M.Sc. Chemistry (2-year) Programme

2024 Batch Onwards

SoC, UoH

	SEMESTERS (I-IV)						
	SEMESTER – I 21				SEMESTER – II 21		
Course ID	**TITLE**	**CREDITS**	**ABBR.**	**Course ID**	**TITLE**	**CREDITS**	**ABBR.**
CY401	Basic Concepts and Coordination Chemistry	3	DSC/Major	CY451	Main group and inner transition elements	3	DSC/Major
CY402	Physical Organic Chemistry	3	DSC/Major	CY452	Organic Reactions and Mechanisms	3	DSC/Major
CY403	Quantum Chemistry	3	DSC/Major	CY453	Molecular Spectroscopy	3	DSC/Major
CY404	Symmetry, Group Theory and Mathematics	3	DSC/Major	CY454	Chemical and statistical thermodynamics	3	DSC/Major
CY405	Advanced Inorganic Chemistry Lab	3	DSC/Major	CY455	Biological Chemistry	3	DSC/Major
CY406	Advanced Organic Chemistry Lab	3	DSC/Major	CY457	Physical Chemistry Lab	3	DSC/Major
CY407	Instrumental Methods of Chemical Analysis	3	DSC/Major	CY456	Industrial Chemistry (Theory and Lab)	3	DSC/Major
Internship (during Summer Break after II Sem) (4 Credits) (To be evaluated during III Sem) Int / RI / CE							
	SEMESTER – III (21)				SEMESTER – IV (21)		
Course ID	**TITLE**	**CREDITS**	**ABBR.**	**Course ID**	**TITLE**	**CREDITS**	**ABBR.**
CY501	Spectroscopic Methods for Organic Compounds	3	DSC/Major	CY551	Chemistry of Materials	3	DSC/Major
CY502	Advanced Organic Synthesis	3	DSC/Major	CY553	Project – II (Research)	9	DSC/Major
CY503	Chemical Dynamics	3	DSC/Major	CY552	Polymer Chemistry	3	DSC/Major
CY504	Chemical Binding	3	DSC/Major	(CY574 - CY587)	Electives (Total = 3); 2 credits each	6	ScSE
CY505	Advanced Inorganic Chemistry	3	DSC/Major				
CY507	Computer Applications and Programing Lab	3	DSC/Major				
CY508	Project – I (Research/Literature/Seminar)	3	DSC/Major				

EXIT OPTIONS

End Semester	Minimum Credit Requirement	Degree / Certificate
II Semester	Total credits (**42**)	**No Exit option**
IV Semester	Total Credits (**88**)	M.Sc. Chem

DETAILED SYLLABUS

Semester I

Basic Concepts and Coordination Chemistry – 3

Prerequisite: None

Shapes of Small Molecules: VSEPR theory - Coordination polyhedra - Enumeration of geometrical and optical isomers. (3 h)

Theory of Acids and Bases: Bronsted and Lewis acids and bases - Gas phase versus solution acidity - Solvent leveling effects - Hardness and softness - Surface acidity. (5 h)

Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams. (6 h)

Coordination Chemistry: d-orbital splitting in various fields – Spectroscopic states and term symbols - Hole formalism - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq. B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries - Bonding involving pi-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements. (18 h)

Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans -effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and -redox reactions, Fluxional molecules. (8 h)

Suggested reading:

(1) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ‘’Inorganic Chemistry’’, 3rd Edn, OUP, 1999.
(2) C. Housecroft, A. G. Sharpe, ‘’Inorganic Chemistry’’, 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(3) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ‘’Advanced Inorganic Chemistry’’, 6th Edn Wiley, 1999).
(4) J. E. Huheey, E. A. Keiter, R. L. Keiter, ‘’Inorganic Chemistry: Principles of Structure and Reactivity’’, 4th Edn, Prentice Hall, 1997 (or a previous edition).
(5) G. L. Miessler, D. A. Tarr, ‘’Inorganic Chemistry’’, 3rd Edn, Pearson Education, 2004.
(6) G. Wulfsberg, ‘’Inorganic Chemistry’’, University Science Books, 2000.

Instrumental Methods of Chemical Analysis – 3

Prerequisite: None

Introductory treatment of the following techniques, including basic instrumentation and illustrative applications from all branches of chemistry.

Absorption and emission spectroscopy (8 h)

Atomic spectroscopy – instrumentation of AAS, AES, ICP-MS/AES Molecular spectroscopy – instrumentation of UV-Vis, IR and CD spectroscopy

Mass spectrometry (8 h)

Basic treatment of ionization methods – FD, EI, CI, ESI, MALDI, FAB Mass analyzers – sectors, quadruple, TOF, ion trap, Detectors – electron multiplier, Faraday cup, array detectors Applications – small molecules, inorganic complexes, polymers, proteins

NMR spectroscopy (8 h)

Basics – Larmor precession, resonance absorption, magnetic fields, shielding and chemical shifts, chemical equivalence, relaxation processes Solution state (^{1}H, ^{13}C) and solid state techniques Instrumentation – block diagram, magnets, sample probe, RF generation and detection,

FT NMR/ESR spectroscopy (6 h)

Introduction – g factor, hyperfine coupling, fine structure Instrumentation – microwaves, waveguides, magnetic field modulation Applications – free radicals, metal complexes, reaction intermediates

Diffraction Techniques (8 h)

X-ray diffraction – Crystal lattices and Miller planes, Bragg condition, Ewald's sphere Instrumentation – X-ray sources including synchrotron, filters, detectors including CCD ,Powder diffraction techniques – Debye-Scherrer Single crystal data collection – 4-circle method, Laue method, rotating crystal

Suggested Reading:

1. Undergraduate Instrumental Analysis by James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, Sixth Ed, Marcel Dekker, New York, 2005.
2. . Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, Fourth Ed., Brooks/Cole Thomson Learning 2009.
3. 3. Physical Chemistry by Peter Atkins and Julio de Paula, 9th Ed., Oxford University Press, 2010.
4. 4. Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds by William Henderson and J. Scott McIndoe, John Wiley & Sons Ltd, 2005.

Quantum Chemistry – 3

Prerequisite: Basic mathematics, differential equations, orthogonal polynomials, and matrix algebra

Review of classical mechanics. Wave-particle duality and Uncertainty principle.
Postulates of quantum mechanics. Operator algebra. Properties of hermitian operators. Eigenvalue problem. Commutators and Uncertainty Principle.
Elementary applications of quantum mechanics- unbound motion in one dimension. Tunneling. Bound motion – particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor. Angular momentum algebra- Hydrogen atom.
Methods of obtaining approximate solution to the time independent Schrödinger equation –perturbation theory and variational method. Application.
Many electron atoms. Spin and Pauli exclusion principle. Hund's rule. Slater determinants. Electronic term symbols.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.
2. Quantum Chemistry, D. A. McQuarrie, University Science Books.
3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Quantum Mechanics, L. Pauling and E. B. Wilson,McGraw Hill International Ed.
5. Quantum Mechanics, N. Zettili, John Wiley and Sons.
6. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
7. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
8. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

Symmetry, Group Theory and Mathematics– 3

Prerequisite: Basic Mathematics

Symmetry elements and operations; matrix representation of symmetry operations; properties of groups and point groups; reducible and irreducible representations, Great Orthogonality Theorem, construction of character tables; direct product representations; projection operators and symmetry adapted linear combinations. Applications to mean observables in molecular spectroscopy. Introduction to molecular space group.

Real and Complex number algebra, Vector algebra: products of vectors, orthonormal vectors; Sequences and series: finite & infinite series, MacLaurin & Taylor series.

Determinants and Matrices: properties of determinants, matrix algebra, orthogonal transformation, rank and inverse of matrix, eigenvalues and eigenvectors.

Functions and variables': limits and continuity; Differential calculus: first- & higher-order derivatives, minima and maxima, partial differentiations, exact and inexact differentials.

Integral Calculus: Indefinite and definite integrals, improper integrals, methods of integration.

Differential Equations: ordinary first- and second-order differential equations and their method of solutions, power series method, Hermite, Legendre, Laguerre and Bessel equations, partial differential equations, Fourier series and transforms.

Probability and Statistics: permutation & combination, discrete and continuous probability distribution functions, joint and conditional probability distributions, moment and error calculations.

Suggested Reading:

1. Symmetry and Group Theory in Chemistry, Mark Ladd, Horwood Publishing Limited
2. Molecular Symmetry and Group Theory. Allan Vincent, John Wiley & Sons, LTD.
3. Symmetry: An introduction to group theory and its applications. R. McWeeny, Dover Publications, Inc.
4. Chemical Applications of Group Theory. F. A. Cotton, John Wiley & Sons, Inc.
5. Symmetry and Structure. S. F. A. Kettle, Wiley.
6. Group Theory in Chemistry: Bonding and Molecular Spectroscopy by Ghosh and Mukherjee
7. Advanced Engineering Mathematics. E. Kreyszig, Wiley.
8. The Chemistry Maths Book, E. Steiner, 2nd Ed., Oxford University Press
9. Mathematics for Physical Chemistry. R. G. Mortimer, Academic Press.
10. Mathematics for Chemistry and Physics. G. Turrell, Academic Press.
11. G. Stephenson, Mathematical Methods for Science Students (510.245 St44M)
12. H. H. Jaffè and M. Orchin, Symmetry in Chemistry (541.2 J18S)

Physical Organic Chemistry – 3

Prerequisite: Basic and intermediate courses in physical and organic chemistry concepts

M.O. and V.B. methods (Hückel's MO Method, pictorial representation of MOs for molecules, qualitative application of MO theory to reactivity. [2]

Electronic effects on the stability of reactive intermediates, non-classical carbocations, anomeric effects. Aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticiy. [3]

Acids and bases, HSAB principle, strain and stability [2]

Stereochemistry: Chirality, chiral compounds without stereocenters – allenes, biphenyls, helicenes, annulenes, cyclophanes, *trans*-cyclooctene (selected examples). Invertomerism. Resolution - kinetic and dynamic kinetic resolutions. Stereoselective and stereospecific reactions. asymmetric reactions, topicity of ligands and faces; *Pro*-R, *Pro*-S, and *Re*/*Si* descriptors. [7]

Conformational analysis of acyclic and cyclic systems: Eclipsed, staggered, gauche and anti, dihedral angle, torsion angle, energy barrier of rotation, relative stability of conformation on the basis of steric effect , dipole-dipole interaction, H-bonding; conformational analysis of alkanes, haloalkanes, 1,2-diols, 1,2-halohydrin. [6]

Conformational analysis of cyclic systems: Baeyer strain theory, mono- and di-substituted cyclohexanes. Stereochemistry of ring systems other than six-membered ring, fused and bridged systems. Effect of conformation on reactivity: Stereoelectronic effects and nucleophilic addition to carbonyls (Cram's, Felkin-Anh and Cieplak models). [7]

Thermodynamics and kinetics: Bond energies and thermochemistry – enthalpy, entropy, transition state theory, kinetic parameters, Hammond's postulate, Curtin-Hammett principle, kinetic and thermodynamic control. Kinetic isotope effects and solvent effects. [6]

Linear free energy relationships - Hammett plots, steric and polar effects-Taft parameters and solvent effects-Grunwald-Winstein plots. [3]

Suggested reading:

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.
2. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry Illustrated Edition, University Science, 2005.
3. M. B. Smith and J. March, March Advanced Organic Chemistry, 7th edition, Wiley, 2015.
4. A. J. Kirby, Stereoelectronic Effects, Oxford University Press, 1996.
5. V. K. Yadav, Steric and Stereoelectronic Effects in Organic Chemistry, 2nd edition, Springer, 2021.
6. P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
7. I. Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds Wiley Student Edition, 2008.

Advanced Inorganic Chemistry Lab - 3

Prerequisite: Basics of Inorganic Chemistry

Part A- Quantitative Analysis

Statistical analysis of data sampling methods.
Redox titrations (permanganometry, dichromatometry, iodometry).
Complexometric titrations using EDTA (estimation of some metal ions, hardness of water).
Precipitation titration (estimation of Ag).
Quantitative separation of metal ions from a binary mixture (e. g., Cu^{2+}/Fe^{3+}).
Gravimetric analysis (e. g., estimation of Ni^{2+}).
Analysis of ores and minerals (e. g., Iron ore, Potassium alum).
Ion exchange separation of metal ions (e. g., Zn^{2+}/Mg^{2+}).

References

1. Laboratory manual provided by teacher
2. Vogel's Qualitative Inorganic Analysis, 7th Edition
3. Vogel's Textbook of Quantitaive Inorganic Analysis, 4th Edition, Revised by J. Bassett, R. C. Denney, G. H. Jeffery, and J. Mendham, Longmann (1982)
4. Quantitative Analysis, R. A. Day and A. L. Underwood, 6th Edition, Pearson Education India (2015).

Part B- Qualitative Analysis

Reactions of some less common metal (TI, W, Mo, V, Zr, Th, U) ions.
Simple reactions to illustrate the aqueous chemistry of some typical transition metal ions
Study of oxidation states of V, Cr, Mn – Oxo and Peroxo ions - Complex formation of Co^{2+}: Reaction with H_2O/HCl.
Group separation of cations (mostly trace elements).

References

1. Laboratory manual provided by teacher
2. Vogel's Qualitative Inorganic Analysis, 7th Edition
3. Vogel's Textbook of Quantitaive Inorganic Analysis, 4th Edition, Revised by J. Bassett, R. C. Denney, G. H. Jeffery, and J. Mendham, Longmann (1982);
4. Quantitative Analysis, R. A. Day and A. L. Underwood, 6th Edition, Pearson Education India (2015).

Part C- Synthesis and Characterization of Inorganic Compounds/ Complexes:

Synthesis of a variety of Inorganic compounds/complexes of 3d metal ions, main group elements and rare earths by using common experimental techniques.
Introduction to various physical measurements (IR, UV-Vis, Mass, NMR, Magnetic susceptibility, EPR and X-ray diffraction) for characterization of the compounds.
Analysis and interpretation of the physical data of the compounds to determine their structures.
Preparation of Scientific Reports.

References:

1. David W. H. Rankin, Norbert W. Mitzel and Carole A. Morrison, Structural Methods in Inorganic Chemistry, John Wiley and Sons, 2013.
2. Relevant literature references.

Advanced Organic Chemistry Lab – 3

Prerequisite: Working knowledge of chemistry laboratory and chemical transformations

Different laboratory techniques: TLC, column chromatography, separation and analysis of organic compounds.

Multistep organic synthesis involving oxidation, reduction, electrophilic substitution, organometallic reagents, cycloaddition, photochemical, rearrangements, radical and enzymatic reactions.

Resolution of racemic organic compounds.

Characterization of the synthesized compounds using different analytical techniques.

Suggested reading:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, A Microscale Approach to Organic Laboratory Techniques, 6th Edition, Cengage Learning, ELBS (2016).
2. A. I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
3. Laboratory manual.

Semester II

Main group and inner transition elements – 3

Prerequisite: Basic Concepts and Coordination Chemistry

Perspectives, periodicity & periodic anomalies; Relativistic effects on chemical properties (2 h)

Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals-Hydrides→classification: electron deficient, electron precise and electron rich hydrides (2 h)

Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, cryptands and organometallic compounds (2 h)

Group 13 elements: Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR3 compounds, Subvalent organo-Al compounds, Organo-gallium, -indium, and –thallium compounds (8 h)

Group 14 elements: Allotropes of Carbon- C60 and its compounds (fullerenes) - carbon nanotubes: synthesis and properties -Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds (6 h)

Group 15 elements: P(V) compounds (structure, bonding, reactivity) - P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, P-S compounds (7 h)

Group 16 elements: Sulfur - polycationic and anionic species - SN compounds.(3 h)

Group 17 elements: Charge-transfer complexes of halogens, interhalogen compounds, halogen oxides and oxygen fluorides, pseudohalogens. (3 h)

Group 18 elements: Noble gas clathrates and compounds. (3 h)

Inner transition elements: Chemistry of f-block elements - Binary compounds - Organometallic compounds - Relation to p-block and d-block chemistry - Transactinides (super-heavy elements). (4 h)

Suggested reading:
(1) A. G. Massey, "Main group chemistry", Wiley, 2000.
(2) N. N. Greenwood and A. Earnshaw, "Chemistry of the Elements", Pergamon Press, 1989.
(3) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Edn, OUP, 1999.
(4) C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Edn, (or 4th Edn in 2012) Prentice Hall/Pearson, 2008.
(5) F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn, John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
(6) J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Edn, Prentice Hall, 1997 (or a previous edition).

Molecular Spectroscopy – 3

Prerequisite: Quantum Chemistry, Symmetry and Group Theory

Interaction of radiation with matter-semiclassical treatment, time-dependent perturbation theory and transition rates. Electric dipole, quadrupole and magnetic dipole transitions. Spectral broadening and line shapes; Pure rotational spectroscopy: classification of rotors, quantum mechanical treatment of selection rules, rigid and non-rigid diatomic rotors, intensity distribution, linear and nonlinear polyatomic molecules; Pure vibrational spectroscopy: harmonic and anharmonic diatomic molecules, quantum mechanical treatment of selection rules, overtone transitions; Ro-vibrational spectroscopy of diatomic molecules, combination difference; Polyatomic molecular vibrations, normal modes, selection rules, overtone and combination transitions; Rotational and vibrational Raman Spectroscopy and selection rules; Electronic spectroscopy of diatomic molecules, electronic states - molecular terms, Franck-Condon principle, Selection rules, vibrational and rotational fine structures, fates of electronic excited states and their lifetimes; Resonance Raman transitions and application; Principles of coherence spectroscopy and wave-packet; Use of Lasers; Electron Spectroscopy- PES, XPS and ESCA; Magnetic resonance: NMR and EPR.

Suggested reading:

1. Molecular Spectroscopy. I. N. Levine, Wiley – Interscience Publication.
2. Molecular Spectroscopy. J. D. Graybeal, McGraw Hill.
3. Spectra of atoms and molecules (3rd edition), Peter F Bernath
4. Modern Spectroscopy. J. M. Hollas, John Wiley & Sons.
5. High Resolution Spectroscopy. J. M. Hollas, Butterworths.
6. Fundamentals of Molecular Spectroscopy. C. N. Banwell and E. M. McCash, Tata McGraw-Hill publishing.
7. Principles of Ultraviolet Photoelectron Spectroscopy, J. W. Rabalais, John Wiley & Sons.
8. Molecular Spectra & Molecular Structure. G. Herzberg, Van Nostrand Reinhold Company.

Chemical and Statistical Thermodynamics – 3

Prerequisite: Basics of thermodynamics, probability theory

Review of classical thermodynamics and Probability (4 h)

Concepts of statistical ensemble, Postulates of Statistical Mechanics, Connection of entropy with probability, extreme value principle (7 h)

Probability descriptions of micro-canonical, canonical and grand canonical ensembles; ergodic principle, Gibbs paradox (6 h)

Boltzmann distribution, Quantum statistics: Fermi-Dirac statistics and Bose-Einstein statistics (6 h)

Partition function, thermodynamic quantities from partition function; translational, rotational, vibrational and electronic partition functions of ideal gas molecules (9 h)

Applications: equilibrium constant, mixing of polymer solutions, Specific heats of solids-Einstein and Debye models (5 h)

Debye-Hückel theory, non-ideal gas-virial equation of state and virial coefficients (3 h)

Suggested reading:

1. Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience (2nd edition) by Ken A Dill and Sarina Bromberg
2. Fundamentals of Statistical and Thermal Physics by Frederick Reif
3. Physical Chemistry (9th edition) by Peter Atkins and Julio de Paula
4. Physical Chemistry (3rd edition) by Thomas Engel & Philip Reid
5. Statistical Mechanics (2nd edition) by Pathria
6. Statistical mechanics a course introduction for chemists by Benjamin Widom

Organic Reactions and Mechanisms - 3

Prerequisite: Knowledge of reaction mechanisms, stereochemistry and physical organic chemistry

Methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related species. [5 h]

Detailed reaction mechanisms and effect of different parameters in the regio-, stereo-, chemo-selective outcome of addition, substitution, elimination, oxidation, reduction, rearrangement and pericyclic reactions. [22 h]

Baldwin ring closure rules [1h]

Heterocycles: Synthesis, properties and reactions – O, S, N containing 3, 4, 5 and 6-membered heterocycles [4h]

Organic photochemical reactions. [4 h]

Suggested reading:

1. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th edition, Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001.
4. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company, 1999.
5. P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
6. I. Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
7. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1991.
8. B. Halton, J. M. Coxon, Organic Photochemistry, Cambridge University Press, 2011.
9. S. Sankararaman, Pericyclic Reactions: A Textbook: Reactions, Applications and Theory, Wiley-VCH, 2005.

Biological Chemistry – 3

Prerequisite: None

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction to biomolecules: Examples of biomolecules and building blocks of biopolymers. Types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

Amino acids, peptides and proteins: Primary structure of proteins, end group determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins α-helix, β-pleated sheet, β-bend and collagen triple helix. Tertiary structure and structural motifs - protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the Michaelis-Menten equation, various types of enzyme inhibition. application of enzymes in chemical synthesis, enzyme models and their applications.

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA. Base pairing, double helical structure of DNA and forces stabilizing nucleic acid structure. Methods used in nucleic acid separation and characterization, nucleic acid sequencing.

Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis. Control of transcription and protein-DNA interactions. The genetic code, tRNA structure and codon-anticodon interactions. Ribosomes and their structure. Gene cloning and site-directed mutagenesis.

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications. Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

Suggested reading:

1. Biochemistry by *D. Voet & J. G. Voet*, 4th Edition (2010) Published by John Wiley (New York).
2. Lehninger's Principles of Biochemistry by *D. L Nelson & M. M. Cox*, 5th Edition (2008) Published by W. H. Freeman (New York) and CBS Publishers (New Delhi).
3. Biochemistry by *J. M. Berg, J. L. Tymoczko & L. Stryer*, 5th Edition (2002) Published by W. H. Freeman (New York).

Industrial Chemistry (Theory & Lab) – 3

Prerequisite: Basic knowledge of organic and inorganic chemistry and laboratory working experience

Fuels, Petrochemicals and petroleum products [2]
Catalysis: Relevant to industrial applications [2]
Industrial organic process: Synthesis of methanol, ethanol, acetic acid, acetone, glycerol and ethyl acetate etc. [3]
Active pharmaceutical intermediates and drugs [2]
Insecticides and pesticides. [1]
Dyes, paints and pigments. [1]
Electroplating, selected metallurgy. [3]
Silicates, glass, ceramics, refractories, cement. [2]
Fertilizers: Nitrogenous and phosphate fertilizers. [1]
Soaps and detergents. Tanning of leather. [1]
Green and environmental aspects of industrial processes. [2]

Suggested reading:

1. P. J. Chenier, Survey of industrial chemistry, 3rd Edition, Kluwer Academic/Plenum Publishers, 2002.
2. K. Weissermel, H.-J. Arpe, Industrial Organic Chemistry, Wiley-VCH, 2003.
3. M. A. Benvenuto, Industrial Inorganic Chemistry, De Gruyter, 2015.
4. S. E. Manahan, Fundamentals of Environmental Chemistry, 3rd edition, CRC press, 2008.

Experiments based on major industrial processes, operations and methods of analysis of Industrial Chemicals and materials. (minimum 6 experiments)

1. Synthesis of paracetamol
2. Synthesis of indigo and dyeing of cloth
3. Estimation of ascorbic acid
4. Preparation of soap
5. Preparation of nylon 6 6
6. Synthesis of molecular sieve – zeolite X and cobalt exchange reaction with it
7. Preparation of super absorbent polymer and exploration of its properties

Suggested reading:

Laboratory manual

Physical Chemistry Lab – 3

Prerequisite: Knowledge and working in organic, inorganic and physical chemistry labs

1. Kinetics of iodine clock reaction
2. Study of an oscillating reaction
3. Determination of dipole moment change on electronic excitation

4. Adsorption of acetic acid on charcoal
5. Estimation of CMC of a micelle using fluorescence
6. Spectrophotometric determination of pKa
7. Estimation of CMC of a micelle using conductance
8. Conductometric titration of a charge transfer complex
9. Phase diagram of a 3-component system
10. Determination of excited state acidity constant
11. Kinetics of an enzyme-catalyzed reaction
12. Potentiometric titration of a redox reaction
13. Differential scanning calorimetric study
14. Determination of the unit cell of a crystal

Suggested reading: Lab manual (http://chemistry.uohyd.ac.in/Files/Other/LabManual%20_CY457.pdf)

Semester III

Advanced Inorganic Chemistry – 3

Prerequisite: CY401

Recent Advances in Main Group Chemistry: Low and hypervalent compounds – p(pi)-p(pi) bonding in heavier main group chemistry. (3 h)

Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor ligands - 16 electron and 18 electron rules – Stability and Reactivity - Isolobal analogy - Structure and bonding - Agostic interaction. (8 h)

Homogeneous and Heterogeneous Catalysis: Hydrogenation, carbonylation, polymerization, Wacker oxidation and other reactions catalyzed by transition metal complexes. (5 h)

Metal Cluster Compounds: Metal-metal bond - Carbonyl and non-carbonyl clusters - Structure and bonding - Low-dimensional solids - Clusters in catalysis. (4 h)

Bioinorganic Chemistry: Biochemistry of iron- its storage, transport and function; Transport and storage of dioxygen- structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin; Electron transport proteins- cytochromes and Fe-S proteins; Copper containing enzymes- blue and non-blue copper enzymes, ascorbate oxidase, tyrosynase, galactose oxidase, superoxide dismutase; Zinc containing enzymes- carboxy peptidase A, carbonic anhydrase, alcohol dehydrogenase; Iron containing enzymes- catalase, peroxidase and cytochrome P-450; Photosynthesis; Nitrogen fixation; Bioinorganic chemistry of alkali and alkaline earth metal cations; Toxicity of metals. (16 h)

Inorganic Photochemistry: Ligand field photochemistry of dn complexes - Photochemistry of carbonyl compounds - Energy conversion (solar) and photodecomposition of water. (4 h)

Suggested reading:

(1) Textbooks suggested for CY-401.

(2) B. D. Gupta, A. J. Elias, "Basic Organometallic Chemistry", University Press, 2010.

(3) I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, "Bioinorganic Chemistry", VLSE with Univ. Sci. Books, 1998.

Spectroscopic Methods for Organic Compounds – 3

Prerequisite: Advanced knowledge of physical, theory of spectroscopic, and organic chemistry

Electronic spectroscopy: Basic principle, electronic transitions and application to structure elucidation. Polarimetry: Optical rotatory dispersion and circular dichroism. [3 h]

Infrared Spectroscopy: organic functional group identification through IR spectroscopy. [5 h]

NMR Spectroscopy: ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift d, inductive and anisotropic effects on d, chemical structure correlations of d, 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 and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation phenomena, DEPT, NOE effects, ^{1}H and ^{13}C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems). 2D NMR spectroscopy. Multinuclear NMR. [16 h]

Mass spectrometry: Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules. [6 h]

Structure elucidation problems using the above spectroscopic techniques. [7 h]

Suggested reading:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. D. L. Pavia and G. M. Lampman Introduction to Spectroscopy 5th Edition, Cengage Learning, 2015.
3. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw Hill, 6th edition 2007.
4. H. Gunther, NMR Spectroscopy, 3rd edition, Wiley-VCH, 2013.
5. J. H. Simpson, Organic Structure Determination Using 2-D NMR Spectroscopy, Academic Press, 2008.
6. J. B. Lambert, E.P. Mazzola, Nuclear Magnetic Resonance Spectroscopy, Pearson Education.
4. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.

Chemical Dynamics – 3

Prerequisite: Kinetics, Transport Phenomenon and Surface Chemistry

Review of basic concepts in kinetics; Fast reactions: experimental techniques; Theories of reaction rates; Unimolecular reactions; rates of photochemical processes, Reactions in solution: reactions between ions, diffusion controlled reactions, electron transfer reactions; Composite reactions including photochemical reactions; Homogeneous and heterogeneous catalysis; Kinetic isotope effect; Molecular reaction dynamics; Transport properties: Diffusion, viscosity, thermal conductivity, ion transport, dynamic electrochemistry

Suggested reading:

1. Physical Chemistry: A Molecular Approach. D. A. McQuarrie and J. D. Simon, University Science books
2. Physical Chemistry. P. W. Atkins and J. de Paula, Oxford University Press.
3. Physical Chemistry. I. N. Levine, McGraw Hill.
4. Chemical Kinetics. K.J. Laidler, Pearson.
5. Chemical Kinetics and Reaction Dynamics, P.L. Houston, Dover Publications, 2006

Advanced Organic Synthesis - 3

Prerequisite: Advanced knowledge of reaction mechanisms, reactive intermediates and chemical transformations

Synthetic analysis and Planning: Retrosynthetic analysis, synthetic equivalent, control of stereochemistry, linear, convergent and divergent syntheses. [3 h]

Use of protecting groups in multi-step synthesis: Different protection and deprotection methods. [3 h]

Modern synthetic methods involving various oxidizing, reducing agents, C-C bond forming reactions by alkylation, acylation, organometallic, radical, pericyclic reactions and rearrangements. [20 h]

Discussion of selected syntheses of natural products. [3 h]

Asymmetric organocatalytic transformations, organometallic catalysis - selected examples. [3 h]

Solid phase organic synthesis, photocatalysis, electrochemical synthesis, NHC catalysis [2 h]

Sustainable and green chemistry [2 h]

Suggested reading:

1. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.
2. A. Carey and and R. J. Sundberg, Advanced Organic Chemistry, Part B, Fifth Edition, 2007
3. E. J. Corey and X. M. Cheng, The Logics of Chemical Synthesis, Wiley, 1989.
4. K. C. Nicolaou, Classics in Total Synthesis, Vol 1, 2 and 3.
5. S. Warren and P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd edition, Wiley, 2008.
6. J. H. Fuhrhop, G. Li, Organic Synthesis: Concepts and Methods, 3rd edition, VCH, 1994.
7. W. Carruthers, Some Methods of Organic Synthesis, Cambridge University Press.
8. H. O. House, Modern Synthetic Reactions, Benjamin-Cummings Publishing Co. 1972.

Project I - 3

Each student is assigned to a faculty supervisor to carry out a research project. The student gets trained on the following aspects:

Literature survey on the assigned research topic using standard search tools such as SciFinder.

Learning presentation tools such as Powerpoint, ChemDraw etc…

Developing scientific writing and presentation skills by writing a report and oral presentation on the assigned topic.

The student will get trained in understanding research problem, addressing the chosen research problem by designing and executing experimental and/or computational experiments and analyse and interpret the results. At the end of the project each student will submit a report of the work done and make a presentation for evaluation.

Computer Applications and Programming Lab – 3

Prerequisite: Quantum Chemistry, Symmetry & Group Theory and Molecular Spectroscopy

Programming in FORTRAN: Introduction to Linux operating system, Program design (algorithm), organization of program, data types and integer constants, complex constants, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmetic, library functions, input/output specification, formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program.

<u>Computational Chemistry Experiments:</u>

C1 - Study of normal modes- optimization of molecular geometry, computation of normal modes and frequencies, analysis of the symmetries of the normal modes, effect of molecular symmetry on the degeneracies, impact of mass on the frequencies

C2 - Determination of equilibrium constants- optimization of molecular geometry of reactant and product, computation of the rotational constants, vibrational frequencies etc., calculation of partition functions, calculation of equilibrium constant at different temperatures

C3 - Determination of rate constants- optimization of molecular geometry of reactant and product, calculation of transition state, computation of the rotational constants, vibrational frequencies etc. for the reactant and transition state, calculation of partition functions, calculation of rates at different temperatures

C4 - 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

C5 - Construction of Walsh diagram- computation of the MO energies at different geometries of a molecule (eg. H_2O, Li_2O), examination of the molecular orbitals and their symmetries, plot of the MO energies versus the geometric parameter reactant, qualitative analysis of the trends in the orbital energy variations

C6 - 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

C7 - Molecular modeling- H-bonded complexes – geometry optimization, analysis of energetics; exciton coupling in chromophore aggregates; effects of solvation

Alternative experiments- Intrinsic reaction coordinate, Natural bond orbital analysis

Suggested Reading:

1. Fortran 77 and Numerical Methods, C. Xavier, New Age International Publishers.
2. Computer Programming in Frotran, V. Rajaraman, PHI Learning Private Limited.
3.Numerical Analysis and Computational Programming, S. A. Mollah, Books and Allied (P) Ltd.
4. Numerical Recipes in Fortran: The art of Scientific Computing, W. H. Press, S. A. Teukolsky, W. T. Vellerling and B. P. Flannery, Cambridge University Press.

Chemical Binding - 3

Prerequisite Course / Knowledge (If any): Courses (Symmetry, Group Theory and Mathematics, Quantum Chemistry, Chemical and Statistical Thermodynamics)

Detailed Syllabus

The Born-Oppenheimer approximation. Electronic structure theory: MO and VB theories, application to H2+ and H2. MO and VB wavefunctions of polyatomic systems. Hϋckel pi-electron theory. Walsh diagram and molecular geometry.

Hartree-Fock theory, Brillouin conditation, Non-orthogonal basis and Roothaan equation, SCF method. Koopmann's theorem.

Post Hartree-Fock methods. Electron correlation. Basis sets.

Density functional theory and application.

Suggested reading:

1. Quantum Chemistry, H. Eyring, J. Walter and G. E. Kimball, John Wiley & Sons.

2. Quantum Chemistry, D. A. McQuarrie, University Science Books.

3. Quantum Chemistry. I. N. Levine, PHI Learning Private Ltd.
4. Molecular Quantum Mechanics. P. W. Atkins and R. S. Friedman, Oxford University Press.
5. The Chemical Bond, J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley and Sons.
6. Modern Quantum Chemistry. A. Szabo and N. S. Ostlund.

Semester IV

Chemistry of Materials – 3

Prerequisite: Knowledge of organic, inorganic, physical, analytical chemistry and symmetry in chemistry

SOLID STATE STRUCTURE

Types of solids; Order - spatial, orientational; Symmetry in crystals - primitive lattice vector – Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - systematic absences - reciprocal lattice - Ewald construction - structure factor - crystal structure solution and refinement - common crystal structure motifs; quasicrystals. **[6 h]**

DEFECTS AND NONSTOICHIOMETRY

Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres.
[2 h]

THERMAL PROPERTIES

Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conduction.
[3h]

ELECTRICAL PROPERTIES

Free electron theory - electrical conductivity and Ohm's law - Hall effect; Energy bands - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; p-n junctions; Semiconductor/metal transition; Superconductivity - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices.
[9h]

MAGNETIC PROPERTIES

Classification of magnetic materials; Langevin diamagnetism; Quantum theory of paramagnetism; Cooperative phenomena - ferro, antiferro and ferrimagnetism - magnetic domains and hysteresis; Superparamagnetism.
[4h]

OPTICAL PROPERTIES

Optical reflectance - plasmon frequency; Raman scattering in crystals; Photoconduction; Photo and electroluminescence; Lasers; Photovoltaic and photoelectrochemical effects. **[3h]**

GENERAL CONCEPTS IN MATERIALS SYNTHESIS

Phase diagrams; Preparation of pure materials; Nucleation and crystal growth; Crystal growth techniques; Zone refining. **[4h]**

INTRODUCTON TO DIFFERENT CLASSES OF MATERIALS

High T_C superconductors, Ionic conductors, Polymers, Liquid crystals, Molecular materials, Nanomaterials. **[15h]**

Reading material

1. H. V. Keer, Principles of the Solid State (541.0421 K25P)*

2. L. E. Smart and E. A. Moore, Solid State Chemistry: an Introduction (541.0421 Sm295)*

3. M. T. Weller, Inorganic Materials Chemistry (546 W45I)*

4. K. J. Klabunde, Nanoscale Materials in Chemistry (660 K66N)*

5. W. D. Callister, Materials Science and Engineering, An Introduction (620.11 C13M)*

6. C. Kittel, Introduction to Solid State Physics (530.41 K65I)*

7. T. P. Radhakrishnan, Core Concepts for a Course on Materials Chemistry (620.112 R11C)*

8. Journals like Chemistry of Materials, Journal of Materials Chemistry, Advanced Materials etc..

Web resource: http://chemistry.uohyd.ac.in/~CY551/

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*Call number of the textbook in the IGML, University of Hyderabad

Polymer Chemistry – 3

Prerequisite: Knowledge of physical, organic and analytical chemistry and basic and intermediate level courses

Definition: Polymer, monomer, repeat unit, polymerization. Classification: Polymers based on source and polymerizations-polymer composition and structure. Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names. Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers). Effect of Polymer structure on their properties

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot)

Physical State and Morphology: Crystalline and Amorphous state, Thermal transitions, Glass-Rubber transition, Mechanical properties– stress-strain behavior, Elastomer, Fibers and Plastics

Polymer Synthesis: Step, chain and miscellaneous polymerizations, Kinetics of polymerization, Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization. Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers. State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc.

Polymer characterization - Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis; Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy; Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension

Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Uses

Application of Synthetic Polymers: Materials and Biological importance and uses. Nanomaterials, Conducting polymers, Polymers for Energy applications. Physical aspects of polymers

Suggested reading:

1. Principles of Polymerization by Geroge Odian
2. Introduction to Physical Polymer Science by L. H. Sperling
3. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall, Inc.
4. F.W. Billmeyer, Jr., Textbook of Polymer Science
5. Relevant topics from modern literature

Project II – 9

The student will continue to work in the same lab which was assigned for the Project-II in the previous semester.

The student will get trained in understanding research problem, addressing the chosen research problem by designing and executing experimental and/or computational experiments and analyse and interpret the results. At the end of the project each student will submit a report of the work done and make a presentation for evaluation.

ELECTIVES

Course Code : CY571
Title of the Course : Organometallic Chemistry

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite: A course on understanding the basic principles of organometallic chemistry

Detailed syllabus (CY571)

1) Organometallic Chemistry of Main Group and Transition metals for applications in organic transformations. [4 h]
2) Carbanionic Organometallics: Organolithium, magnesium, zinc , copper and titanium reagents. [4 h]
3) Chemistry of Organoboron, aluminium, silicon and tin compounds. [4 h] Organomercurials and organothalium compounds. [1 h]
4) Chemistry of Metal carbonyls: chromium, iron and cobalt carbonyl reagents. [2 h]
5) Metal carbon multiple bonds: carbenes, carbynes, and N-heterocyclic carbenes. [2 h]
6) Chemistry of Metallocenes: Ferrocene and related compounds. [2 h]
7) Organometallic Chemistry of the Noble Metal: Pd, Rh, Ru and Au catalyzed reactions, involving metal catalyzed coupling, C-H activation and metathesis reactions. [5 h]

Suggested Text Books:

1. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
2. J. F. Hartwig, Organotransition metal chemistry, University Science Books, 2010.
3. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4^{th} edition, Wiley, 2005.
4. L. S. Hegedus, B. C. G. Södenberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books, 2010.

Course Code : CY572

Title of the Course : Supramolecular Chemistry

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite: MSc courses in the I – III semesters

<u>Detailed Syllabus</u>

CONCEPTS **[3 h]**

Definition, Development and Classification, Binding Constants, Supramolecular interactions

SUPRAMOLECULAR CHEMISTRY IN LIFE **[3 h]**

Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly

CATION BINDING HOSTS **[6 h]**

Podand, Crown Ether, Cryptand, Spherand - Nomenclature, Selectivity and Solution Behaviour. Alkalides, Electrides, Calixarenes, Siderophores

ANION BINDING HOSTS **[3 h]**

Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods

ION PAIR RECEPTORS **[2 h]**

Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction

HOSTS FOR NEUTRAL GUEST **[6 h]**

Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins

CRYSTAL ENGINEERING **[3 h]**

Concepts, Crystal Nucleation and Growth, Understanding Crystal Structures, Polymorphism, Co-crystals

Reading material

1. J. W. Steed & J. L. Atwood (2009), Supramolecular Chemistry, 2nd Edition, John Wiley
2. G.R. Desiraju (1989), Crystal Engineering. The Design of Organic Solids, Elsevier

3. G. R. Desiraju, J. J. Vittal, A. Ramanan (1989), Crystal Engineering -A Textbook, World Scientific-IISc Press
4. Recent papers from journals and reviews and monographs, etc

Course Code : CY573

Title of the Course : Stereoselective Organic Synthesis

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite: CY452, CY502 (or equivalent)

<u>Detailed syllabus</u>

Brief review of stereochemistry (1 h)

Chiral pool approach, Acyclic stereoselection: reactions at □-and □□positions of a chiral center. Auxillary econtrolled stereoselection: Evans oxazolidones, Oppolzer sultams, Myers amides, Enders RAMP/SAMP, Shollkopf. (8 h)

Enantioselective alkylation allylation and crotylation reactions (2 h)

Asymmetric oxidation [epoxidation (Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], reduction (Noyori, Corey, Pfaltz) (3 h)

Organocatalyzed asymmetric synthesis (2 h)

Desymmetrization, Kinetic resolution reactions (3 h)

Application of the above methods in synthesis of selected biologically relevant molecules. (5 h)

Suggested reading:

1. M. Nogrady, *Stereoselective Synthesis: A Practical Approach*, Wiley, 2008.

2. E. M. Carreira, L. Kvaerno *Classics in Stereoselective Synthesis*, Wiley-VCH: Weinheim, Germany, 2009.

3. K. C. Nicolaou, E. J. Sorenson, *Classics in Total Synthesis*, Wiley-VCH.

4. K. C. Nicolaou, S. A. Snyder, *Classics in Total Synthesis II*, Wiley-VCH.

Course Code : CY574

Title of the Course : Advanced Magnetic Resonance

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Detailed Syllabus

Review of electron and nuclear spins - angular momentum and magnetic moment: classical and quantum descriptions

Larmor precession, energy levels, and Bloch equation

Angular momentum operators of single and coupled spins: density matrix, unitary transformation, spin angular momentum product operators, spin Hamiltonians, transformations under the influence of rf and microwave pulses, coherence transfer

Spin Relaxation

Scalar and Dipolar interactions, Fermi contact and hyperfine interactions

Chemical shift, g-value, anisotropy

Effect of distortion of structure and symmetry on g-value

Molecular structure determination from J-coupling and NOE constraints

Magnetic field gradients, molecular diffusion, NMR and EPR imaging

Suggested reading :

R R Ernst, G Bodenhausen, A Wokaun "Principles of Nuclear Magnetic Resonance in One and Two Dimensions" (Oxford Science)

Course Code : CY575

Title of the Course : Density Functional Theory

L-T-P : L ~~/ T / P~~

Credits **:** 2 – 0 – 0

Prerequisites: CY403 (or equivalent)

Detailed Syllabus

Many-electron wave functions; electron distributions and densities.

The Thomas-Fermi and Hartree-Fock Model. Slater Exchange Approximation.

The Hohenberg–Kohn theorems and the Kohn–Sham (KS) approach.

The Exchange-Correlation Functional. The Local Density Approximation (LDA).

The Generalized Gradient Approximation (GGA).

Hybrid functionals and the meta-GGA approaches.The Random Phase Approximation (RPA).

Implementations of density functional theory.

Course Code : CY576
Title of the Course : Advanced Chemical Dynamics

L-T-P : L / ~~T/ P~~
Credits : 2 – 0 – 0

Prerequisite Course: CY403, CY404, CY453, CY454, CY504

Detailed Syllabus

Gas Phase Dynamics: Molecular beam scattering, Review of potential energy surface.
Dynamics of Molecular Collisions: Quasi-classical and quantum dynamics, cross section and rate constant. Microscopic mechanism of selected chemical reactions. Roming atom mechanism.
Microscopic interpretation of Arrhenius parameters.
Introduction to condensed phase dynamics, Krammer's theory and solvent effects.
Microscopic reversibility and detailed balance.
Marcus theory of electron transfer.
Femtochemistry- spectroscopic probing of transition state and control of chemical reactivity.

Suggested reading:

1. Theories of Molecular Reaction Dynamics, N. E. Henriksen and F. Y. Hansen, Oxford University Press.

2. Molecular Reaction Dynamics, R. D. Levine, Cambridge University Press.

3. Molecular Reaction Dynamics and Chemical Reactivity, R. D. Levine and R. B. Bernstein, Oxford University Press.

4. Tutorials in Molecular Reaction Dynamics, Eds. M. Brouard and C. Vallance, RSC Publishing.

Course Code : CY577

Title of the Course : Computational Chemistry

L-T-P : L /~~T~~/ P
Credits : 1 – 0 –1

Prerequisite: CY403, CY504

Detailed Syllabus

One hour lecture + two hours laboratory per week

Review of Electronic Structure Theory: Hartree-Fock, MP2, DFT and configuration interaction. Basis sets, convergence.

Geometry optimization, frequency calculation, location of transition state, intrinsic reaction coordinates, population analysis, natural bond orbital analysis, calculation of thermodynamic parameters.

Calculation of molecular excited electronic states.

Representative examples.

Suggested reading:

1. Quantum Chemistry, I. N. Levine, PHI Learning Private Limited.
2. Essentials of Computational Chemistry- Theories and Models, C. J. Cramer, John Wiley and Sons, Ltd.
3. Introduction to Computational Chemistry, F. Jensen, John Wiley and Sons, Ltd.
4. Computational Chemistry- a Practical Guide for Applying Techniques to Real-World Problems, D. C. Young, John Wiley and Sons, Ltd.

Course Code : CY578

Title of the Course : Physical Methods for Inorganic Chemistry

L-T-P : L / ~~T/ P~~
Credits : 2 – 0 – 0

Detailed Syllabus

Prerequisite: M.Sc. Semesters 1-3 courses in inorganic chemistry

Electronic and Photoelectron Spectroscopy: Excitation and ejection of electrons- Core level and valence- electron level photoelectron spectroscopy- Valence excitation spectroscopy- - Electronic spectra of transition metal complexes (3 h)

Vibrational Spectroscopy: Applications to Inorganic systems- Raman Spectra (1.5 h)

NMR Spectroscopy- Time scale- Multinuclear and Organometallic NMR spectroscopy - More common spin-1/2 nuclei, 19F, 31P, 29Si, 119Sn, 195Pt - Quadrupolar nuclei, e.g. 6Li, 11B, 14N, 17O and their characteristics and applications- Relaxation - Fluxional Processes- NMR spectroscopy of paramagnetic compounds- Lanthanide shift reagents, Shiftless reagents- Multiple resonance (3 h)

ESR Spectroscopy – Hamiltonian, Zeeman interaction, g-tensor, g–spread, g-value anisotropy, hyperfine coupling, and hyperfine anisotropy - dipolar contributions spin densities; exchange coupling, zero-field splitting- magnetic anisotropy - liquid, powder and single crystal studies - Variable temperature techniques- Examples from bioinorganic, coordination compounds and clusters (4.5 h)

Magnetism- Overview - Curie and Curie-Weiss law – Super exchange mechanism, Heisenberg- Dirac-van Vleck (HDvV) operator – Bleaney Bowers model- Spin ladder - Magnetic Measurements, Mechanisms of magnetic coupling - coupling in dimers - Single molecule magnets – Quantum tunneling - magneto structural correlations- Examples: Cu dimers, Spin clusters of Mn, Fe, and Cr, Mixed valence species (3 h)

Mössbauer Spectroscopy- Principles- 57Fe - Isomer shift, quadrupole splitting, magnetic hyperfine splitting, selected applications in Fen+ systems, Fe-S systems- Bioinorganic systems, Carbonyl compounds (1.5 h)

Diffraction methods: Distinction among X-ray, neutron and electron diffraction techniques- Single crystals and interpretation of results from X-ray crystallography (1.5 h)

Suggested readings:

(1) E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, ELBS, (Blackwell), 1987.
(2) R. S. Drago, Physical Methods in Chemistry (Saunders publishing)
(3) R. A. Scott and C. M. Lukehart (Editors) Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, 2007 [also available as Encyclopedia of Inorganic Chemistry, 5

Course Code : CY579
Title of the Course : Elementary Polymer Chemistry

L-T-P : L ~~/ T / P~~
Credits : 2 – 0 – 0

Prerequisite: MSc courses in the I - III semesters

Detailed Syllabus

Definition: Polymer, monomer, repeat unit, polymerization- Classification: Polymers based on source and polymerizations-polymer composition and structure- Nomenclature- IUPAC, Non-IUPAC, structure-based, and trade names- Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers)- Effect of Polymer structure on their properties (3 h)

Polymer Synthesis: Step, chain and miscellaneous polymerizations- Kinetics of polymerization- Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization- Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers- State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc. (6 h)

Polymer characterization - Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis- Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy- Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension (4.5 h)

Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot) (3 h)

Physical State and Morphology: Crystalline and Amorphous state- Thermal transitions- Glass-Rubber transition - Mechanical properties– stress-strain behaviour - Elastomer, Fibers and Plastics (3 h)

Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Uses (1.5 h)

Application of Synthetic Polymers: Materials and Biological importance and uses. Nanomaterials, Conducting polymers, Polymers for Energy applications. Physical aspects of polymers (1.5 h)

Suggested readings:

1. L. H. Sperling, Introduction to Physical Polymer Science, Wiley (1986)
2. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall (1990)
3. George Odian, Principles of Polymerization, 4th Edn, John Wiley (2004)
4. M. P. Stevens, Polymer Chemistry: An Introduction (2nd Edn), Oxford University Press (1990)
5. F.W. Billmeyer, Jr., Textbook of Polymer Science (1984), paperback
6. Relevant topics from modern literature

Course Code : CY580

Title of the Course : Natural Products and Medicinal Chemistry

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite: MSc courses in the I – III semesters

Detailed Syllabus

Biosynthesis, total synthesis, structure elucidation and biological significance of selected natural products. (12 h)

Introduction to drug discovery: Sources of drugs-natural products, drugs from organic synthesis, drug discovery and development (2 h)

Drug structure and biological activity-pharmaceutically important functional groups physicochemical properties of drugs, electronic effects, spatial properties of drugs Fate of drugs in the body-absorption, distribution, metabolism, and excretion. Chemistry of drug metabolism, modifications to decrease metabolism, prodrugs Molecular mechanism of drug action-drug targets, receptors, enzymes, nucleic acids, non-receptor targets (5 h)

Chemistry of selected drug classes-pharmacodynamic, chemotherapeutic, antibacterial, antiviral, antineoplastic, cardio-vascular, CNS, antihistamine, diabetic, analgesic and antiinflammatory drugs. (5 h)

Suggested readings:

1. K. C. Nicolaou, Classics in Total Synthesis, Vol 1, 2 and 3.
2. J. H. Fuhrhop, G. Li, Organic Synthesis: Concepts and Methods, 3rd edition, VCH, 1994.
3. J. Mann, Chemical Aspects of Biosynthesis, Oxford University Press, 1994.
4. R. B. Silverman, The Organic Chemistry of Drug Design and Action, 2nd edition, Elsevier, New York, 2004.
5. G. L. Patrick, An Introduction to Medicinal Chemistry-5, Oxford University Press, 2013.

Course Code : CY581

Title of the Course : Introduction to High Energy Materials

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite: A course on undergraduate level physical and organic chemistry

<u>Detailed Syllabus</u>

Brief review of thermodynamics **[3 h]**
Laws of thermodynamics, Definition of heat, energy, internal energy, enthalpy, free energy and entropy. Relationship between ΔE and ΔH, Cp and Cv. Bond energy.

Thermo chemistry
[2 h]
Standard enthalpy of formation, enthalpy changes in reactions, thermo chemical equations, heat of combustion, Hess Law, calculations of enthalpies for various types of reactions.

Requirement for High Energy Materials (HEM) **[5 h]**
Explanation for energy release using bond energy calculations, energy release with respect to heats of formation, heat of explosion, Density factor, oxygen balance.

Power of HEM **[2 h]**
Volume of gas and heat releases in an explosion, Pressure and temperature rise in an explosion reaction, explosive power and power index.

Decomposition reactions **[4 h]**
Decomposition products from explosion reactions: Kistiakowesky-Wilkinson rule, modified K-W rule, Springer-Robert rule, water-gas equilibrium, determination of composition of decomposition products using equilibrium chemistry.

Characterization of HEM
[4 h]
Bomb calorimeter, Use of TG-DTA and DSC for determination of various energetic parameters of HEM.

Classification of HEM **[3 h]**
Classification based on chemical groups present, Activation energy required for initiation of HEM, Classification based on explosive power and energy required for initiation of HEM.

Burning of HEM
[2 h]
Combustion, detonation and deflagration processes; propellants, explosives and pyrotechnics. Propellant and explosive compositions, fuel, oxidizers, binders, plasticizers, thermite mixture, and other ingredients.

Designing of HEM
[3 h]
Synthesis of representative examples of HEM. Research directions, Specific applications of HEM

Reading materials:

1. Book: The Chemistry of Explosives, ISBN 0-85404-640-2, RSC Paperbacks 2004, Jacqueline Akhavan.
2. Book: Demystifying Explosives: Concepts in High Energy Materials, ISBN 978-0-12-801576-6, Elsevier 2015. _S. Venugopalan , HEMRL, Pune, India
3. Book: Introduction to Physics and Chemistry of Combustion: Explosion, Flame, Detonation, ISBN 3540787593, Springer 2008, Liberman Michael.

Course Code : CY582

Title of the Course : Molecules and Materials for Electricity Production and Storage

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisites: None

Detailed Syllabus

Molecules and Materials for Electricity Storage Devices: Primary and secondary batteries and their working principles, electrode reactions, Inorganic and Organic Materials for anodes, cathodes and for transport of electrons and ions. Liquid and solid electrolytes used in the batteries.

Molecules and Materials for Renewable Electricity Harvesting Devices: Photovoltaic effect. Various types of solar cells and their operating principles. Inorganic and Organic Semiconductors, electron transport and hole transport in solar cells, efficiency of the solar cells and energy payback time.

Course Code : CY583

Title of the Course : C-H functionalization

L-T-P : L / ~~T / P~~
Credits : 2 – 0 – 0

Prerequisite: CY402, CY452, CY502

<u>Detailed Syllabus</u>

1) Origin and earlier reports: Concept and classification of C-H functionalization, C-H functionalization of acidic C-H bonds, C-H functionalization of less acidic C-H bonds
2) Friedel-Crafts reaction, intramolecular Friedel-Crafts reaction, asymmetric intramolecular Friedel-Crafts reaction, application to synthesis of natural products and bioactive compounds
3) Free radical mediated C-H functionalization reactions, Breslow remote functionalization and applications, other reactions
4) Fujiwara–Moritani reaction, Heck reaction including asymmetric Heck reaction, intramolecular Heck reaction, asymmetric intramolecular Heck reaction, application to synthesis of natural products and bioactive compounds, Catellani reaction
5) Baylis-Hillman reaction, asymmetric Baylis-Hillman reaction, intramolecular Baylis-Hillman reaction, asymmetric intramolecular Baylis-Hillman reaction, application to synthesis of natural products and bioactive compounds
6) C-H functionalization *via* C-H activation, origin of C-H bond activation and earlier reports, development of concept of C-H functionalization *via* C-H activation, asymmetric C-H functionalization *via* C-H activation, intramolecular version, asymmetric intramolecular version, application to synthesis of natural products and bioactive compounds
7) Miscellaneous reactions

References

Books: (1) Smith, M. B. March, J. J. *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th ed.; Wiley: New York, 2013**.** (2) Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry*; *Part A & B*, 5th ed.; Springer: New York, 2007. (3) Mundy, B. P ; Ellerd, M. G. ; Favaloro, F. G. *Name Reactions and Reagents in Organic synthesis* (2005) second edition John-Wiley and Sons Inc. New Jersey.

Reviews: (1) Rueping, M.; Nachtsheim, B. J. A review of new developments in the Friedel–Crafts alkylation–from green chemistry to asymmetric catalysis. *Beilstein J. Org. Chem.* **2010**, *6*, 6. doi:10.3762/bjoc.6.6. (2) Breslow, R. Biomimetic control of chemical selectivity. *Acc. Chem. Res.* **1980***, 13*, 170-177. (3) Mc Cartney, D.; Guiry, P.J. The asymmetric Heck and related reactions. *Chem. Soc. Rev.* **2011,** *40*, 5122–5150. (4) Beletskaya, I. P.; Cheprakov, A. V. The Heck reaction as a sharpening stone of palladium catalysis. *Chem. Rev.* **2000**, *100*, 3009-3066 (5) Basavaiah, D.; Veeraraghavaiah, G. The Baylis-Hillman reaction: A novel concept for creativity in chemistry. *Chem. Soc. Rev.* **2012**, *41*, 68-78. (6) Basavaiah, D., Reddy, B. S.; Badsara, S. S. Recent contributions from the Baylis-Hillman reaction to organic chemistry. *Chem. Rev.* **2010**, *110,* 5447–5674. (7) Gandeepan, P.; Müller, T.; Zell, D.; Cera, G.; Warratz, S.; Ackermann, L. 3d Transition metals for C−H activation. *Chem. Rev.* **2019**, *119,* 2192–2452. (8) Abrams, D. J.; Provencher, P. A.; Sorensen, E. J. Recent applications of C–H functionalization in complex natural product synthesis. *Chem. Soc. Rev.* **2018***, 47,* 8925−8967. (9) Wencel-Delord, J.; Glorius, F. C–H bond activation enables the rapid construction and late-stage diversification of functional molecules. *Nat. Chem.* **2013**, *5,* 369–375.

Course Code : CY584
Title of the Course : Flow Chemistry and Process Intensification

L-T-P : L / ~~T / P~~ Lectures only

Credits : 2 – 0 – 0 (2 lectures per week of 1 hour each)

Prerequisite: M.Sc. courses up to 3rd year of Integrated 5 year MSc / B.Sc. degree courses for 2 year M.Sc.

<u>Detailed syllabus</u>

Introduction to flow chemistry and its advantages (2)

Recapitulate basic concepts of physical chemistry and reaction kinetics (2)

Principles and equations of flow chemistry (3)

Heterogeneous catalysis in flow chemistry reactions (4)

Pharmaceutical synthesis in flow reactors (5)

Different types of flow reactors (2)

Hazardous batch reactions done with ease in flow (3)

Handling of solids, liquids and gases reactants in flow (2)

Manufacture of Entresto/ commercial drugs in flow chemistry process (2)

Crystallization of polymorphs, cocrystals and salts in flow mode (4)

Important safety aspects essential in flow chemistry (2)

Video illustration of flow reactions (1)

Lectures by eminent academics covering recent research (3)

Brainstorming on design / development of batch to flow reactions by students (2)

Suggested Reading:

1. Masuda et al. Flow fine synthesis with heterogeneous catalysts. Tetrahedron 2018, 74, 1705-1730.

2. Domokos et al. Integrated Continuous Pharmaceutical Technologies-A Review. Org. Process Res. Dev. 2021, 25, 721-739.

3. Mascia et al. End-to-End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation. Angew. Chem. Int. Ed. 2013, 52, 12359-12363.

4. Bedard et al. Science, 2018, 361, 1220-1225.

5. Plutschack et al. The Hitchhiker's Guide to Flow Chemistry. Chem. Rev. 2017, 117, 11796-11893.

6. Cole et al. Kilogram-scale prexasertib monolactate monohydrate synthesisvunder continuous-flow CGMP conditions. Science, 356, 2017, 1144-1150.

7. Drahl, C&EN, March 12, 2018, p. 12.

8. Thaisrovings et al. Development of an Organometallic Flow Chemistry Reaction at Pilot-Plant Scale for the Manufacture of Verubecestat. Org. Process Res. Devp. 2018, 22, 403-408.

9. Akwi & Watts, Continuous flow chemistry: where are we now? Recent applications, challenges and limitations. Chem. Commun. 2018,54, 13894-13928.

10. Kleinbeck et al. Application of Transition-Metal Catalysis, Biocatalysis, and Flow Chemistry as State-of-the-Art Technologies in the Synthesis of LCZ696. J. Org. Chem. 2020, 85, 11, 6844–6853.

11. Narala et al. Pharmaceutical Co-crystals, Salts, and Co-amorphous Systems: A novel opportunity of hot-melt extrusion. Journal of Drug Delivery Science and Technology, 2021, 61, 102209.

12. Gerardy & Monbaliu. Multistep Continuous-Flow Processes for the Preparation of Heterocyclic Active Pharmaceutical Ingredients. Top. Heterocycl. Chem. DOI: 10.1007/7081_2018_21.

13. Hartman, McMullen, Jensen. Deciding Whether To Go with the Flow: Evaluating the Merits of Flow Reactors for Synthesis. Angewandte Chemie International Edition, 2011, 50, 33, 7502-7519.

14. Gutmann, Cantillo, Oliver Kappe. Continuous-Flow Technology—A Tool for the Safe Manufacturing of Active Pharmaceutical Ingredients. Angewandte Chemie International Edition, 2015, 54, 23, 6688-6728.

15. Norbert Kockmann et al. Safety assessment in development and operation of modular continuous-flow processes. React. Chem. Eng., 2017, 2, 258-280.

Web resource: http://chemistry.uohyd.ac.in/~CY584/

Course Code : CY585
Title of the Course : Introduction to Molecular Simulation Techniques

L-T-P : L ~~/ T / P~~

Credits : 2 – 0 – 0

Prerequisite: Quantum chemistry, Statistical thermodynamics and Fortran Programming

Detailed Syllabus

Classical Statistical Mechanics, Liouville operator, Ergodicity (3)

Ensembles, Fluctuations and Time Correlation Functions (2)

Introduction to Computer Simulations, Force fields, Periodic Boundary (2) Conditions

Monte Carlo Simulations; Importance Sampling and Metropolis Method (4)

Molecular Dynamics Simulations (Verlet and Great Predictor-corrector (4)

algorithm, Neighbour List)

Long-range forces (Ewald Sum) (1)

Analysis of Liquid Structure (2)

Free energy estimation Methods (2)

Rare Event Simulations (1)

Applications: Melting, Protein-drug binding, Transport Properties of Liquids, (3) Adsorption Isotherms

Suggested Reading:

1. Computer Simulation of Liquids by D. J. Tildesley and M.P. Allen
2. Understanding Molecular Simulation: From Algorithms to Applications by Berend Smit and Daan Frenkel

Course Code : CY586

Title of the Course : AI-ML and Blockchain in Chemistry

L-T-P : L / T / P
Credits : 1– 0 –1

Prerequisite: Familiarity with any computer programming language and interest to learn new concepts and algorithms.

Detailed Syllabus

1. **Introduction to Artificial intelligence, Machine Learning, Deep Learning and Blockchain Algorithms.**
2. **Python Programming Language:**
   - **2.1 Introduction to Python:** Basic structure of Python programs and Data Structures.
   - **2.2 Python for Data Science:** Two important libraries of Python – *NumPy* and *Pandas.*
   - **2.3 Mathematics for Machine Learning:** Linear Algebra, Matrices, Multi-Variable Calculus and Vectors.
   - **2.4 Data Visualization in Python:** Graphs plotting using Python.
   - **2.5 Basic and Data Analysis using SQL:** Basics of SQL.

3. **Basics of Machine Learning:** Basics of Machine Learning and algorithms.
   3.1 Linear Regression: Basics of linear regression and applications in chemistry.
   3.2 Logistic Regression: Multivariate Logistic Regression and Implementation in Python.

4. **Advanced Machine Learning:** ML models such as supervised and unsupervised algorithms.
   4.1 Advanced Regression: Generalized Linear Regression and Regularized Regression techniques.
   4.2 Support Vector Machine: SVM algorithm, its working, kernels and implementation.
   4.3 Tree Models: Basics of Tree models, their structure, splitting techniques and pruning.
   4.4 Unsupervised Learning: Clustering, its types, basics of PCA, its working and implementation in Python.

5. **Deep Learning:** Types of Neural Networks covered along with implementation.
   5.1 Neural Networks: Basics of Neural Networks, activation functions, and Feed Forward network.
   5.2 Convolutional Neural Network (CNN): CNN structure, layers, and working.
   5.3 Recurrent Neural Networks (RNN)**:** RNN and LSTM with their implementations.

6. **Practical Hands-on Sci-Kit Learn and Keras/TensorFlow software packages.**

Suggested reading:

1. Bishop, C. M. (2006) Pattern Recognition and Machine Learning.
2. Goodfellow, I., Bengio, Y. and Courville, A. (2016) Deep Learning. MIT Press.
3. Bengio, Y., LeCun, Y., Hinton, G. (2015). Deep Learning. Nature 521: 436-44.
4. Stuart J. Russell and Peter Norvig, (2015) Artificial Intelligence: A Modern Approach, Pearson.
5. Schmidhuber, J. (2015) Deep Learning in Neural Networks: An Overview.
6. Aurélien Géron, (2019) Hands-On Machine Learning with Scikit-Learn and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems, O'Reilly.
7. ScikitLearn
8. Keras: https://keras.io/
9. TensorFlow: https://www.tensorflow.org/

Course Code : CY587

Title of the Course : Essentials of Nanoscience and Technology

L-T-P : L / T / P
Credits : 2– 0 –0

Prerequisite: None

Detailed Syllabus

Basic concepts: Applications of quantum mechanics and Maxwell's electromagnetic field equations. The analogy between quantum particles and electromagnetic wave - Dispersion, density of states, confinement and tunneling.

Light polarization states. CW and pulse lasers. Interaction of electron/light with matter. Localized and propagating light in metals, organic and inorganic crystals - excitons and polaritons. Far and nearfield, resolution (diffraction limit, gratings, numerical aperture), scattering, interference.

Non-linear optics (order of electric-susceptibility, multiphoton absorption and frequency up-conversion).

Nanoparticle growth and shape – thermodynamic and kinetic aspects, surface effects. Nanoelectronics – Coulomb blockade and quantum dots, Nanomagnetism – superparamagnetism, quantum tunneling of magnetization (10)

Instrumentation:

- Atomic force microscopy (AFM), and scanning tunneling microscopy (STM).
- Electron microscopy (SEM/TEM), Dual-beam (FIB-SEM) microscopy.
- Confocal optical micro-spectroscopy, near-field optical micro-spectroscopy, and non-linear optical micro-spectroscopy.
- Powder X-ray diffraction (indexing, line broadening effect), micro-XRD, electron diffraction.
- Visit to instruments facility (8)

Fabrication, characterizations and selected applications:

Metals and soft nano/microstructures (including single atom and single molecule devices).

Top-down and bottom-up fabrication approaches - Self-Assembly, sol-gel, vapour deposition, epitaxy, template-based synthesis, vapor (solution)-liquid-solid growth.

Lithography- Photo, electron beam, ion-beam, scanning-probe, PDMS-stamping and two-photon polymerization lithography.

Applications: Integrated Circuits, Medical imaging and theranostics, Drug-delivery, Sensors, Catalysis and high-energy materials. (6)

References:

1. Principles of Physical Chemistry, Kuhn, Försterling, Waldeck, Wiley, 2009.
2. Nanoscale Materials in Chemistry, Kenneth J. Klabunde and Ryan M. Richards, Wiley, 2009.
3. Physical and Chemistry of interfaces, Butt, Graf and Kappl, Wiley VCG, 2nd edition, 2008.
4. Nonlinear Optics, Robert W Boyd, 3rd Edition, Academic Press, Elsevier.
5. Nano- The Essentials, T. Pradeep, Tata McGraw-Hill Publishing Company Limited. 2007.
6. Materials Science and Engineering - An Introduction, William D. Callister, Jr. John Wiley & Sons, 2007.
7. Nanosurface Chemistry, Morton Rossoff, Marcel Dekker AG
8. Introduction to Nanophotonics, Sergey V Gaponenko, Cambridge University Press.
9. Reviews and literatures