistry Laboratory II</td><td>Course No</td><td colspan="4">CY3026</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to synthesize and characterize various inorganic systems.

Course Contents:

1. Coordination Chemistry: Steroisomerism & Jahn-Teller effect: Synthesize, characterization and estimation of manganese in $Mn(acac)_3$.
2. Coordination Chemistry: Verification of spectrochemical series with Nickel(II) complexes: $[Ni(en)_3]Cl_2$, $NiCl_2{\bullet}6H_2O$ and $[Ni(NH_3)_6]Cl_2$.
3. Coordination & Photochemistry: Potassium tris(oxalato)ferrate(III): Synthesis, analysis and photochemistry.
4. Organometallic Chemistry: Preparation and characterization of *Ortho* and *para* (chloromercury(II))-phenol, $(C_6H_5O)HgCl$.
5. Bioinorganic Chemistry: Preparation of tetraphenylporphyrin (H_2TPP) and its zinc(II) complex.
6. Synthesis and characterization of an N-hetercyclic carbene.
7. Solid state chemistry: Synthesis and characterization of calcium manganite, Ca_2MnO_4.
8. Phase transition in solid: Synthesize, characterization and phase transition study of copper(I) tetraiodomercurate(II), Cu_2HgI_4.
9. Nanoparticles: Synthesis and Characterization of CdS nanoparticles.

Text Books:

1. Practical inorganic chemistry, G. Pass and H. Sutcliffe, Chapman & Hall, 2nd Ed., 1974.
2. Text book of quantitative inorganic analysis. I. Vogel, (revised), ELBS publications, 4th Ed., 1978.
3. Preparation and properties of potassium trisoxalatoferrate(III) trihydrate – A laboratory exercise. *J. Chem. Educ*., **1974**, *51*, 129.
4. Infrared and Raman spectra of inorganic and coordination compounds. K. Nakamoto, Wiley Interscience, 5th ed., 1997, Part B.
5. A simplified synthesis for *meso*-tetraphenylporphin. *J. Org. Chem*., **1967**, *32*, 476.
6. A facile route to preparation of CdS nanorods. *Materials Chemistry and Physics* **2003,** *77* (3), 734-737.

<table>
<tr><td>Course title</td><td colspan="9">Physical Chemistry Laboratory II</td><td>Course No</td><td colspan="4">CY 3028</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to conduct experiments by applying the basic principles of chemical kinetics

Course Contents:

1. Alkaline Hydrolysis of an ester by
   (a) Analytical method
   (b) Conductivity method
2. Acid hydrolysis of an ester
3. Kinetics of oxidation of iodine by persulphate (a) order, (b) salt effect
4. (a) Kinetics of oxidation of formic acid using bromine – by potentiometry
   (b) Determination of enthalpy of solution using solubility principles-heat of solution
5. (a) Adsorption isotherm-study of adsorption of a solute on activated charcoal
   (b) Ammonia chemisorption technique
6. a) Iodination of acetone using spectrophotometer
   b) Decomposition of benzene diazonium chloride

Text Books:

1. Shailendra K Sinha, Physical Chemistry: A Laboratory Manual, Narosa Publications, 2014.
2. A. O. Thomas, Practical Chemistry, Scientific Book Centre, Kannur, 7th Edn., 1999.
3. W. G. Palmer, Experimental Physical Chemistry, Cambridge University Press, 2009.

SEMESTER VIII

<table>
<tr><td>Course title</td><td colspan="9">Spectroscopy of Inorganic and Organometallic Compounds</td><td>Course No</td><td colspan="4">CY 4020</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to apply spectroscopic principles for structure analysis of inorganic compounds

Course Contents:

Nuclear Magnetic Resonance Spectroscopy: Principles and interpretations of NMR (^{1}H and ^{13}C) spectra of organometallic compounds, fluxionality; NMR (^{31}P, ^{11}B, ^{19}F and ^{29}Si) of main group compounds; solid-state NMR, Instrumentation.

Electron Paramagnetic Resonance Spectroscopy: Principle and theory of EPR, g-factor, hyperfine interactions, interpretation of spectra of simple organic free radicals, spin-trap, and of transition metal (copper, chromium, molybdenum) complexes; instrumentation.

Infrared & Raman Spectroscopy: Basic concepts and principles- modes of vibrations, active/inactive modes using simple Inorganic molecules (CO_2, H_2O, etc.), Interpretation of the spectra of a variety of transition metal complexes with different inorganic ligands (carbonyl, nitrosyl, dinitrogen, oxygen, nitride, cyanide, carboxylate, etc.); d^1, d^9, d^5 (low spin systems); instrumentation-components, sample preparation and procedures.

Mass spectrometry: Basic principles, ionization techniques, isotope abundance, molecular ion; illustrative examples from coordination, supramolecular and organometallic compounds.

Mössbauer Spectroscopy: Basic principle, concepts and applications - isomer shift, quadrupole splitting, hyperfine splitting, Mossbauer active nuclei, interpretation of spectra of simple iron complexes with variations in valence, spin-state and coordination geometry; limitations; instrumentation.

Text Books:

1. D. W. H. Rankin, N. W. Mitzel and C. A. Morrison, *Structural Methods in Molecular Inorganic Chemistry*, 1st Edition, Wiley, 2013
2. R. S. Drago, *Physical Methods for Chemists*, 2nd Edition, Surfside.
3. M. Weller, T. Overton, J. Rourke, and F. Armstrong, *Inorganic Chemistry*, 7th Edition, Oxford University Press, 2018.
4. C. E. Housecroft, and A. G. Sharpe, *Inorganic Chemistry*, 5th Edition, Pearson, 2018.

Course title	**Modern Spectroscopic Methods for Structural Elucidation**									Course No	**CY 4022**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes:

Learners should be able to analyze and interpret the spectral data, and elucidate the structure of organic molecules.

Course Contents:

Electronic spectroscopy: Basic principle, electronic transitions in organic molecules and application to structure elucidation. Optical rotatory dispersion and circular dichroism (ORD and CD) spectroscopy, underlying principle, plane curves, Cotton effects, octant rule, axial halo-keto rule, applications to assignment of configuration of chiral molecules.

Infrared spectroscopy: Basic principle, and organic functional group identification.

NMR spectroscopy: NMR phenomenon, spin ½ nuclei, (^{1}H, ^{13}C, ^{31}P and ^{19}F), ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ: inductive and anisotropic effects, chemical structure correlations; chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects: examples of AB, AX, AA'BB' and ABX systems, simplification of second order spectrum. ^{13}C NMR, introduction to FT technique, relaxation of nuclear spins, NOE effects, chemical shift.

^{1}H and ^{13}C chemical shifts to structure correlations: stereochemical assignments, selective decoupling, chemical shift reagents; dynamic processes by VT NMR (restricted rotation, cyclohexane ring inversion, and degenerate rearrangements).

Mass spectrometry: Basic principles, ionization techniques (including ESI and MALDI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, illustrative examples from simple organic molecules.

Structure elucidation problems using the above spectroscopic techniques.

Text Books:

1. L. Pavia, G. M. Lampman, G. S. Kriz, and J. R. Vyvyan, Introduction to Spectroscopy, CENGAGE Learning., 5th Ed., 2015.
2. R. M. Silverstein, F. X. Webster, and D. J. Kiemle, Spectrometric Identification of Organic Compounds John Wiley & Sons Inc., 7th Ed., 2005.
3. W. Kemp, Organic Spectroscopy, Macmillan Education, 3rd Ed., 1991.

Course title	**Advanced Quantum Chemistry & Applications**									Course No	**CY 4024**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: The students will be able to learn basic and advanced concepts of Quantum Chemistry and Group Theory to structure, bonding, and spectroscopy.

Course Contents:
Self-Consistent Field and Hartree-Fock Theory, Electronic Population Analysis, The Koopman's theorem, Electron correlation, Configuration Interaction, Brillioun theorem

Introduction to DFT, Electron density, Pair density, Self-interaction correction, Kohn-Sham theorems, Exchange correlation

Molecular symmetry and its applications**:** Normal Mode Analysis of Molecular Vibrations, Irreducible representations, Symmetry-adapted linear combinations, Woodward-Hoffmann Rules, Frontier Orbital Theory, Vibrational and Electronic Spectroscopy of simple molecules, Perturbations and Orbital splitting, Vibronic coupling, and Jahn-Teller effect & their implications

Text Books:

1. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press, 4th ed., 2005.
2. I. Levine, Quantum Chemistry, Pearson Press, 6th ed., 2009.
3. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994
4. A. Szabo and S. Ostuland, Modern Quantum Chemistry, Dover Publications, 1996.
5. F A Cotton, Chemical Applications of Group Theory, Wiley Student Ed., 2008.
6. E. B. Wilson, J. C. Decius, and P. C. Cross, *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra*, Dover, 1980.

<table>
<tr><td>Course title</td><td colspan="9">Computational Chemistry Lab</td><td>Course No</td><td colspan="4">CY 4026</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to demonstrate the application of the principles/ methods, learnt in Quantum Mechanics and Spectroscopy (CY 2017) and Chemical Bonding (CY 3015) courses, to chemical problems. The applications involve quantum chemistry calculations at various levels of theory using the Gaussian/Mopac software package for different chemical problems, as listed below. The learning outcomes of the course are: (i) describe different computational approaches and their application in chemistry, and, (ii) design and perform electronic structure calculations for a chemical problem of interest and use the expertise gained from the course in experimental chemistry areas that require routine use of computations.

1. Basic Linux commands and writing Z-matrices for various chemical systems (e.g. H_2O, C_6H_6) with dummy atoms.

2. Geometry optimization: Identification of the lowest energy structure of different molecules (Eg. C_2H_6, Cyclohexane etc.), visualisation of orbitals and electrostatic potential, population analysis, and atomic charges

3. Spectroscopy: IR, Raman, NMR, and ESR spectra of molecules

4. Analysis of non-covalent interactions: H-bond, van der Waals interactions (e.g. H_2O cluster, Benzene dimer, DNA base pair/stack)

5. PES surface scan calculations and calculations of bond dissociation energy (e.g. H_2, O_2, ethane, butane, 2-chlorobiphenyl, etc.)

6. Koopman's theorem: Calculation of ionization potential and electron affinity and comparison with experiments (e.g. H_2, Li_2, etc.)

7. Woodward–Hoffman correlation diagrams- optimization of the geometries of cyclobutene and butadiene, computation of the molecular orbitals and their energies as a function of ring opening of cyclobutene under con- and dis-rotatory modes, plot of the frontier MO energies vs the ring opening coordinate (maintenance of symmetry), analysis of the plots and discussion about thermal/photochemical processes.

8. Chemical reactivity descriptors: Computation of different local and global reactivity descriptors and applications to chemical reactivity prediction (eg. Nucleophilic attack on carbonyl compounds, halogenation of benzene)

9. Thermochemistry - Normal mode analysis, IR and Raman spectra, analysis of the symmetries of the normal modes, computation of the rotational constants, vibrational force constant, partition functions

10. Reaction mechanism and kinetics – Free energy calculation and reaction barriers, identification of transition state, determination of rate constant, IRC profile, computation of rate as a function of temperature

11. Computational drug discovery: Visualisation of protein-ligand interaction, structure-based screening using docking

12. Modeling excited states- Franck-Condon spectral calculations, optimization of the geometry of the ground, excited and ionized excited states, calculation of the vibrational frequencies of these states, calculation of the transition energies and oscillator strengths for the photo-electron spectra, Electronic circular dichroism (Eg. Butadiene, Benzene excitation energies, dye molecules)

Text Books:

1. F. Jensen, Introduction to Computational Chemistry, Wiley-Blackwell, 2nd edition, 2006.
2. A. Szabo and S. Ostuland, Modern Quantum Chemistry, Dover Publications, 1996.
3. A. R. Leach, Molecular Modelling Principles and Applications, Prentice Hall, 2001.
4. Jan H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
5. Daan Frenkel B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2001.
6. Michael P. Allen and Dominic J. Tildesle, Computer Simulation of Liquids, Oxford University Press, 1991
7. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, Wiley: Chichester, England. 2002.

DEPARTMENT FREE ELECTIVE BASKET

BS@CHEMISTRY, IIT MADRAS

SEMESTER VIII

CY XXXX:	Supramolecular Chemistry
CY XXXX	Advanced Bioinorganic Chemistry
CY XXXX	Advanced Organometallic Chemistry
CY XXXX	Advanced Organic Chemistry
CY XXXX	Organic Photochemistry
CY XXXX	Medicinal Chemistry
CY XXXX	Advanced physical organic chemistry
CY XXXX	Stochastic theory of molecular catalysis
CY XXXX	Experimental Methods in Chemistry
CY XXXX	Molecular Thermodynamics of Liquid Mixtures
CY XXXX	Modern Electronic Structure Methods for Molecules
CY XXXX	Machine Learning in Chemistry

(students should choose three courses of their choice)

SEMESTER IX*

CY XXXX	Organometallics for Polymer Synthesis
CY XXXX	Molecules and Clusters: Structure, Bonding and Applications
CY XXXX	Magnetism for Molecule-based Future Electronics
CY XXXX	Asymmetric synthesis
CY XXXX	Stereoselective synthesis of biologically active molecules
CY XXXX	Application of Organometallics in Organic Synthesis
CY XXXX	Green and Sustainable Chemistry
CY XXXX	Organic Functional Materials
CY XXXX	Transient Absorption Spectroscopy
CY XXXX	Advanced Optical Spectroscopy
CY XXXX	Statistical Thermodynamics
CY XXXX	Quantum Computing and Quantum Chemistry
CY XXXX	Numerical Methods & Computational Chemistry

(students should choose three courses of their choice)

*Applicable only for MS students

<table>
<tr><td>Course title</td><td colspan="9">Supramolecular Chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: Students will be able to identify the design strategies used in developing supramolecular structures

Course Content:

Introduction to supramolecular chemistry: Historical perspective, Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-π, anion-π, π–π, and van der Waals interactions, Supramolecular chemistry of life

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complementarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Crystal engineering: concepts, polymorphism, cocrystals, supramolecular synthons, halogen bonding, role of H-bonding and other weak interactions.

Self-assembly molecules: design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, discrete coordination cages, coordination polymers, mechanical bond, catenanes, rotaxanes, helicates and knots.

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis and supramolecular nanomaterials etc. Dynamic covalent bonding and complex systems

Examples of recent developments in supramolecular chemistry from current literature

Text Books:

1. J. -M. Lehn; Supramolecular Chemistry-Concepts and Perspectives, Wiley-VCH, 1995
2. W. Steed and J. L. Atwood; Supramolecular Chemistry, Wiley, 3rd Edition, 2022

<table>
<tr><td>Course title</td><td colspan="9">Advanced Bioinorganic Chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes: Students will be able to identify the structure-property relation in bioinorganic systems

Course Content:

Chemical elements in biology. Recapitulation of trace transition metal ions and ligands in biology. Biodistribution, thermodynamic, and kinetic factors of metal ions; tetrapyrrole macrocyclic skeletons (porphin, chlorin, corrin, and corphin). Hemoglobin and myoglobin; O_2 binding to hemoglobin, cooperativity and its interpretation using theoretical models. Bohr effect. Active site structure of carbonic anhydrase and its role in the functioning of hemoglobin. Non-heme O_2 carrier hemocyanin and hemerythrin. Resonance Raman spectroscopic characterization of oxy forms of heme or nonheme metalloproteins. Representative synthetic models of O_2 carrier metalloproteins.

Enzymes-nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts kinetics of enzyme-catalyzed reactions. Michaelis-Menten's constant, effect of pH and temperature on the catalytic efficiency of enzymes.

Iron transport and storage proteins in bacterial and mammalian systems – siderophores, ferritin and transferrin.

Electron transport proteins: Blue copper proteins, cytochromes, iron-sulfur proteins – rubredoxin, ferredoxins, HiPIP; electron transport chain (ETC) in respiration and photosynthesis. Role of manganese in photosynthesis and O_2 evolving complex (4 Mn cluster): Photosystem I and II; Antenna chlorophylls.

Redox enzymes: Structure, function, and mechanism of several selected enzymes: Methane monooxygenase (MMO), ribonucleotide reductase (RNR), tyrosinase, dopamine β-monooxygenase (DβM), peptidyl glycine α-hydroxylating monooxygenase (PHM), cytochrome *c* oxidase, vitamin B-12, cytochrome P-450, catalase, peroxidase, and superoxide dismutase (Cu-Zn). Structure, function, and mechanism of action of a few non-redox enzymes: Urease, peptidases, phosphatases, and carboxypeptidase.

Nitrogen-cycle enzymes: Mo in N, and S-metabolism by Mo-pterin cofactors and Mo-Fe-cofactors. NO_x reductases, sulfite oxidase, xanthine oxidase, nitrogenase, P and M-clusters in nitrogenase, transition-metal N_2 complexes and insights into N_2 binding, and reduction to ammonia.

Metals in medicine: Anti-cancer agents, cisplatin, diagnostic (Gd in MRI), radio-pharmaceuticals (^{99m}Tc, ^{131}I), and therapeutic agents. Toxicity of ions (Hg, Cd, Pb, As) including Cr^{6+} in biology and chelation therapy.

Text Books:

1. Bertini, Gray, Lippard and Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd. 1994.
2. Shriver, Weller, Overton, Rourke, Armstrong, *Inorganic Chemistry*, 6^{th} Ed., 2014.
3. R. Crichton, *Biological Inorganic Chemistry*, 3^{rd} Ed., 2019.
4. Lippard and Berg, *Principle of Bioinorganic Chemistry*, Univ. Sci., Books, 1994.
5. Kaim, Schwederski and Klein, *Bioinorganic Chemistry: Inorganic Perspective in the chemistry of life*, 2^{nd} Ed., 2013.
6. Mathews, Holde, Appling and Anthony-Cahill, *Biochemistry*, 4^{th} Ed., 2013.

Course title	**Advanced Organometallic Chemistry**									Course No	**CY XXXX**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: Students will be able to identify structure and reactivity of organometallic compounds

Synthesis, reactivity, and bonding of metal hydride, allyl, dienyl, arenes, and other acyclic ligands; cyclobutadiene-based metal complexes; Polyene and polyenyl complexes, MCp_2 complexes, bent sandwich compounds, and their properties; Davis-Green-Mingos (DGM) rule

Neutral spectator ligands: Steric and electronic properties of phosphines; Basicity of phosphines, and different phosphine ligands; Synthesis, structure, and properties of different types of N-heterocyclic carbenes; Metal-ligand multiple bonds

Organometallic compounds of elements: Organo-alkali metal, -beryllium and -magnesium compounds, mixed metal containing compounds; Organometallic compounds of B, Al, Ga, and In; Divalent compounds of group 14 elements (heavier analogues of carbenes): synthesis, properties, reactivity towards small molecule activation and catalysis

Fluxionality and dynamic equilibria in Organometallic Compounds: Stereochemical non-rigidity in organometallic compounds; fluxionality in Cp complexes and other organometallic compounds

Different types of organometallic reactions: ligand substitution; oxidative addition (polar and non-polar reagents) and reductive elimination (different types of mechanism); agostic interaction, intramolecular oxidative addition: C-H activation and orthometalation reactions; Nucleophilic and electrophilic attack on coordinated ligands, (de)insertion reactions with mechanistic aspect of CO insertion; β-hydride elimination; transmetalation reaction

Organometallic catalysis: Homogeneous *vs* Heterogeneous catalysis; Different important terminologies used in catalysis; Hydrofunctionalization (e.g. hydrosilylation, hydroboration, hydrocyanation) and oxidative functionalization of olefins; Fishcher-Tropsch reaction; Hydroamination reactions; Ziegler-Natta polymerization of olefins; Transition metal catalyzed various types of C-C (Kumada, Heck, Sonogashira, Negishi, Stille, Suzuki, and Hiyama couplings) and C-N cross coupling reactions (Ullmann, Buchwald-Hartwig, and Chan-Lam coupling): Mechanistic aspects and application to industrially relevant compounds and drug molecule synthesis; Classification and significance of metathesis reactions, mechanism of olefin metathesis; Catalytic C-H bond functionalization

Text Books:

1. B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, 2nd Edition, Universities Press (India), 2013.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition metals, 4th Edition, Willey Interscience, 2005
3. J. F. Hartwig, Organotransition Metal chemistry: From Bonding to Catalysis, University Science Books, 2010
4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 5th Edition, Pearson, 2018.

Course title	**Advanced Organic Chemistry**									Course No	CY XXXX			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes:

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

Understand the principles of advanced synthetic strategies and aspects of regio- and stereoselective methods.

Analyze the mechanistic implications of organic reactions and predict or rationalize their outcomes.

Strategically design, plan, and propose efficient routes for synthesizing simple to complex organic molecules.

Course Contents:

Regio- and stereoselective synthesis, Synthesis under steric control, Protecting groups.

Asymmetric synthesis: organocatalysis and metal-based catalysis.

Methodologies for constructing small to medium-sized carbocycles and heterocycles and applications in organic synthesis.

Transition and main group elements based reactions; Advanced C-C and C-hateroatom bond forming and breaking reactions; SET, XAT, and HAT reaction pathways; Cross-coupling strategy and C-H bond activation reaction.

Linear and convergent synthesis, Formal Synthesis and introduction to total synthesis, Synthetic aspects using Domino reactions, Principles of atom economy and pot economy.

Illustration through the synthesis of small molecules.

Text Books:

1. Carey and Sundberg, Advanced Organic Chemistry, Part A and B, 5th ed., 2007.
2. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge, 4th Ed, 2004.
3. M. B. Smith, Organic Synthesis, McGraw Hill Higher Education, 3rd Ed., 2010.
4. Garry Procter, Asymmetric Synthesis, OUP Oxford, 1996
5. Jonathan Clayden, Nick Greeves, and Stuart Warren, Organic Chemistry, 2nd ed., 2012
6. P. G. M. Wuts, T. W. Greene, Greene's Protective Groups in Organic Synthesis, John Wiley & Sons, Inc., 4th Ed, 2006.
7. A. de Meijere, F. Diederich, Metal-Catalyzed Cross-Coupling Reactions, Wiley-VCH Verlag GmbH, Weinheim, 2nd Ed, 2004.

Course title	Organic Photochemistry									Course No	CY XXXX			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes: Students will be able to identify the principles governing the organic photochemistry reactions

Course Contents:
Introduction to photochemistry; photochemical and photophysical process
Photochemistry of organic compounds Photochemistry of alkenes; cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3- and 1,4-dienes; di- π-methane rearrangements, dimerization, electrocyclisation and Sigmatropic rearrangements,
Photochemistry of aromatic compounds: Isomerisation, skeletal isomerisations, Dewar and prismanes in isomerisations. Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loeflier Freytag reaction.
Photochemistry of carbonyl compounds: cyclic and acyclic ketones; α, β and β,γ-unsaturated ketones; cyclohexadienons (cross-conjugated & conjugated); photoreductions.
Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides.
Energy transfer reactions

Text Books:

1. N. J. Turro, Modern Molecular Photochemistry, University Science Books, US; 1991
2. N. J. Turro, V. Ramamurthy, and J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, US; 2010.
3. J. M. Coxon and B. Halton, Organic Photochemistry, Cambridge University Press, New York;1974.
4. J. Kagan, Organic Photochemistry: Principles and Applications, Academic Press, London; 1993.
5. V. Balzani, P. Ceroni, and A. Juris, Photochemistry and Photophysics, Wiley-VCH, Verlag GmbH & Co; 2014.

<table>
<tr><td>Course title</td><td colspan="9">Principles of Drug Discovery and Development</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes: The learners will be able to:
Describe various stages in drug development, describe drug-likeness and ADMET aspects in terms of chemical structure and physicochemical properties, predict possible metabolic fates of drugs, describe drug-target interactions and molecular basis of drug action, categorize inhibitors based on their target interaction, describe hit-identification and lead optimization strategies, describe the criteria for biomolecules to be considered as therapeutic targets with examples. Laboratory component: Estimate the physicochemical properties such as LogP value, Assess and analyze drug stability and degradation profile, perform basic enzyme inhibition and cell viability assay, perform computational docking for drug design; perform natural product extraction.

Course Contents:

Historical perspectives on the discovery of drugs; Concept of pharmacophore; Drug targets: enzymes, receptors, ion channels, nucleic acids; Stereochemical aspects and energetics of drug-target interactions; Drug administration and ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity), Structural and biological factors affecting ADMET profiles of drugs; Types of inhibitors (competitive, non-competitive and allosteric inhibitors, transition-state analogs and suicide substrates).

Drug discovery process; Combinatorial and diversity-oriented synthesis in drug discovery; Hit identification and lead optimization strategies; Structure-activity relationships, concepts such as bioisosteres and scaffold hopping in medicinal chemistry, pro-drugs and drug delivery systems; drug resistance and combination therapy; Examples of drug development process through specific examples of anticancer, antiviral, antimalarial and antibacterial drugs.

Laboratory component: LogP/LogD calculation; Drug stability/degradation and impurity profiling; Enzyme inhibition assay; Computational docking; Natural product extraction, Synthesis of a representative drug; Protein secondary structure determination by CD, Drug binding assays through ITC, Bioinformatics tools for drug discovery

Text Books:

1. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 7th Ed., 2023.
2. Richard B Silverman, Mark W Holladay, The Organic Chemistry of Drug Design and Drug Action, Academic Press, 3rd ed., 2014.
3. Victoria F. Roche, S. William Zito, Thomas L. Lemke, David A. Williams, Wolters Kluwer, Foye's Principles of Medicinal Chemistry, 8th Ed., 2020.
4. Camille Georges Wermuth, David Aldous, Pierre Raboisson, Didier Rognan, The Practice of Medicinal Chemistry, 4th ed., 2015.

Course title	**Asymmetric synthesis**										Course No	**CY XXXX**				
Department	Chemistry	New Credits	L	T	E	P	O	C	TH		Old Credits	L	T	P	C	
			3				6	9				3		0	3	
Offered for	BSMS										Status					
Faculty	**CY Faculty**										Type	Elective				
Pre-requisite skills	Basics of thermodynamics and reaction kinetics										To take effect from	July 2025				
Submission date	Date of approval by DCC		Date of approval by BAC								Date of approval by Senate					

Course Learning Outcomes: Students will be able to identify strategies and applications of asymmetric synthesis

Course Contents:

Stereoselective synthesis: Selectivity, Stereospecific reactions, Stereoselective reactions: diastereoselective reactions and their application.
Asymmetric synthesis: Importance and principle, Classification: Chiral pool synthesis, resolutions, chiral auxiliary, chiral reagents and chiral catalysts.
Chiral Metal catalyzed asymmetric reduction, oxidation, C-C bond forming reactions, allylic substitution, cyclization, and other important reactions.
Asymmetric organocatalysis: Importance, classification, covalent organocatalysts and non-covalent organocatalysts including phase transfer catalysts and hydrogen-bonding catalysts, supported chiral metal- and organocatalysts.
Resolution: Kinetic, parallel kinetic, dynamic kinetic and Dynamic Kinetic Asymmetric Transformation. Desymmetrization. Nonlinear effect: autocatalysis, auto-induction.
Determination of optical purity using NMR, GC, and HPLC techniques and absolute configuration using NMR, X-ray crystallography.
Application of asymmetric synthesis in industrially relevant molecules.

Text Books:

1. I. Ojima (Ed.), Catalytic Asymmetric Synthesis, John Wiley & Sons, New Jersey, 3rd Ed., 2010.
2. Eric N. Jacobsen, Andreas Pfaltz, Hisashi Yamamoto (Eds.), Comprehensive Asymmetric Catalysis I-III; Springer-Verlag Berlin Heidelberg, Germany, 1999.
3. P. J. Walsh and M.C. Kozlowski, Fundamentals of asymmetric catalysis, University science books, USA, 2009.
4. M. Christmann and S. Brase (Eeds.), Asymmetric Synthesis – The Essentials, Wiley-VCH Verlag GmbH, Weinheim, 2007.

<table>
<tr><td>Course title</td><td colspan="9">Advanced physical organic chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes: The students will be able to apply physical organic chemistry principles to explain the reaction mechanisms

Course Contents:

Through bond and remote stereoelectronic effects

Steric and Stereoelectronic effects on reactivity: Acetals, Esters, Amides and related functional groups.

Reactions at sp^3, sp^2, and sp carbons.

Examples in synthesis and biological processes.

Strains, Strained organic molecules, Stereocontrol in reactions

Organic solid-state reactions

Text Books:

1. J. Kirby,, Stereoelectronic effects, Oxford Chemistry Primers, 2011.
2. V. K. Yadav, Steric and Stereoelectronic Effects in Organic Chemistry, Springer, 2016.
3. Ian Fleming, Molecular orbitals and organic chemical reactions, Wiley, 2009.
4. I. V. Alabugin, Stereoelectronic effects, Wiley, 2016.
5. P. Deslongchamps, Stereoelectronic effects in organic chemistry, Pergamon Press, 1983.

Course title	**Stochastic theory of molecular catalysis**									Course No				
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes:

At the end of the course, the learners should be able to apply the stochastic theory of molecular catalysis to understand how quantum and thermal fluctuations manifest in catalysis at the molecular scale and how they are measured in single-molecule experiments.

Course Contents:

Fundamentals of stochastic reaction kinetics: Molecular fluctuations in reaction mechanisms and stochastic trajectories, uncertainty in reaction completion times, chemical kinetics as discrete-state continuous-time Markovian process, reaction probabilities, chemical master equation (CME) for complex reaction mechanisms, generating function method, exact solution and generalized rate laws, classical chemical kinetics as the asymptotic limit of the CME.

Classical enzyme catalysis: Conformational fluctuations in enzymatic mechanisms and hyperbolic saturation curves, statistical models and binding equations; thermodynamic and kinetic models of enzyme cooperativity and inhibition; asymptotic assumptions of stationarity and equilibrium and chemical detailed balance.

Stochastic enzyme catalysis: Single-enzyme catalytic networks; CME for single- and mesoscopic enzyme catalysis; count and point process descriptions; number and temporal fluctuations in single- and multi-site catalysis; classical and statistical velocity. Statistical measures for non-stationary (transient) and stationary (steady) states in catalytic networks: randomness parameter and dynamic disorder, turnover time correlations and molecular memory. Generalized (statistical equilibrium) conditions for stationarity and detailed balance; inferring mechanisms and rate parameters from single-molecule (statistical) kinetic data. Onsager symmetry of number correlations and microscopic reversibility; Kolmogorov loop criterion for kinetic cooperativity and inhibition.

Text Books:

1. C. W. Gardiner, Handbook of Stochastic Methods for Physics, Chemistry and Natural Sciences, Springer, 2004.
2. N. G. Van Kampen, Stochastic Processes in Physics and Chemistry, Elsevier, 2007.
3. K. P. Frank, Reversibility and Stochastic Networks, Cambridge University Press. 2011.
4. A. Cornish-Bowden, Fundamentals of Enzyme Kinetics, Wiley-Blackwell, Weinheim 2012.
5. A.F. Bartholomay, A stochastic approach to statistical kinetics with application to enzyme kinetics, Biochemistry 1(2), 223–230, 1962.
6. D. A. McQuarrie,: Stochastic approach to chemical kinetics, Journal of Applied Probability 4(3), 413-478, 1967.
7. D. T. Gillespie, Stochastic simulation of chemical kinetics, Annual Review of Physical Chemistry 58(1), 35–55, 2007.

<table>
<tr><td>Course title</td><td colspan="9">Advanced Experimental Methods in Chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td>Department</td><td>Chemistry</td><td>New Credits</td><td>L
3</td><td>T</td><td>E</td><td>P</td><td>O
6</td><td>C
9</td><td>TH</td><td>Old Credits</td><td>L
3</td><td>T</td><td>P
0</td><td>C
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: Students will be able to identify the basic principles used in experimental chemistry

Course Contents:

Concepts of vacuum; kinetic theory concepts

Two-dimensional materials; low energy electron diffraction (LEED).

Basic concepts in surface imaging; secondary electron microscopy (SEM); secondary Auger microscopy (SAM); scanning probe microscopy (SPM); scanning tunneling microscopy (STM); transmission electron microscopy (TEM); surface imaging; depth profiling. Associated techniques of microscopy and spectroscopy.

Wavelength and energy dispersive X-ray fluorescence spectroscopy (WDS and EDS); X-ray absorption spectroscopy (XANES and EXAFS); secondary ion mass spectrometry (SIMS); temperature programmed desorption (TPD); thermal desorption spectroscopy (TDS).

Atomic absorption spectroscopy (AAS); inductively coupled plasma-atomic emission spectroscopy (ICP-AES).

Voltametry; coulometry; amperometry; potentiometry; polarography; electrolytic conductivity; impedance spectroscopy.

Normal and reversed-phase liquid chromatography (NP- & RP-LC); Gas Chromatography (GC); GC-MS; High Performance Liquid Chromatography (HPLC); Size-Exclusion Chromatography (SEC); Ion Chromatography (IC).

Text Books:

1. Wiesendanger, *Scanning Probe Microscopy and Spectroscopy,* Cambridge University Press, 1994.
2. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
3. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Susses, 2002.
4. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/ColeCengage learning, New Delhi, 2004.
5. Atkins and J. de Paula, Atkins‘ Physical chemistry, Oxford University Press, New Delhi, 8th Ed., 2008.
6. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
7. Scholz, Electroanalytical Methods, Springer, 2nd Ed., 2010.

<table>
<tr><td>Course title</td><td colspan="9">Molecular Thermodynamics of Liquid Mixtures</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: Students will be able to identify the theories and modern experimental techniques in molecular thermodynamics of liquid mixtures

Course Contents:

Ideal and non-ideal solutions. Mixing and excess properties of liquid-liquid mixtures.

Theories of electrolyte and non-electrolyte solutions: van Laar, van der Waals, Scatchard-Hildebrand, Lattice, Prigogine Cell, Flory equation of state, Prigogine-Flory-Patterson, Extended Real Associated Solution model, and Kirkwood-Buff theory.

Modern experimental techniques: determination of vapour-liquid equilibrium (static and dynamic methods), calorimetric measurements of heat capacity and heat of mixing, volumetric, transport, acoustic, and optical properties of liquid-liquid mixtures

Thermodynamic relations: excess Gibbs energy, excess entropy, excess enthalpy, excess volume, viscosity deviation, excess heat capacity, excess compressibility

Partial molar properties, their physical significance, and determination methods

Non-ideal behaviour of solutions: nonpolar + nonpolar, polar + nonpolar, polar + polar, hydrogen-bond formation, and charge transfer complexes

Empirical and semi-empirical formulas, theoretical expressions, correlations, and group contribution methods for predicting thermodynamic properties

Computational models for thermodynamic property prediction in liquid mixtures

Text Books:

1. J. M. Prausnitz, R.N. Lichtenthaler, E.G. Azevedo, Molecular Thermodynamic of Fluid-Phase Equilibria, Prentice Hall, 3rd edition, 1998.
2. J. S. Rowlinson, Liquid and Liquid Mixtures, Springer; 1st edition, 1995.
3. W. E. Acree, Thermodynamic Properties of Nonelectrolyte Solutions, Academic Press, 1984.
4. Bevan Ott, Juliana Boerio-Goates, Chemical Thermodynamics: Advanced Applications, Academic Press, 1st edition, 2000.
5. Prigogine, The Molecular Theory of Solutions, North Holland Publishing Co. Amsterdam 1957.
6. Arieh Ben-Naim, Molecular Theory of Solutions, Oxford University Press, USA, 2006.

<table>
<tr><td>Course title</td><td colspan="9">Modern Electronic Structure Methods for Molecules</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BS-MS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: Students will be able to use various computational methods to calculate excited electronic states

Course Contents:

Hartree product wave function; electron spin and antisymmetry; Slater determinant; second quantization; Hartree-Fock self-consistent field methods; Gaussian and Slater type basis sets; semiempirical Hartree-Fock methods; configuration interaction; multiconfiguration self-consistent field; coupled cluster theory; perturbation theory.

Density matrices; Thomas-Fermi model; Hohenberg-Kohn theorem; Kohn-Sham approach; approximate exchange-correlation functionals; self-interaction error; local density and local spin density approximation; generalized gradient approximation; adiabatic connection; hybrid functionals; density functional tight binding method.

Implicit models for condensed phase; Hybrid quantum/classical models; ONIOM; Born-Oppenheimer molecular dynamics

Calculation of excited electronic states; variational excited state methods; configuration interaction singles; equation of motion coupled cluster methods; time-dependent Hartree-Fock and density functional theory.

Text Books:

1. A. Szabo, and N.S., Ostlund, Quantum Chemistry, Dover, New York 1996.
2. T. Helagaker, P. Jorgenson, and J. Oslen, Molecular Electronic Structure Theory, John Wiley & Sons, New York, 2000.
3. C. J. Cramer, Essentials of Computational Chemistry, John Wiley & Sons, 2013.
4. W.C. Koch, and M.C. Holthausen, A Chemist's Guide to Density Functional Theory, Wiley-VCH, Germany, 2000
5. R.G. Parr, and W. Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford, 1989.

<table>
<tr><td>Course title</td><td colspan="3">Machine Learning in Chemistry</td><td>Course No</td><td></td></tr>
<tr><td>Department</td><td>Chemistry</td><td>New Credits</td><td>L: 3 | T: 1 | E: | P: | O: 6 | C: 10 | TH:</td><td>Old Credits</td><td>L: 3 | T: 1 | P: 0 | C: 4</td></tr>
<tr><td>Offered for</td><td colspan="3">BS-MS</td><td>Status</td><td></td></tr>
<tr><td>Faculty</td><td colspan="3">CY Faculty</td><td>Type</td><td>Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="3">Nil</td><td>To take effect from</td><td>July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td>Date of approval by BAC</td><td colspan="2">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to apply basic concepts of machine learning in solving chemical problems

Course Contents:

1. Introduction to ML and Linear Regression: Introduction to AI and ML; features and labels; supervised and unsupervised learning; regression and classification; ML in chemistry; linear regression.

2. Fingerprint and Polynomial Regression: Train-test Splitting; feature identification for chemical problems; experimental, computational and graph features; introduction of non-linearity; polynomial features; polynomial regression.

3. Core Concepts and Improving ML Models: Overfitting; standardization; regularization; K-fold cross-validation; curse of dimensionality; recursive feature elimination (RFE).

4. Popular ML Models and Libraries: Probabilistic models; gaussian process regressor; decision tree models; ensemble learning; random forest regressor; gradient boosting regressor; deep learning and neural networks

Text Books:

1. Andrew White, Deep Learning for Molecules and Materials by , https://dmol.pub
2. C. M. Bishop, Pattern recognition and machine learning; Springer:New York, 2006.

Course title	**Organometallics for Polymer Synthesis**									Course No	**CY XXXX**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes:

Course Content:

Organometallic Catalysts for Polymerization: Overview of polymerization mechanisms (chain growth, step growth, coordination); Ziegler-Natta polymerization: Catalysts, mechanism, and control of polymer stereochemistry; Metallocene polymerization: Catalyst design, polymerization characteristics, and applications; Late transition metal catalysts and their role; boranes and alanes as cocatalysts

Ring-Opening Metathesis Polymerization (ROMP): Mechanism of ROMP; Grubbs catalysts and their evolution; Applications of ROMP in the synthesis of well-defined polymers

Ring-Opening Polymerization (ROP): Organometallic catalysts for ROP of cyclic esters, epoxides, and lactides; Mechanism and kinetics of ROP; Biodegradable polymers and sustainable materials

Other Polymerization Techniques: Living polymerization and controlled radical polymerization; Coordination polymerization of polar monomers; organometallic-mediated click chemistry for polymer synthesis

Characterization Techniques: Gel Permeation Chromatography (GPC); Differential Scanning Calorimetry (DSC); X-ray diffraction

Textbooks:

1. George Odian, Principles of Polymerization, John Wiley & Sons, 4th Edition, 2004.
2. Paul C. Hiemenz and Timothy R Lodge, Polymer Chemistry, CRC Press, 2nd Edition, 2007.
3. V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Polymer Science, New Age International, 2005.

Course title	Organometallics for Polymer Synthesis										Course No	CY XXXX			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH		Old Credits	L	T	P	C
			3				6	9				3		0	3
Offered for	BSMS										Status				
Faculty	**CY Faculty**										Type	Elective			
Pre-requisite skills	Basics of thermodynamics and reaction kinetics										To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC								Date of approval by Senate				

Course Outcomes:

Introduction: Molecules and molecular clusters.

Main-group clusters: Geometric and electronic structures, Three-, four- and higher connect clusters, *closo-, nido-, arachno*-borane structural paradigm, Wade-Mingos Rules, Jemmis electron counting rules, When e-counting rules fail, Structure, synthesis and reactivity of boranes and polyhedral boranes, Clusters with nuclearity 4-12 and beyond 12, Nanoclusters and magic number

Transition-metal clusters: Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms, Structure, synthesis and reactivity, Isolobal relationships between main-group and transition metal fragments, metal-ligand complexes vs heteronuclear cluster.

Main-group-Transition-metal clusters: Isolobal analogues of p-block and d-block clusters, limitations and exceptions. Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters.

Molecular clusters in catalysis: Clusters to materials, Boron-carbides and metal-borides.

Nanomaterials: Synthesis and properties of nanomaterials, Characterization of nanomaterials - an overview, Luminescent nanomaterials, Applications of nanomaterials: Scientific and technological aspects

Illustrative examples from recent literature.

Textbooks:

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

<table>
<tr><td>Course title</td><td colspan="9">Magnetism for Molecule-based Future Electronics</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Basics of thermodynamics and reaction kinetics</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Outcomes:

Course Content:

Importance of magnet and magnetic field: History of magnet and its utility in navigation, cosmic phenomena, human life, civilization and biological systems.

Origin of magnetism: Basic concepts on the origin of magnetism, electronic spin, hard and soft magnets, electro-magnet and their utilities in daily life.

Magnetic phenomena: Bulk magnets; ferro-, ferri-, antiferro-, meta-, canted/weak magnet. Kagome, spin-frustrated, spin-ice, spin-liquid systems; Key features, characteristics, similarities and differences. Molecular magnets; paramagnets, super-paramagnets, single-molecule, single-chain and single-ion magnets; bulk magnet vs molecular magnet for technological advantage. Critical temperature and critical field. Magnetism in pure metals and Curie temperatures.

Important magnetic parameters: Spin Hamiltonian in isotropic and anisotropic bimetallic systems. Super exchange, double exchange and physical meaning of *J* and g. Zero-field splitting parameters (D), rhombic parameters (E), uni-axial and easy-plane anisotropies, and their effects of D- and g-tensors. The sign and physical meaning of D and g and their influences in magnetism. The effect of change in coordination numbers on g and D. Synthetic strategies on the increment of single-ion D-values. Experimental EPR studies towards the evaluation of g and D. Zeeman effect and Boltzmann distribution.

Magnetic energy levels: Spin-spin coupling in bi-, tri-, tetra-metallic paramagnetic/exchange-coupled metal complexes/clusters; magnetic energy levels, spin structures; energy spectrum in ferromagnetic and antiferromagnetic complexes. Magnetic structures of Mn_{12}-Ac, Fe_4 and Fe_8 coordination clusters.

Magnetic measurements: DC and AC susceptibilities, physical meaning temperature dependent in-phase and out-of-phase susceptibilities, Arrhenius law and extraction of energy barrier for reorientation between up-spin and down-spin states. Temperature and field dependent hysteresis loops, blocking temperature.

Mechanism of magnetic relaxation: Direct process, Raman process, quantum tunnelling pathways, Orbach process and mixed pathways; effect of uni-axial and rhombic anisotropies on different relaxation pathways.

High Temperature Magnets: Bulk/molecular magnets with high blocking temperatures; synthetic strategies; control on coordination geometry; effect of meta-metal bond; advantage single-ion magnetic-anisotropy of 4f-ions over 3d metal ions. Stark effect in 4f ions; effect of ligand field and covalency on energy barrier.

Dynamics of spin/magnetization: Dynamics of reorientations; photon and phonon mechanism; vibration energy levels, spin-spin vs spin-lattice relaxation.

Text Books:

1. O. Kahn, *Molecular Magnetism*, VCH Publishers, Inc. 220 East 23rd Street New York, 1993.
2. C. Benelli and D. Gatteschi; *Introduction to Molecular Magnetism: From Transition Metals to Lanthanides,* Wiley-VCH; 1st edition, 2015.

<table>
<tr><td>Course title</td><td colspan="9">Asymmetric synthesis</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

Stereoselective synthesis: Selectivity, Stereospecific reactions, Stereoselective reactions: diastereoselective reactions and their application.

Asymmetric synthesis: Importance and principle, Classification: Chiral pool synthesis, resolutions, chiral auxiliary, chiral reagents and chiral catalysts.

Chiral Metal catalyzed asymmetric reduction, oxidation, C-C bond forming reactions, allylic substitution, cyclization, and other important reactions.

Asymmetric organocatalysis: Importance, classification, covalent organocatalysts and non-covalent organocatalysts including phase transfer catalysts and hydrogen-bonding catalysts, supported chiral metal- and organocatalysts.

Resolution: Kinetic, parallel kinetic, dynamic kinetic and Dynamic Kinetic Asymmetric Transformation. Desymmetrization. Nonlinear effect: autocatalysis, auto-induction.

Determination of optical purity using NMR, GC, and HPLC techniques and absolute configuration using NMR, X-ray crystallography.

Application of asymmetric synthesis in industrially relevant molecules.

Text Books:

1. I. Ojima (Ed.), Catalytic Asymmetric Synthesis, John Wiley & Sons, New Jersey, 3rd Ed., 2010.
2. Eric N. Jacobsen, Andreas Pfaltz, Hisashi Yamamoto (Eds.), Comprehensive Asymmetric Catalysis I-III; Springer-Verlag Berlin Heidelberg, Germany, 1999.
3. P. J. Walsh and M.C. Kozlowski, Fundamentals of asymmetric catalysis, University science books, USA, 2009.
4. M. Christmann and S. Brase (Eeds.), Asymmetric Synthesis – The Essentials, Wiley-VCH Verlag GmbH, Weinheim, 2007.

<table>
<tr><td>Course title</td><td colspan="8">Stereoselective synthesis of biologically active molecules</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="8">BS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="8">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="8">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="6">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

Comprehend the fundamental principles of chemical synthesis and stereoselective reactions.

Analyze and apply disconnection strategies to effectively synthesize diverse classes of natural products (secondary metabolites).

Apply these strategies in the design and synthesis of key pharmaceutical compounds.

Course Contents:

Overview of the chemistry of natural products with emphasis on secondary metabolites, their occurrence, structure, biosynthesis, and properties. Stereo/enantioselective synthesis of representative examples from the domain of Alkaloids, Steroids, Terpenes, Hormones, Pheromones, and Macrolides. Synthesis of lead molecules based on natural products for different therapeutic areas. Total synthesis of Penicillin, Endiandric Acid A and B, Prostaglandin, Reserpine, Perhydrohistrionicotoxin, Gibberellic Acid, Strychnine, Epothilones, Platensimycin, Spirotryprostatin, Erythronolide B, Discodermolide, and Taxol.

Text Books:

1. K. C. Nicolaou & E. J. Sorensen, Classics in Total Synthesis, VCH, 1996.
2. K. C. Nicolaou & S. A. Snyder, Classics in Total Synthesis II, VCH, 2003.
3. E. J. Corey & X-M. Cheng, The Logic of Chemical Synthesis, Wiley-Interscience, 1st Ed., 1995
4. S. V. Bhat, B. A. Nagasampagi, S. Meenakshi, Natural Products Chemistry & Applications, Narosa Publishing House, 2009
5. E. M. Carreira, L. Kvaerno, Classics in Stereoselective Synthesis, Wiley VCH, 2009
6. Francis A. Carey and Richard J. Sundberg, Advanced Organic Chemistry, Springer 2008

Course title	**Application of Organometallics in Organic Synthesis**									Course No	**CY XXXXX**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	CORE			
Pre-requisite skills	Nil									To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Learning Outcomes:

Organometallic chemistry has served as a bridge between traditional inorganic and organic chemistry and contributed to the development of several important discoveries in synthetic organic chemistry. At the end of this course, students will thoroughly understand the classification and mechanistic aspects of several organometallic reactions. They will be able to identify the role of organometallic complexes in organic synthesis and industrial applications.

Course Contents

1. Review of formalisms such as oxidation state, 18-electron rule, classes of ligands, structure and bonding.
2. Review of reaction mechanisms, ligand substitution, oxidative addition, reductive elimination, migratory insertion, hydride elimination, transmetallation, nucelophilic and electrophilic attack on the ligands coordinated to metals.
3. Synthetic application of transition metal hydrides, homogenious hydrogenation, transfer hydrogenations and hydrofunctionalization reactions. Organotitanium and zirconium reagents, metallocene complexes in C-C bond forming reactions. Addition to enynes and diynes, hydrozirconation, metallocycle formation and their synthetic utility.
4. Metal (W, Cr, Rh, Ru, Mo) carbene complexes, Fischer, Schrock and Grubbs type carbene complexes, comparison of their stability and reactivity, reactions of Fischer carbene complexes and their synthetic utility, Dötz reaction, simple and cross metathesis reactions, ring opening, ring closing metathesis in organic synthesis, examples from macrocycles synthesis.
5. Metal (Fe, Cr, Mo, Ni, Co, Rh) carbonyl compounds in organic synthesis. C-C bond forming. Cyclooligomerization of alkenes, enynes and alkynes, Vollhardt reaction. Carbonylation and decarbonylation reactions and hydroformylation reaction.
6. Metal (Fe, Pd) ene, diene and dienyl complexes, metal complexes as protecting groups, activation towards nucleophilic addition reaction and rules governing such additions, synthetic utility. pi-allyl palladium, nickel and iron complexes, synthesis and their synthetic utility. Various Wacker type oxidation and cyclization reactions including asymmetric version.

7. Metal (Co, Zr) alkyne complexes, protection of triple bond, C-C bond forming reactions such as Pauson-Khand reaction, alkyne cyclotrimerization and oligomerization reaction. Metal (Cr, Fe, Ru) arene complexes, synthesis and structure. Activation of arene nucleus and side chain. Nucleophilic substitution and addition of arene.

Textbooks:

1. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley & Sons, 6th Ed., 2014.
2. Louis S. Hegedus, Bjorn C. G. Soderberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books, Sausalito, California, 3rd Ed., 2009
3. Jonathan Clayden, Nick Geeves, Stuart Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012.
4. Anil Elias, Gupta B. D., Basic Organometallic Chemistry, University Press, 2nd Edition, 2013.

Course title	**Green and Sustainable Chemistry**										Course No	**CY XXXX**			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH		Old Credits	L	T	P	C
			3				6	9				3		0	
Offered for	BSMS										Status				
Faculty	**CY Faculty**										Type	Elective			
Pre-requisite skills	Nil										To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC								Date of approval by Senate				

Course Learning Outcomes:

At the end of the course, the learners should be able to have a clear understanding of Green and Sustainable practices in chemistry. Create awareness for design strategies for reducing waste, minimizing energy consumption in organic synthesis. Implement techniques of green synthesis in organic reactions.

Course Contents

1) Current Challenges for Sustainable Development: Role of Chemistry

Sustainable Development, Current challenges for sustainable development: Pollutions (Water, Air, Greenhouse effect, Acid rains), energy conservation, Deforestation.

The role of Chemistry in addressing these challenges.

Need for Green Chemistry,

Green Chemistry Definition

Evolution of Green Chemistry

12 principles of Green Chemistry

2) Water Management

Ground water contamination and contamination of water bodies.

Role of chemistry in developing appropriate technological solutions (reverse osmosis, electrodialysis, resin-based water purification, etc) for addressing these issues.

Role of chemistry in providing technical solutions for water treatment and wastewater management in leather and textile sector.

3) Sustainable agriculture

Design of green pesticides for agriculture. Role of NKP fertilizer that causes the increase in salinity of the soil. Approaches to improve the salinity of agri-soil.

4) Green and Sustainable Synthetic Approaches:

A) Green Chemistry Metrics: Atom Economy, E-factor, RME, Carbon efficiency, etc

B) Classification and study of organic reactions under Atom Economy:

i) Atom economic and non-toxic byproduct reactions: rearrangements, addition reaction, condensations, cascade strategies under catalysis etc

ii) Atom uneconomic reactions: substitutions, eliminations, Wittig reactions, degradation reactions etc

C) Alternate/Green Reaction Techniques:

Principles of, i) Microwave, ii) Sonochemsitry/Ultrasound, iii) Ball mill technique, iv) Electrochemical reactions, v) Photochemical reactions, vi) Reactions at Room Temperature, vii) Reagent Free reactions

D) Alternate/Green Solvents

i) Water, ii) Ionic liquids, iii) Supercritical liquids (SCL), iv) Fluorous biphasic Solvents, v) Solvent Free Organic Synthesis

E) Catalysis for Green Chemistry

F) i) Domino/Cascade approaches; ii) Multicomponent reactions.

G) Use of CO2 as 1-C source in organic synthesis

H) Renewable resources for small molecules and Biofuels

Selected industrial case studies: drugs, polymers, like ibuprofen, Propylene oxide; Nylon production; Biodiesel; Vitamin B3; Polyethylene and others

Textbooks:

1. Green Chemistry: An Introductory Text, M. Lancaster, Royal Society of Chemistry, Edition 3, 2016.
2. P. Anastas and P. Trevorrow, Handbook of Green Chemistry, Green Processes, Designing Safer Chemicals, 2013.
3. A. Lapkin and D. Constable, Green Chemistry Metrics: Measuring and Monitoring Sustainable Processes, 2008.
4. J. H. Clark, A. Hunt, C. Topi, G. Paggiola and J. Sherwood, Sustainable Solvents: Perspectives from Research, Business and International Policy (Green Chemistry Series, 2017.
5. M. North, J.H. Clark, Sustainable Catalysis (Green Chemistry Series), 2015.
6. G. Stefanifis, A. Stankiewicz, J.H. Clark, A. de la Hoz, J. Fan, R. Mato Chain, J. Santamaria, Alternative Energy Sources for Green Chemistry (Green Chemistry Series), , 2016.
7. R. Höfer, A.S. Matharu, Z. Zhang, Green Chemistry for Surface Coatings, Inks and Adhesives: Sustainable applications Green Chemistry Series, 2019

Course title	**Organic Functional Materials**									Course No	**CYXXXX**				
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C	
Offered for	BS-MS									Status					
Faculty	**CY Faculty**									Type	CORE				
Pre-requisite skills	Nil									To take effect from	July 2025				
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate					

Course Learning Outcomes: The students will be able to identify the basic principles of designing functional materials for desirable applications

Course Contents:

Organic Photonic, Electronic, Magnetic and Energy materials: Basic principle and function, Molecular design, examples and application

Molecular switches, motors, machines, memories, logic gates

Organic superconductors, thermoelectric materials

Text Books:

1. T. J. J. Müller and U. H. F. Bunz, Functional Organic Materials, Wiley-VCH, 2007
2. A. Kohler and H. Bassler, Electronic Processes in Organic Semiconductors: An Introduction, Wiley-VCH, 2015
3. A. Credi, S. Silvi and M. Venturi, Molecular Machines and Motors: Recent Advances and Perspectives, Topics in Current Chemistry (Springer), 354, 2014.

Course title	Transient Absorption Spectroscopy									Course No	CY XXXX			
Department	Chemistry	New Credits	L	T	E	P	O	C	TH	Old Credits	L	T	P	C
			3				6	9			3		0	3
Offered for	BSMS									Status				
Faculty	**CY Faculty**									Type	Elective			
Pre-requisite skills										To take effect from	July 2025			
Submission date	Date of approval by DCC		Date of approval by BAC							Date of approval by Senate				

Course Outcomes: At the end of this course, students will be able to:

1. Explain the fundamental principles of transient absorption spectroscopy.
2. Interpret TAS experiments.
3. Analyze kinetic and spectral data from TAS experiments.

Course Content:

Introduction to Transient Absorption Spectroscopy (TAS)

Fundamentals of excited-state dynamics, Time scales of photophysical and photochemical processes, Overview of TAS and its significance in modern research

Ultrafast Laser Systems

Principles of ultrafast laser pulses (femtosecond & picosecond), Mode-locking and chirped pulse amplification, Tunable lasers

Pump-Probe Spectroscopy

Principles of pump-probe techniques**;** Optical layout of a TAS experiment**,** White-light continuum generation**,** Sample preparation considerations

Data Analysis and Kinetic Modeling

Global and target analysis methods, Fitting transient absorption decay curves, Singular value decomposition (SVD) and other advanced techniques

Text Books:

1. Atanu Bhattacharya, Ultrafast Optics and Spectroscopy in Physical Chemistry, World Scientific Publishing Company, 2018
2. Ahmed H Zewail, Femtochemistry: Ultrafast Dynamics of the Chemical Bond (Volumes I & II), World Scientific Publishing Co Pte Ltd., 1994

<table>
<tr><td>Course title</td><td colspan="9">Advanced Optical Spectroscopy</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9"></td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: Students will be able to identify basic principles of photophysical chemistry and the modern techniques and instrumentation required to analyze the excited state dynamics

Course Content:

Overview of basic concepts: Light-matter interaction, Einstein coefficients, introduction to lasers, transition dipole moment, selection rules for electronic transitions, Jablonskii diagram, fluorescence and phosphorescence, kinetics of unimolecular and bimolecular processes.
Advanced concepts: Theory of nonradiative transitions, spin-orbit coupling and singlet-triplet transitions, polarized light absorption and emission: fluorescence anisotropy, solvation dynamics, energetics and dynamics of bimolecular processes like excimer and exciplex formation, resonance energy transfer, mechanisms of fluorescence quenching, introduction to non-linear spectroscopy.
Techniques and instrumentation: Uv-Vis spectrophotometry, steady-state fluorimetry, lasers as excitation sources, time-resolved fluorimetry, transient absorption spectroscopy, surface plasmon spectroscopy, evanescent wave spectroscopy, multiphoton spectroscopy, single-molecule spectroscopy, fluorescence correlation spectroscopy.
Applications: Microscopy (optical, phase-contrast, confocal, FLIM). Applications in biology and analytical chemistry.

Text Books:

1. J M Hollas, Modern Spectroscopy, , John Wiley & Sons, 4th Edn, 2004
2. William W Parson, Modern Optical Spectroscopy, , Springer, Student Edn, 2009
3. K K Rohatgi-Mukhejee, Fundamentals of Photochemistry, Wiley Eastern Ltd., 1992.
4. J R Lakowicz, Principles of Fluorescence Spectroscopy, , Springer, 3rd Edn., 2006
5. W. Demtroder, Laser Spectroscopy- Basic concepts and instrumentation, Springer, 3rd edition, 2004.

<table>
<tr><td>Course title</td><td colspan="9">Statistical Thermodynamics</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td>Department</td><td>Chemistry</td><td>New Credits</td><td>L
3</td><td>T</td><td>E</td><td>P</td><td>O
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<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9"></td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes:

At the end of the course, the learners should be able to:
Explain the laws of thermodynamics as consequences of the statistical properties of ensembles.
Relate the thermodynamic properties with the partition functions.
Calculate the absolute value of thermodynamic quantities (U, H, S, A, G) and equilibrium constant (K) from the spectroscopic data.
Obtain the heat capacity (Cv, Cp) of an ideal gas of linear and non-linear molecules from the fluctuations of the rotational and vibrational degrees of freedom.
Derive the temperature dependence of the second Virial coefficient (real gases) from interatomic potentials.
Predict the temperature range in which the classical statistics is recovered from the quantum statistics.
Understand the molecular origins of the temperature dependence of the rate parameters.

Course Content:

Introduction: Review of the thermodynamic laws and systems; macrostates, microstates and the concept of ensembles; probability distributions, means and fluctuations; statistical entropy and the method of most probable distribution, time versus ensemble average and ergodic hypothesis.

Partition functions and thermodynamic properties: microcanonical, canonical and grand-canonical ensembles; microcanonical partition function, residual entropy and its relation to the third law; canonical partition function, Boltzmann distribution and thermodynamic properties as ensemble averages.

Ideal gases: Boltzmann statistics and molecular partition function; translational, rotational and vibrational partition functions; Absolute values of thermodynamic quantities for ideal monoatomic, diatomic and polyatomic gases; heat capacity of linear and non-linear molecules; the equipartition theorem; temperature dependence of heat capacity.

Quantum ideal gases: Grand-canonical partition function and chemical potential; Fermi-Dirac and Bose-Einstein Distributions for fundamental particles; free electron model and density of states, Fermi Function and Fermi energy.

Solids: Thermodynamics of solids – Einstein and Debye models; heat capacity of solids at low temperatures (universal features).

Real gases: Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients. Temperature dependence of the second virial coefficient and equation of state.

Chemical Equilibrium: Equilibrium constant from the partition function; molecular origins of entropic and enthalpic contributions to equilibrium constant.

Applications to chemical kinetics: Kinetic theory of gases, Maxwell-Boltzmann distribution; reaction rate theories and equilibrium assumption; basics of collision theory, transition state theory, Eyring equation.

Textbooks:

1. T. L. Hill, An Introduction to Statistical Thermodynamics. New York, NY: Dover, 1987.
2. R. Silbey, R. Alberty, and M. Bawendi. Physical Chemistry, New York, NY: John Wiley & Sons, 4th ed., 2004.
3. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford 2014.
4. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004.
5. L. Nash, Elements of Statistical Thermodynamics, New York, NY: Dover, 2nd ed. 2006.
6. D. A. McQuarrie, Statistical Mechanics, University Science Books, California 2005.
7. B. Widom, Statistical Mechanics – A Concise Introduction for Chemists, Cambridge, University Press, 2002

<table>
<tr><td>Course title</td><td colspan="11">Quantum Computing and Quantum Chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td colspan="2" rowspan="2"></td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Faculty</td><td colspan="11">CY Faculty</td><td>Type</td><td colspan="4">Elective</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="11"></td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
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Course Learning Outcomes: (a) Comprehensive understanding of quantum computing principles and their application to chemistry. (b) Develop proficiency in mapping chemical problems to quantum algorithms.

Introduction:

Qubits and Quantum States: Quantum Superposition and Entanglement, Bloch Sphere representation of qubits, Product States and Hartree Approximation, Entanglement and its relation to electron correlation, Measurement of Qubits, Measurement Basis (X, Y, Z),

Quantum Gates and Operations: Single Qubit Gates (Pauli Operators(X, Y, Z), Hadamard Gate, Rotational Gates (Rx, Ry, Rz)), Two Qubit Gates (CNOT, CZ, SWAP), Basis Transformation using gates (e.g., Hadamard for X- and Z-basis transitions)

Quantum States*:* Product states vs Entangled States (e.g. Bell States), Action of Two qubit gates (e.g. CNOT) on Quantum states.

Foundation of Quantum Chemistry for Quantum Computing:

Electronic structure: Hartree Fock Approximation and the Mean-Field Approach; Electron Correlation and its role in Chemistry; Many-body methods like Coupled Cluster theory, Multiconfiguration Self-Consistent Field theory, and Configuration Interaction; Chemical Basis Sets: STO-nG, split-valence basis sets, and correlation-consistent basis sets.

Second Quantization: Basics, Representation of one- and two-electron operators in second quantization, Commutation relations between Fermionic operators, Writing Hamiltonian in the second quantized form with examples.

Femionic-to-Qubit Mappings**:** Jordan-Wigner, Parity, and Bravyi-Kitaev mappings, and their application to small molecules like H2.

Variational Method and Ground State Energy Calculations:
The Variational Principle and its application to simple systems like He atom, Variational Quantum Eigensolver (VQE), Chemistry-Inspired Ansatzes (UCCSD, k-UpCCGSD, LUCJ, etc.), Hardware-efficient Ansatzes (Ry, Rz, SwapRz, Excitation Preserving, Two Local, Givens Rotations, etc.), Frozen Core Approximations and Active Space Transformations, Exponential operators in Quantum Circuit form, Trotter-Suzuki Decomposition for Exponential Operators, Error Mitigation Techniques (e.g. TRex, and Zero noise Extrapolation (ZNE)).

Quantum Circuit Optimization and Measurement Techniques:
Pauli Groupings, Optimization Techniques (SPSA, CG, COBYLA, L-BFGS, ADAM, etc.), Preparation of Quantum States, Choosing the initial point (Random, HF, and MP2 initial points).

Embedding Theory:
HF/DFT Embedding, Density Matrix Embedding Theory (DMET): Concepts and Applications

Advanced Quantum Algorithms for Chemistry:
Ground State Algorithms: (a) Variational Quantum Eigensolver (VQE), (b) Adaptive VQE (Adapt-VQE), (c) Quantum Phase Estimation (QPE), Sample Based Quantum Diagonalization (SQD) with Configuration Recovery.

Excited State Algorithms: (a) Variational Quantum Deflation (VQD), (b) Quantum Subspace Expansion (QSE), (c) Quantum Equation of Motion (q-EOM), (d) Subspace Search VQE (SS-VQE).

Text Books:

1. Nielsen, M. A., and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge: Cambridge University Press, 2010.
2. P. R. Surján, *Second Quantized Approach to Quantum Chemistry*; Springer: Berlin, Heidelberg, 1989.
3. T. Helgaker, P. Jørgensen, J. Olsen *Molecular Electronic-Structure Theory*; John Wiley & Sons, 2000.
4. C. Hughes, J. Isaacson, A. Perry, R. F. Sun, Turner J *Quantum computing for the quantum curious*; Springer Cham, 2021.
5. S. McArdle, S. Endo, A. Aspuru-Guzik, S.C. Benjamin and X. Yuan, *Quantum computational chemistry Rev. Mod. Phys.* 92 015003, 2020.
6. Y. Cao, J. Romero,J. P. Olson, M. Degroote, P. D. Johnson, M. Kieferová, I. D. Kivlichan, T. Menke, B. Peropadre, N. P. D. Sawaya, S. Sim, L. Veis, A. Aspuru-Guzik, *Quantum Chemistry in the Age of Quantum Computing*. *Chem. Rev. 119* (19), 10856– 10915, 2019.
7. D. Claudino, The basics of quantum computing for chemists; *Int. J. Quantum Chem.* , 122(23), e26990, 2022.
8. J. Tilly et. al. *The variational quantum eigensolver: a review of methods and best practices Phys. Rep.* 986 1–128, 2022.
9. H. Liu, G. H. Low, D. S. Steiger, T. Häner, M. Reiher, and M. Troyer, “Prospects of quantum computing for molecular sciences,” *Mater. Theory* 6, 11, 2021.
10. IBM Quantum Documentation.

<table>
<tr><td>Course title</td><td colspan="9">Numerical Methods & Computational Chemistry</td><td>Course No</td><td colspan="4">CY XXXX</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemistry</td><td rowspan="2">New Credits</td><td>L</td><td>T</td><td>E</td><td>P</td><td>O</td><td>C</td><td>TH</td><td rowspan="2">Old Credits</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
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<tr><td>Offered for</td><td colspan="9">BSMS</td><td>Status</td><td colspan="4"></td></tr>
<tr><td>Faculty</td><td colspan="9">CY Faculty</td><td>Type</td><td colspan="4">CORE</td></tr>
<tr><td>Pre-requisite skills</td><td colspan="9">Nil</td><td>To take effect from</td><td colspan="4">July 2025</td></tr>
<tr><td>Submission date</td><td colspan="2">Date of approval by DCC</td><td colspan="7">Date of approval by BAC</td><td colspan="5">Date of approval by Senate</td></tr>
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Course Learning Outcomes: The students will be able to apply basic concepts of numerical methods to various computational problems in Chemistry using the Numerical Programming recipes in FORTRAN language.

Course Contents:
Numerical Methods
Linear Algebra- Systems of linear equations, Matrix inversion, Eigenvalues and eigenfunctions of Hermitian (real symmetric and complex) Matrices, LU decomposition, Diagonalization, Iterative methods for large-scale eigenvalue problems, Jacobi rotation method, Lanczos recursion,
Data regression, Numerical interpolation, polynomial & cubic spline interpolation, fitting with exponentials and orthonormal basis functions.

Calculus- Finite difference methods, evaluation of the first and the second derivatives, Nonlinear equations and roots of polynomials, Scant and Newton-Raphson methods for finding roots of an equation, data interpolation by Newton polynomial method
Numerical integration: trapezoidal and the Simpson methods, Gaussian quadrature, Gauss-Hermite, and Gauss-Legendre intervals
Integration of coupled first-order and second-order differential equations, Runge-Kutta and Predictor-corrector methods
Fourier transformations, Fast Fourier Transformations, spectral analysis

FORTRAN Programming- Brief introduction and usage of available Numerical Recipes

Applications- of numerical methods to various aspects of Computational Chemistry problems involving data fitting, thermodynamics, kinetics, quantum mechanics & spectroscopy using the Numerical Recipes.

Text Books:

1. R W Hamming, Numerical Methods for Scientists and Engineers, Dover Books on Mathematics, 2nd Revised ed. Edition,1987.
2. S S Sastry, Introductory Methods of Numerical Analysis, 5^{th} Edition, PHI Learning Pvt. Ltd., New Delhi, 2012.
3. V Rajaraman, Computer Programming on Fortran 90 and 95, Prentice Hall of India, New Delhi, 2006.
4. W H Press, S A Teukolsky, W T Vetterling and B P Flannery, Numerical Recipes; The art of Scientific Computing, Cambridge University Press, New York, 2007.