M. Sc.

IN

CHEMISTRY

CURRICULUM AND SYLLABI

(Applicable from 2023 admission onwards)

तमसो मा ज्योतिर्गमय

Department of Chemistry
NATIONAL INSTITUTE OF TECHNOLOGY CALICUT
Kozhikode - 673601, KERALA, INDIA

The Program Educational Objectives (PEOs) of M.Sc. in Chemistry

PEO1	Develop in-depth understanding on the fundamental concepts in chemistry and its relevance to science, society, and technology
PEO2	Give adequate exposure to laboratory practices and experimental protocols to make ‘research-ready’ students
PEO3	Instil critical thinking and problem-solving abilities along with good communication and interpersonal skills in students

Programme Outcomes (POs) & Programme Specific Outcomes (PSOs) of M.Sc. in Chemistry

PO1	Deliver the fundamental theoretical concepts and propose experiments to support the concept.
PO2	Identify research problems, propose and execute methodologies, collect and analyze the data, and draw conclusions with future outlooks.
PO3	Demonstrate competence in assignments they take and should be able to perform individually and in a team.
PSO 1	Apply the scientific knowledge for the betterment of society.
PSO 2	Develop human resources for scientific research and education in the area of chemical science

CURRICULUM

Total credits for completing M. Sc. in Chemistry are 75.

COURSE CATEGORIES AND CREDIT REQUIREMENTS:

The structure of M. Sc. programme shall have the following Course Categories:

Sl. No.	Course Category	Minimum Credits
1.	Program Core (PC)	56
2.	Program Electives (PE)	6
3.	Institute Elective (IE)	2
4.	Projects	11

The effort to be put in by the student is indicated in the tables below as follows:
L: Lecture (One unit is of 50 minute duration)
T: Tutorial (One unit is of 50 minute duration)
P: Practical (One unit is of one hour duration)
O: Outside the class effort/self-study (One unit is of one hour duration)

PROGRAMME STRUCTURE

Semester I

Sl. No.	Course Code	Course Title	L	T	P	O	Credits	Category
1.	CY6301E	Basic Concepts of Inorganic Chemistry and Main Group Elements	3	0	0	6	3	PC
2.	CY6302E	Basic Concepts of Organic Chemistry	3	0	0	6	3	PC
3.	CY6303E	Chemical and Statistical Thermodynamics	3	0	0	6	3	PC
4.	CY6304E	Principles of Quantum Mechanics	3	0	0	6	3	PC
5.	CY6305E	Analytical Chemistry	3	0	0	6	3	PC
6.	CY6391E	Inorganic Chemistry Laboratory	0	0	6	3	3	PC
7.	CY6392E	Physical Chemistry Laboratory	0	0	6	3	3	PC
		Total	**15**	**0**	**12**	**36**	**21**	**--**

Semester II

Sl. No.	Course Code	Course Title	L	T	P	O	Credits	Category
1.	CY6311E	Chemistry of Coordination Compounds	3	0	0	6	3	PC
2.	CY6312E	Chemistry of Multiple Bonds and Rearrangement Reactions	3	0	0	6	3	PC
3.	CY6313E	Chemical Kinetics and Surface Chemistry	3	0	0	6	3	PC
4.	CY6314E	Molecular Quantum Mechanics and Basics of Computational Chemistry	2	0	4	6	4	PC
5.	CY6315E	Group Theory and Principles of Molecular Spectroscopy	3	0	0	6	3	PC
6.	CY6393E	Organic Chemistry Laboratory	0	0	6	3	3	PC
7.	CY7397E	Mini Project	0	0	0	6	2	Projects
		Total	**14**	**0**	**10**	**39**	**21**	**--**

Semester III

Sl. No.	Course Code	Course Title	L	T	P	O	Credits	Category
1.	CY7301E	Organometallic and Bioinorganic Chemistry	3	0	0	6	3	PC
2.	CY7302E	Synthetic Methodologies in Organic Chemistry	3	0	0	6	3	PC
3.	CY7303E	Electrochemistry	3	0	0	6	3	PC
4.	CY7304E	Solid State and Materials Chemistry	3	0	0	6	3	PC
5.	CY7305E	Applications of Molecular Spectroscopy	3	1	0	8	4	PC
6.	XXXX	Institute Elective Basket	2	0	0	4	2	IE
7.	CY7398E	Project Phase I	0	0	0	9	3	Projects
		Total	**17**	**1**	**0**	**45**	**21**	**--**

Semester IV

Sl. No.	Course Code	Course Title	L	T	P	O	Credits	Category
1.	XXXX	Elective I$	3	0	0	6	3	PE
2.	XXXX	Elective II$	3	0	0	6	3	PE
3.	CY7399E	Project Phase II/Internship	0	0	0	18*	6	Projects
		Total	**6**	**0**	**0**	**30**	**12**	**--**

$ Electives can be credited in Semester II, Semester III or Semester IV, without overloading of the total credits in each semester.

* In the case of Internship, it is decided by the organization at which the internship is done

Institute Elective Basket

Sl. No.	Course Code	Course Title	L	T	P	O	Credits
1.	ZZ6003E	Research Methodology	2	0	0	4	2
2.	MS6174E	Technical Communication and Writing	2	1	0	3	2
3.	IE6001E	Entrepreneurship Development	2	0	0	4	2

List of Electives

Sl. No.	Course Code	Course Title	L	T	P	O	Credits
1.	CY7351E	Nuclear Chemistry	3	0	0	6	3
2.	CY7352E	Porphyrins and Metalloporphyrins	3	0	0	6	3
3.	CY7353E	Medicinal Chemistry	3	0	0	6	3
4.	CY7354E	Principles of Biochemistry	3	0	0	6	3
5.	CY7355E	Orbital Interactions in Chemistry	3	0	0	6	3
6.	CY7356E	Advanced Materials	3	0	0	6	3
7.	CY7357E	Raman Spectroscopy	3	0	0	6	3
8.	CY7358E	Metal Based Drugs	3	0	0	6	3
9.	CY7359E	Metal Complexes in Molecular Systems and Devices	3	0	0	6	3
10.	CY7360E	Applied Coordination Chemistry	3	0	0	6	3
11.	CY7361E	Chemistry of Macromolecules	3	0	0	6	3
12.	CY7362E	Lubricant Chemistry	3	0	0	6	3
13.	CY7363E	Heterocyclic Chemistry	3	0	0	6	3
14.	CY7364E	Chemistry at Interfaces.	3	0	0	6	3
15.	CY7365E	Green Chemistry	3	0	0	6	3
16.	CY7366E	Organometallic Chemistry of Main group elements	3	0	0	6	3
17.	CY7367E	Metal Catalysed Asymmetric Synthesis	3	0	0	6	3
18.	CY7368E	Supramolecular Chemistry	3	0	0	6	3
19.	CY7369E	Bioinorganic Chemistry	3	0	0	6	3
20.	CY7370E	Advanced Quantum Chemistry	3	0	0	6	3
21.	CY7371E	Polymer Science and Technology	3	0	0	6	3

CY6301E BASIC CONCEPTS OF INORGANIC CHEMISTRY AND MAIN GROUP ELEMENTS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Learn about the basic concepts and principles of inorganic chemistry and be able to think innovatively
CO2: Study various properties of main group elements and their related compounds to enable the synthesis of new inorganic compounds.
CO3: Know about the importance of nuclear chemistry, its related reactions and their applications.

Chemical bonding-Valence bond theory, hybridization, VSEPR theory, molecular orbital theory, wave mechanical description of orbitals, applications of MOs for homo and heteronuclear diatomic molecules, symmetry of molecular orbitals, theories of bonding in metals.

Introduction to acid-base concepts-Bronsted-Lowry definition, solvent system definitions, Lux-Flood definition, Lewis definition, Hard and Soft Acids and Bases concept (HSAB), classification of hard, border line, and soft acids and bases.

Main Group Chemistry-General discussion on the properties of main group elements, boron cage compounds, structure and bonding in polyhedral boranes, carboranes and metalloboranes, styx notation, Wade's rule, electron count, synthesis of polyhedral boranes and carboranes, silicones, silicates, boron nitride, borazines and phosphazenes, hydrides, oxides and oxoacids of nitrogens (N, P), chalcogens (S, Se & Te) and halogens, xenon compounds, pseudo-halogens and interhalogen compounds, allotropes of carbon, synthesis and reactivity of inorganic polymers of silicon and phosphorous. Reduction potentials-Latimer and Frost diagrams.

Inner Transition Metals- Introduction to lanthanides and actinides, position of lanthanides/ actinides, physical properties including electronic structure and oxidation states, lanthanide and actinide contractions, actinide hypothesis, optical spectra and magnetic properties of lanthanides, applications of lanthanide complexes, trans actinide elements.
Nuclear chemistry-Introduction, radioactivity and measurement, radioactive series, half-life, nuclear decay, Bethe's notation of nuclear process, types of nuclear reactions, nuclear fission.

References:

1. J. E. Huheey, E. A. Keiter, R.L. Keiter, and O. K. Medhi, *Inorganic Chemistry, Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
2. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, Inc., New York, 2009.
3. J. D. Lee, *Concise Inorganic Chemistry*, Blackwell Science, Oxford, 2008.
4. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins: Inorganic Chemistry*, 5th edition, Oxford University Press, Oxford, 2010.
5. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Pearson, 2012.
6. G. Choppin, J. Rydberg and J. O. Liljenzin, *Radiochemistry and Nuclear Chemistry*, Butterworth-Heine-mann, 3rd Edition, 2002.
7. W. D. Loveland, D. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, John Wiley & Sons, 2006.

CY6302E BASIC CONCEPTS OF ORGANIC CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the principles of stereochemistry to organic reactions.
CO2: Deliver the fundamental concepts of reaction mechanism in organic chemistry.
CO3: Deliver the functions of biomolecules and categorize the natural products.

Stereochemistry: stereoisomers – configurational isomers, conformational isomers, enantiomers and diastereomers; projection representation of stereoisomers and their interconversion; absolute configuration, R and S notation, prostereoisomerism – topicity of ligands and faces and their absolute configuration; stereoisomerism of molecules with axial, planar, and helical chirality, *cis-trans* isomerism – π and ring diastereomers, diastereoselectivity – Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk models, Cieplak and cation coordination models, and Zimmerman-Traxler transition state model; Conformational analysis – acyclic and cyclic molecules, Klynen-Prelog conformational terminology, Cahn conformational selection rules, conformational analysis of cyclohexane and substituted cyclohexanes, cyclohexane ring with sp^2 carbons – cyclohexene, conformation of fused polycyclic systems.

Organic reactive intermediates: Generation, stability and reactivity of carbocations - nonclassical carbocations, neighbouring group participation, carbanions, free radicals, carbenes, benzynes and nitrenes, relation between structure and thermodynamic stability, Hammond's postulate, chemical kinetics, energetics of reactions, potential energy changes in reactions, relation between thermodynamic stability and reaction rates, kinetic versus thermodynamic control, correlation between kinetic and thermodynamic aspect of reactions, Curtin-Hammett principle, primary and secondary kinetic isotope effects, linear free energy relationships, acid, base and nucleophilic catalysis, Lewis acid catalysis, solvent effects in reactions.

The concept of aromaticity, criteria for aromaticity, Huckel's rule, aromatic and antiaromatic compounds - annulenes, charged rings, fused ring systems and heterocyclic rings; homoaromaticity, aromatic electrophilic and nucleophilic substitution of benzoid and heteroaromatic systems – intermediates, orientation, structure – reactivity relationships, selected aromatic substitutions, C-C bond formation involving aromatic substitution reactions – Skraup synthesis, Vilsmeier-Haack formylation, Reimer-Tiemann reaction, Kolbe-Schmidt carboxylation, Gattermann-Koch reaction, Gattermann formylation.

Introduction to biomolecules, structure and functions of carbohydrates, lipids, physicochemical properties of amino acids, chemical synthesis of peptides, structural features of proteins and nucleic acids, fundamentals of steroids, terpenoids, carotenoids and alkaloids.

References:

1. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry,* Part A: Structure and Mechanisms, 5th edition, Springer, Boston, USA, 2007.
2. D. Nasipuri, *Stereochemistry of Organic Compounds. Principles and Applications*, 3rd edition, New Age International Publishers, India, 2011.

3. D. G. Morris, *Stereochemistry*, *Basic Concepts in Chemistry*, Royal Society of Chemistry, Cambridge, UK, 2002.
4. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, 1st edition, John Wiley & Sons, Inc., 2008.
5. R. Bruckner, *Advanced Organic Chemistry, Reaction Mechanisms*, 1st edition, Academic Press, California, USA, 2002.
6. J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, 7th edition, W.H. Freeman and company, New York, 2011.
7. D. L. Nelson and M. M. Cox, Lehninger, *Principles of Biochemistry*, 6th edition, W.H. Freeman and Company, New York, 2013.
8. R. K. Murray, D. A. Bender, K. M. Botham, Peter J. Kennelly, Victor W. Rodwell and P. Anthony Weil, *Harper's Illustrated Biochemistry* 28th edition, McGraw-Hill Medical, New Delhi, 2009.
9. A. B. Hughes, *Amino Acids, Peptides and Proteins in Organic Chemistry: Protection Reactions, Medicinal Chemistry, Combinatorial Synthesis*, Volume 4, Wiley-VCH, Federal Republic of Germany, 2011.
10. S. V. Bhat, B. A. N. Sampagi, M. Shivakuman, *Chemistry of Natural Products*, Revised edition, Narosa Publishing House Pvt. Ltd., New Delhi, 2018.

CY6303E CHEMICAL AND STATISTICAL THERMODYNAMICS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Assess and apply the laws of thermodynamics to industry-based applications and practical systems
CO2: Apply the equilibrium thermodynamic concepts to chemical reactions
CO3: Apply phase rule to various industry-based applications
CO4: Apply the principles of statistical mechanics to selected problems to relate the thermodynamic parameters in classical thermodynamics with statistical thermodynamics

Review of classical thermodynamics, laws of thermodynamics, internal energy, enthalpy, absolute entropy, residual entropy - free energy functions, fundamental equations of thermodynamics; properties of the internal energy, Maxwell’s relations, temperature and pressure dependence of thermodynamic quantities.

Thermodynamics of mixtures, ideal and nonideal solutions; chemical potential, partial molar quantities; excess thermodynamic functions; colligative properties; spontaneity and equilibria, criterion for chemical equilibrium; equilibrium constants from thermodynamic data, chemical affinity and thermodynamic functions, equilibrium constant.

Phase equilibrium, Gibbs phase rule and its derivation; one, two, and three component systems, simple eutectic systems, cooling curves; activity, activity coefficient, fugacity, and fugacity coefficient; Ehrenfest classification of phase transitions; general theory of nonequilibrium processes, entropy production and phenomenological relations.

Concept of ensembles, microcanonical, canonical and grand canonical ensembles; probability distribution of particles, most probable distribution; distribution laws – Boltzmann, Fermi-Dirac and Bose-Einstein distributions; partition function; thermodynamic information in partition function; molecular partition function- Translational, rotational and vibrational partition functions; Calculation of thermodynamic properties.

References:

1. P. Atkins, J. de Paula, Atkin’s *Physical Chemistry*, 11th Ed, Oxford university press, Oxford, 2018.
2. S. Glasstone, *Thermodynamics for Chemists, East-West Press*, 2008.
3. J. B. Ott, J. Boerio Goates, *Chemical Thermodynamics-Principles and Applications*, Academic Press, Elsevier Science & Technology Books, 2000.
4. D. A. Mcquarrie, *Statistical Thermodynamics*, University Science books, California 2004.
5. F. W. Sears, G. L. Salinger, *Thermodynamics, Kinetic Theory, and Statistical Thermodynamics*, 3 Ed, Narosa Publishing House, New Delhi, 1988
6. B. R. Puri, L. R. Sharma, M. S. Pathania, *Principles of Physical Chemistry*, 48th Ed, Vishal Publishing Co, Jalandhar, 2021
7. R. E. Sonntag, C. Borgnakke, G. J. Van Wylen, *Fundamentals of Thermodynamics*, 6th Ed, John Wiley & Sons, 2002.

CY6304E PRINCIPLES OF QUANTUM MECHANICS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the concepts of quantum mechanics to simple chemical systems.
CO2: Demonstrate the application of fundamental laws to solve chemical problems.
CO3: Apply suitable approximation to solve the Schrödinger equation for simple systems.

Wave-particle duality - postulates - operators, linear and Hermitian operators, commutation relations, eigenvalue problem - Heisenberg and Schrödinger representations of quantum mechanics - solution for Schrödinger equation - particle in 1D, 2D, 3D boxes and their applications - degeneracy - particle in a box of finite barrier and quantum mechanical tunneling.

Simple harmonic oscillator - Solution by the method of power series, Hermite equation, Hermite polynomials, recursion relation, wave functions and energies - Particle in a sphere and hydrogen atom -Wave equation in spherical polar coordinates, separation of center of mass motion from relative motion, separation of variables, Legendre and associated Legendre polynomials, spherical harmonics, polar diagrams, wave functions and energies of hydrogen-like atoms, Laguerre and associated Laguerre polynomials, radial functions, radial distribution functions, angular functions and their plots - Postulate of spin, discovery of spin, spin orbitals.

Angular momentum, quantum mechanical operators, commutation relations, Eigen functions, Ladder operator method for angular momentum, space quantization.

Many electron atoms (He), approximation methods: independent particle method, perturbation method (treatment of the ground state of He atom), variation method (treatment of the ground state of He atom), self-consistent field approximation, Slater type orbitals, symmetric and antisymmetric wave functions, Pauli's exclusion principle, vector model of atom; spin-orbit coupling, spectroscopic term symbols for atoms, Russel-Saunder's terms and coupling schemes, introduction to SCF methods, Slater determinants, Hartree and Hartree-Fock's SCF.

References:

1. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, New York, 2005.
2. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, Mill Valley CA.,1983.
3. M. W. Hanna, *Quantum Mechanics in Chemistry*, Benjamin/Cummings, Melano Park, CA, 1981.
4. R. K. Prasad, *Quantum Chemistry*, Oscar Publications, New Delhi, 2000.
5. I. N. Levine, *Quantum Chemistry*, 5th Edition, Pearson Educ., Inc., New Delhi, 2000.
6. S. N. Datta, *Lectures on Chemical bonding and quantum chemistry*, Prism Books, Bangalore, 1997.
7. J. P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
8. A. K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill, 1994.

CY6305E ANALYTICAL CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Suggest the appropriate separation, purification and analysis methods for various chemical compounds and their mixtures
CO2: Correlate the principles and methodologies of modern sophisticated instruments.
CO3: Detail the chemistry of biochemical and water quality analyses methods.

Lab safety protocols in analysis, Analytical methods for the separation and analysis of compounds, theory of gravimetric analysis, gravimetric factor and calculations, solubility product, common ion effect, precipitation methods, inclusion, occlusion, coprecipitation and post precipitation, solvent extraction - theory and applications, uses of dithiocarbamates, crown ethers, dithiozone and oxine in extraction, electrophoretic methods, capillary electrophoresis.

Chromatography: mechanisms, retention volume, retention time, chromatographic performance, column chromatography, ion exchange chromatography: action of cation and anion exchange resins, applications, size exclusion chromatography, theory and instrumentation of paper, thin layer, liquid and gas chromatography, gel permeation chromatography (GPC), HPLC.

Theory, instrumentation and applications of spectrophotometry, fluorimetry, phosphorimetry, Atomic Absorption Spectroscopy, Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Dynamic Light Scattering (DLS). Use of Dynamic Mechanical Analyzer for material characterisation, Theory, instrumentation and applications of TG, DTA, and DSC, coulometry, amperometry, cyclic voltammetry, cathodic and anodic stripping analysis.

Radiochemical methods: carbon dating, neutron activation analysis, isotope dilution techniques, Estimation of biological fluids: haemoglobin, cholesterol and blood sugar, Water quality parameters, standards and analysis, Chemical pollutants analysis in water.

References:

1. D. A. Skoog and D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole, Florence, 2013.
2. G. D. Christian, *Analytical Chemistry*, 7th Edition, John Wiley & Sons, Singapore, 2013.
3. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd., New Delhi, 2009
4. H. H. Williard, L. L. Merrit, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, Wadsworth Publishing Company, Belmont, California, 2004.
5. D. Harvey, *Modern Analytical Chemistry*, McGraw Hill Higher Education, New York, 2000

CY6391E INORGANIC CHEMISTRY LABORATORY

Pre-requisites: NIL

L	T	P	O	C
0	0	6	3	3

Course Outcomes:

CO1: Carry out the experiments in order to attain more technical/practical skills.
CO2: Estimate/quantify the presence of metal ions in a given mixture.
CO3: Synthesis and purifications of inorganic compounds.
CO4: Apply various spectroscopic techniques for the characterization of inorganic and coordination compounds through hands-on practice with the instruments.

Syllabus / List of Experiments:

Introduction to lab safety protocols, Qualitative and quantitative estimations of inorganic salts containing mixtures of metal ions. Synthesis, separation, purification, characterization, and property measurements of inorganic compounds with an emphasis on different techniques of reaction set-up (air-sensitive, moisture-sensitive, etc.).

Characterization of inorganic compounds/complexes using various spectroscopic techniques (UV-visible, IR, etc), and by thermal analysis (TGA, DSC, etc). Magnetic moment determination for the transition metal complexes by Evans method using NMR.

References:

1. G. H. Jeffery, J. Bassett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, Bath Press, Avon, 1989.
2. D. A. Skoog and D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole, Florence, 2004.
3. W. G. Palmer, *Experimental Inorganic chemistry*, Cambridge University Press, London, 1970.
4. E. J. Meehan, S. Bruckenstein and I. M. Kolthoff and E. B. Sandell, *Quantitative Chemical Analysis*, Mac-millan, London, 1969.
5. D. F. Evans, D. A. Jakubovic, *J. Chem, Soc. Dalton Trans.*, 1988, 2927-2933.

CY6392E PHYSICAL CHEMISTRY LABORATORY

Pre-requisites: NIL

L	T	P	O	C
0	0	3	3	2

Course Outcomes:

CO1: Hands-on experiments in various areas of physical chemistry.
CO2: Apply different instrumental methods in physical chemistry.
CO3: Develop different physical chemistry experiments.

Syllabus / List of Experiments:

Experiments on thermodynamics, kinetics, catalysis, electrochemistry, spectroscopy, photochemistry and macromolecules

References:

1. B. Visvanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, 2010.
2. A. M. Halpern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Text Book*, 3rd edition, W. H. Freeman, 2006.
3. J. Raveendran, L. Sreejith and S. Murugan, *Microscale Experiments Manual*, Proc. of FDP on Green environment for Academic Campus,2013.

CY6311E CHEMISTRY OF COORDINATION COMPOUNDS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Understand the theories of bonding in coordination complexes.
CO2: Acquire enough knowledge of the electronic spectral properties of coordination complexes.
CO3: Learn the inorganic reaction mechanisms to design the new metal complexes.

Coordination Chemistry-Transition elements and their oxidation states, valence bond theory, crystal field theory, high spin, low spin configurations, calculation of crystal field stabilization energy, effects of crystal field on octahedral, tetrahedral and tetragonal symmetries, spectrochemical series, applications of crystal field theory, molecular orbital theory of octahedral, tetrahedral and square planar complexes, π-acceptors and π-donors and experimental evidences of π-bonding.

Inorganic Reaction Mechanism-Substitution reactions of square planar and octahedral metal complexes, inert and labile complexes, trans effect, associative, dissociative and interchange mechanisms, solvent effect, formation of ion pairs and conjugates of complexes, kinetics of octahedral substitution, factors affecting reaction mechanism, aquation reactions, acid and base hydrolysis, redox reactions, outer sphere and inner sphere mechanisms and electron transfer reactions

Electronic absorption spectra of transition metal complexes-calculation of number of microstates, term symbols, selection rules, prediction of electronic transitions, Orgel diagrams showing splittings in octahedral, tetrahedral and square planar complexes, Tanabe-Sugano diagrams, tetragonal distortions from octahedral symmetry, Jahn Teller effect and charge transfer spectra

Magnetism of transition metal complexes-ferro and antiferromagnetic metal complexes, measurement of magnetic susceptibility, variation of magnetic properties of complexes with temperature.

References:

1. F. A. Cotton, G. Wilkinson and P. L. Gaus, *Basic Inorganic Chemistry*, Wiley India Ltd., New Delhi, 2009.
2. J. E. Huheey, E. A. Keiter, R.L. Keiter, and O. K. Medhi, *Inorganic Chemistry, Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
3. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, Inc., New York, 2009.
4. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins: Inorganic Chemistry*, 5th Edition, Oxford University Press, Oxford, 2010.
5. J. D. Lee, *Concise Inorganic Chemistry,* Blackwell Science, Oxford, 2008.
6. F. A. Carey, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley Inter-science, 2003.
7. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Pearson, 2012.

CY6312E CHEMISTRY OF MULTIPLE BONDS AND REARRANGEMENT REACTIONS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Deliver methods for the synthesis of compounds containing C=C / C=X bonds and their reactions.
CO2: Deliver the principles and application of pericyclic and photochemical reactions.
CO3: Predict the outcome of the reactions based on the various rearrangement reactions.

Formation and selected reactions of C-C double bond: β-Elimination reactions, stereoselective and regioselective eliminations, β-eliminations *via* cyclic transition states: sulfoxides, selenoxides, *N*-oxides, acetates and xanthates eliminations; Wittig, Horner Wadsworth Emmons, Peterson, Bamford, Stevens, Shapiro, Corey-Winter reactions, Julia olefination, McMurry coupling - Selected reactions of alkenes: hydration of alkenes, hydroboration reactions, halolactonization.

Chemistry of carbonyl group: nucleophilic addition to the carbonyl group, the addition of nitrogen, oxygen and sulphur nucleophiles: imine, enamine, hemiacetal, acetal and thioacetals; C-C bond formation via enolates and enamines, methods of formation, kinetic/thermodynamic control and regio- and stereoselectivity in enolate formation; reactions of enolates, acetoacetic and malonic ester synthesis, condensation with carbonyl compounds, Aldol and Michael reactions, reactions of enamines, enamines in Aldol and Michael reactions; Claisen, Dieckmann, Knoevenagel, Stobbe, Perkin and Darzen condensations.

Pericyclic reactions: classification, Woodward Hoffmann rules, FMO analysis, orbital symmetry correlations and transition state aromaticity methods for electrocyclic, cycloaddition and sigmatropic reactions; pericyclic reaction in organic synthesis – Diels-Alder reactions, 1,3-dipolar additions, Cope, Claisen and Ireland-Claisen rearrangements; chelotropic, group transfer and ene reactions.
Photochemistry: Introduction to photochemistry and photochemical reactions: isomerization, reduction, Paterno-Buchi reaction, Norrish Type I and Norrish Type II reactions, rearrangements: di-pi methane, oxa di-pi methane and aza di-pi methane rearrangements, Barton nitrite ester reaction.

Types of rearrangements, rearrangement involving carbocations: Wagner Meerwein rearrangement, Pinacol and semipinacol rearrangement, Demjanov rearrangement, benzylic acid rearrangement; rearrangement to electron-deficient oxygen: Baeyer Villiger oxidation, hydroperoxide rearrangement, Dakin reaction; rearrangement to electron-rich carbon: Steven's rearrangement, Sommelet-Hauser rearrangement, Wittig rearrangement, Favorskii rearrangement; rearrangement to electron-deficient nitrogen: Wolf, Hofmann, Curtius, Schmidt, Lossen and Beckmann rearrangements.

References:

1. R. Bruckner, *Advanced Organic Chemistry, Reaction Mechanisms*, 1st Edition, Academic Press, California, USA, 2002.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5th Edition, Springer, Boston, USA, 2007.
3. J. J. Li, *Name Reactions: A Collection of Detailed Mechanism and Synthetic Applications*, 4th Edition, Springer, New York, 2009.
4. I. Fleming, *Pericyclic Reactions,* 2nd edition, Oxford University Press, UK, 2015.
5. S. Sankararaman, *Pericyclic reactions – A Textbook*: *Reactions, Applications and Theory,* Wiley-VCH, Weinheim, Germany, 2005.

6. M. B. Smith, March's, *Advanced Organic Chemistry*: *Reactions, Mechanisms and Structure*, 7th Edition, John-Wiley & Sons, Inc., New Jersey, 2013.
7. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edition, Cambridge University Press, UK, 2004.
8. J. D. Koyle, *Introduction to Organic Photochemistry*, Wiley, New York, 1991.
9. P. Klan and J. Wirz, *Photochemistry of Organic Compounds: From Concepts to Practice*, John Wiley and Sons Ltd, UK, 2009.
10. R. O. C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, 3rd edition, CRC Press, UK, 1993.

CY6313E CHEMICAL KINETICS AND SURFACE CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Calculate the rate of reaction and kinetic triplet for chemical reactions.
CO2: Elucidate the reaction mechanisms using established reaction rate theories.
CO3: Postulate surface reactions in catalyzed chemical reactions.
CO4: Correlate the theory, predictions and mechanisms for industrially relevant chemical reactions.

Empirical Rate Laws - Complex Reactions, Parallel, Opposing and Consecutive Reactions - Collision and Transition State Theories of Rate Constants, Thermodynamic Formulation of Transition State Theory, Linear and Non-linear Arrhenius equations, Arrhenius Parameters; Activation Energy, Statistical Distribution of Molecular Energies - Steady State Approximation - Unbranched and Branched Chain Reaction - Determination of Reaction Mechanisms, Theories of Unimolecular Reactions - Radical and Ionic Polymerization Reactions - Photochemical Reactions - Potential Energy Surfaces ($D + H_2 \rightarrow DH + H$, $D_2 + H_2 \rightarrow 2DH$) - Kinetics of Fast Reactions and Relaxation Kinetics.

Kinetics of Reactions in Solution - Comparison Between Gas Phase and Solution Phase Reactions, Cage Effect, Factors Determining the Reaction Rates in Solution, Reactions Between Ions, Ion Dipole and Dipole-Dipole Reactions - Structure, Pressure Effect, Primary and Secondary Salt Effects - Homogeneous Catalysis, General Catalytic Mechanisms, Acid-Base Catalysis, Catalysis by Enzymes, Inhibition, Transient, Phase Kinetics, Sigmoid Kinetics.

Processes at Solid Surfaces, Thermodynamics and Kinetics of Adsorption, Adsorption Isotherms, Adsorption Entropies, BET equation and its Applications, Adsorption on Porous Solids, Hysteresis - Langmuir Blodgett Films - Heterogenous Catalysis, Adsorption and Catalysis, Unimolecular Surface Reactions, Bimolecular Surface Reaction, Langmuir-Hinshelwood Mechanism.

Micelles, Emulsions, and Foams, Critical Micelle Concentration (CMC) - Temperature Dependence, Influence of Chain Length and Salt Concentration, Surfactant Parameter, Thermodynamics of Micellization, Aging and Stabilization of Emulsions, Micelles and Microemulsion as Templates for Synthesis of Nanostructures.

References:

1. P. Atkins, J. de Paula, *Physical chemistry*, 10th Edition, Oxford university press, Oxford, 2014.
2. J. I Steinfeld, J.S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics*, 2nd Edition, Prentice Hall, 1998.
3. K. J. Laidler, *Chemical Kinetics*, 3rd Edition, 1997, Benjamin-Cummings, Indian reprint - Pearson, 2009.
4. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, Wiley, 1997.
5. H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2006.
6. H. Kuhn, H. -D. Forsterling and D.H. Waldeck, *Principles of Physical Chemistry*, Wiley, 2009.
7. G. A. Somorjai and Y. Li, *Introduction to Surface Chemistry and Catalysis*, 2nd Edition, 2010.
8. R. J. Silbey, R. A. Alberty and M. G. Bawendi, *Physical Chemistry*, 4th Edition, 2014.
9. B. R. Puri, L. R. Sharma, M. S. Pathania, *Principles of Physical Chemistry*, 48th Edition, Vishal Publishing Co, Jalandhar, 2021

CY6314E MOLECULAR QUANTUM MECHANICS AND BASICS OF COMPUTATIONAL CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
2	0	2	6	4

Total Sessions: 26L + 52P

Course Outcomes:

CO1: Deliver the basis of wave function and density functional methods.
CO2: Deliver the basic principles of computational chemistry.
CO3: Perform simple computational calculations and analysis the output of simple computational quantum mechanical calculations.

Molecular Quantum Mechanics - Born-Oppenheimer approximation, MO theory, LCAO approximation, MO theory for the ground state and excited state of H_2^+, hydrogen molecule - MO treatment and calculation of energy, molecular term symbols, VB theory - H_2^+ and H_2 molecule, MO and VB treatment of diatomic molecules, polyatomic molecules, hybridization - construction of sp, sp^2, sp^3, $dsp^2$and d^2sp^3 hybrids, Walsh's rules, conjugated π systems, HMO theory and charge on an atom, Hellman-Feynman theorem and its simple applications.

Molecular mechanics and force fields, various potential energy terms, parameterization, potential energy surface - local minima, global minima, saddle point and transition states, ab initio methods - self-consistent theory of molecules, Hartee-Fock method, Roothan's equations, Koopmans' theorem, basis sets, Slater and Gaussian functions, classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

Hartree-Fock limit, electron correlation, post Hartree-Fock methods, qualitative description of configuration interaction, coupled cluster and Møller-Plesset Perturbation theory, semi-empirical methods and its basic principles. Introduction to Density Functional Theory (DFT) methods - Hohenberg-Kohn theorems, Kohn-Sham orbitals, exchange-correlation functional, local density approximation, generalized gradient approximation and hybrid functionals.

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, analysis of Gaussian output files, minimum and stable structure, saddle point and transition state structure, computing multipole moments and molecular electrostatic potential, partial atomic charges and atomic spin, ionization potentials, electron affinities, infrared spectra and NMR spectra. Electronic Energy, zero-point vibrational energy, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions, use of graphics programs like Chemcraft, Molden in analyzing Gaussian output data, identification and visualization of normal modes of vibration, calculation and interpretation molecular orbitals

References:

1. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, New York, 2005.
2. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, McGraw Hill Education, New Delhi, 2017.
3. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, Mill Valley CA.,1983.
4. M. W. Hanna, *Quantum Mechanics in Chemistry*, Benjamin/Cummings, Melano Park, CA, 1981.
5. R. K. Prasad, *Quantum Chemistry,* Oscar Publications, New Delhi, 2000.
6. I. N. Levine, *Quantum Chemistry,* 5th Edition, Pearson Educ., Inc., New Delhi, 2000.
7. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st edition, revised, Dover, 1989.
8. F. Jensen, *Introduction to Computational Chemistry*, Wiley, New York, 1999.
9. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons, 2002.
10. J. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
11. E. G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics,* 2nd edition, Springer 2011.

CY6315E GROUP THEORY AND PRINCIPLES OF MOLECULAR SPECTROSCOPY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the concepts of symmetry and group theory to chemical problems.
CO2: Demonstrate the application of fundamental laws to solve chemical problems.
CO3: Apply suitable approximation to solve the Schrödinger equation for simple systems.

Symmetry elements and operations, point groups, group multiplication table, matrix representation of symmetry operations. Representations using different basis, reducible and irreducible representations, construction of irreducible representation, great orthoganality theorem (GOT). Construction of character tables (C2v, C3v, C2h and C4v), Mülliken symbols, reduction formula, direct sum and direct products, connection between group theory and quantum mechanics.

Interaction of radiation with matter, Uncertainty relation and natural line width - line shapes – Line intensity- transition moment - selection rules for electric dipole, magnetic dipole, electric quadrupole transitions. Born-Oppenheimer approximation - rotational, vibrational and electronic energy levels.
Rotation of rigid bodies, pure rotational spectroscopy of diatomic, linear, symmetric and asymmetric tops molecules, selection rules, structure determination, vibrational spectroscopy of diatomic molecules, selection rules, anharmonicity and centrifugal effects, determination of dissociation energies, vibration -rotation transitions, FTIR, ATR, Raman effect, classical and quantum mechanical model, rotational Raman of diatomic molecules, Vibrational Raman spectroscopy, vibration-rotation Raman Spectroscopy of diatomic molecules, SERS, SEIRS, RRS, CARS.

Molecular vibrations- symmetry aspects of molecular vibrations- selection rules for vibrational absorption- complementary character of IR and Raman spectra- determination of the number of active IR and Raman lines (H_2O, NH_3, CH_4, SF_6).
Polar versus non-polar molecules - Chirality - Symmetry adapted linear combinations (SALC), projection operator, overlap integrals - construction of hybrid orbitals-BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Application to MO theory of H_2O, NH_3 and octahedral complexes.

Electronic spectroscopy of diatomic and polyatomic molecules, Franck-Condon principle, Fortrat diagram- Dissociation and pre-dissociation- calculation of heat of dissociation. charge transfer spectra, effect of solvent and conjugation, Woodward's rules, fluorescence spectroscopy, photoelectron spectroscopy-XPES and UPES theory, Auger electron spectroscopy, XRF and EELS

References:

1. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley Interscience, New York, 2006.
2. P. H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., New York, 1998.
3. L. H. Hall, *Group Theory and Symmetry in Chemistry*, Mc Graw Hill, New York, 1969.
4. R. Mc Weeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.
5. Jaffe and Orchin, *Symmetry in Chemistry*, Wiley Eastern, New Delhi, 1991.
6. C. N. Banwell and Elaine M. McCash, *Fundamentals of Molecular Spectroscopy*, McGraw-Hill, International, UK, 1995.
7. P. F. Bernath, *Spectra of Atoms and Molecules*, Oxford University press, New York, 2005.
8. S. Hufner, *Photoelectron Spectroscopy*, Springer-Verlag, Berlin, 1995.
9. T. Engel, *Quantum Chemistry and Spectroscopy*, 3rd Edition, Pearson Education, New Delhi, 2015.

CY6393E ORGANIC CHEMISTRY LABORATORY

Pre-requisites: NIL

L	T	P	O	C
0	0	6	3	3

Course Outcomes:

CO1: Execute basic laboratory techniques.
CO2: Set up and monitor different types of reactions.
CO3: Carry our purification and structural characterization of products obtained.

Syllabus:

Introduction to basic laboratory techniques: isolation and purification processes- filtration, recrystallization, solvent extraction, distillation, vacuum distillation, chromatography- purification of organic solvents.
Methods of separation of mixtures and analysis.
Natural products extraction and characterization.
Synthesis, isolation, purification and characterization of organic compounds.

References:

1. B. S. Furniss, A. J. Hannaford, P. W.G. Smith, A. R. Tatchell, *Vogel's Text Book of Practical Organic Chemistry*, 5th Edition, Pearson India, 2003.
2. F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, 4th Edition, Pearson India, 2009.

CY7397E MINI PROJECT

Pre-requisites: NIL

L	T	P	O	C
0	0	0	6	2

Course Outcomes:

CO1: Carry out literature survey in a particular research topic.
CO2: Identify research problems and seek solutions.
CO3: Write technical notes and scientific reports.

Syllabus:

The student under the supervision a faculty at the institute carries out state of the art research in the frontier areas of chemistry. The final report/thesis describing the details of the entire project work has to be submitted to the Department, in a prescribed format. Presentation of the work and evaluation are to be done before an expert committee.

CY7301E ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Learn about the structure, bonding, preparation and reactivity of organometallic compounds.
CO2: Describe the mechanism of the catalytic processes of organometallic complexes.
CO3: Elaborate on the details of biological inorganic processes.

Structure of organometallic compounds-Molecular orbital theory and 18 electron rule, metal carbonyl complexes – preparation and properties, metal-metal bridging in polynuclear carbonyls, carbonylate anions, isolobal fragments, linear and bent nitrosyl complexes, Fischer and Schrock carbenes, synthesis and reactivity of ferrocenes

Main group organometallics – preparation and use as synthetic reagents, Grignard reagents, organolithium compounds and organomagnesium compounds, organoboranes, organometallic compounds of aluminium, and silicon, preparation, and properties of transition metal – alkyl and aryl compounds

Catalytic processes, substitution reactions, oxidative addition, reductive elimination, migratory insertion, and hydride elimination reactions in homogeneous and heterogeneous catalysis, hydrogenation catalysis (Wilkinson's catalyst), Ziegler-Natta catalysts, hydroformylation reactions, alkene polymerization and isomerization, Wacker process, hydroamination and hydroboration, olefin metathesis.

Bioinorganic Chemistry-Transition elements in biology, occurrence, beneficial and toxic effects of metal ions and their role in the active-site structure and function of metalloproteins and enzymes, metal deficiency, toxicity, MRI agents and therapeutic applications, electron transfer reactions, vitamin B_{12} and cytochrome P450 and their mechanisms of action, chlorophyll, water-oxidation reactions, nitrogen fixation, O_2 binding properties of heme and non-heme proteins, their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr Effect; characterization of O_2 bound species by Raman and infrared spectroscopic methods, synthetic models for oxygen binding in heme and non-heme systems

References:

1. J. E. Huheey, E. A. Keiter, R.L. Keiter, and O. K. Medhi, *Inorganic Chemistry, Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
2. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, Inc., New York, 2009.
3. C. Elschenbroich, *Organometallics*, Wiley-VCH, Germany, 2006.
4. B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry, Concepts, Syntheses and Applications, University Press*, 2013.
5. I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, *Bioinorganic chemistry*, University Science Books, 1994.
6. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, 1994.
7. W. Kaim and B. Schwederski, *Bioinorganic chemistry: Inorganic Elements in the Chemistry of Life – An Introduction and Guide*, John Wiley & Sons, 1994.
8. R. M. Roat-Malone, *Bioinorganic Chemistry – A Short Course*, John Wiley & Sons, Inc., Hoboken, New Jersey, 2007.
9. L. Que, *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism*, Univ. Science Books, 2000.

CY7302E SYNTHETIC METHODOLOGIES IN ORGANIC CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Recommend reagents and methods for functional group interconversions.
CO2: Design synthetic strategies for C-C bond formation.
CO3: Deliver the concepts and methods of stereoselective synthesis and retrosynthesis.

Oxidation: Alcohols to carbonyls-chromium, manganese, ruthenium, silver and aluminium reagents, DMSO mediated oxidations- oxidations with TEMPO - oxonium salts - hypervalent iodine reagents: IBX and DMP-oxidation of phenols-Fremy's salt, CAN oxidations, DDQ, SeO_2, Corey-Kim oxidation- oxidations of alkenes - hydroxylation reactions, OsO_4-Sharpless asymmetric dihydroxylation, aminohydroxylation- Woodward and Prevost dihydroxylation reactions- asymmetric epoxidation of alkenes using peroxy acids and DMDO-epoxidation of allylic alcohols –peroxy acids and transition metal catalyzed- Sharpless asymmetric epoxidation- Jacobsen asymmetric epoxidation.

Reduction: Catalytic hydrogenation- heterogeneous and homogeneous catalysts- reduction with metal hydrides: lithium aluminium hydride, alkoxyaluminates, sodium borohydride, lithium and Zn borohydrides, alkoxy and alkylborohydrides, cyanoborohydrides, superhydrides, selectrides, boranes- selectivity in the reduction of carbonyl compounds.

Asymmetric synthesis: Control of stereochemistry- resolution- chiral pool-chiral auxiliary- methods of asymmetric induction: substrate, reagent and catalyst-controlled reactions- determination of enantiomeric and diastereomeric excess- enantio-discrimination.

C-C bond formation:Organometallic reagents: organo-lithium, magnesium, titanium, copper, chromium, zinc, boron and silicon reagents- palladium catalyzed coupling reactions: Suzuki, Sonogashira, Negishi, Stille, Hiyama, Fukuyama, Kumada and Buchwald–Hartwig coupling reactions- C-C bond formation reactions: Baylis–Hillman reaction, Henry reaction, Sakurai reaction- Baldwin rules- acyloin condensation.

C-C bond formation in polymerization reactions: Living polymerization: anionic polymerization, cationic polymerization, ring-opening metathesis polymerization (ROMP), free radical polymerization: stable free radical mediated polymerization (SFRP), atom transfer radical polymerization (ATRP), reversible addition-fragmentation chain transfer (RAFT) polymerization, iodine-transfer polymerization.

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

Retrosynthetic analysis: Basic principles and terminology of retrosynthesis- one group and two group C-X disconnections- one group C-C and two group C-C disconnections- important strategies of retrosynthesis- functional group transposition- important functional group interconversions.

References:

1. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5th Edition, Springer,2007.
2. J. J. Li, *Name reactions: A collection of detailed mechanism and synthetic applications*, 4th Edition, Springer, 2009.
3. S. Warren and P Wyatt, *Organic Synthesis: The disconnection Approach*, 2nd Edition, John-Wiley & Sons, Inc., 2008.

4. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons,1994.
5. M. B. Smith, March's, *Advanced Organic Chemistry*: *Reactions, Mechanisms and Structure*, 7th Edition, John-Wiley & Sons, Inc., 2013.
6. W. Carruthers and I.Coldham, *Modern Methods of Organic Synthesis,* 4th Edition, Cambridge University Press, 2004.
7. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3rd Edition, CRC Press, 1993.

CY7303E ELECTROCHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the fundamentals of Electrochemistry.
CO2: Demonstrate and practically develop different electrochemical cells.
CO3: Identify and handle the electrodes and cells.

Electrode potentials, Activity and activity coefficients of electrolytes, ionic strength, Debye-Huckel theory and limiting law, Nernst equation, EMF of a galvanic cell, Thermodynamics of cell reactions, EMF and temperature, pH, solubility product, potentiometry measurements and titrations. Polarisable and non-polarisable electrodes, reversible cells, reversible electrodes.

Basic electronics-capacitors, resistors, inductors, AC circuits, diodes, p-n junction, transistors, LED, solar cells, integrated circuits.

Faraday's laws of electrolysis, conductance and its measurements, theory of electrolytic dissociation, mechanism of electrolytic conduction, transport number, molar conductivity and its measurements, degree of dissociation, Debye-Huckel-Onsagar equation, Debye-Falkenhagen effect, Wein effect.

Primary and secondary batteries, fuel cells-polymer electrolyte and membranes, solid oxide fuel cells, electrochemical capacitors, pseudo capacitors, photo electrochemical solar cells, photo electrochemical water splitting, Bioelectricity, Na-K pump, corrosion and its applications

Electrified interface-structures, model and thermodynamics, kinetics of electrochemical reactions, electro catalysis, Butler-Volmer equation, Tafel equation and plots, overvoltage, microelectrodes, gas sensing electrodes, enzyme electrodes, chronomethods, spectroelectrochemistry.

References:

1. S. Glasstone, *Introduction to Electrochemistry*, East-West Press., 2006.
2. J. O. M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. I and II, Kluwer, Academic/Plenum Publishers, 2000.
3. R.G. Compton, G.H.W. Sanders, *Electrode Potentials*, Oxford University Press, New York, 1996
4. Allen J Bard, *Electrochemical Methods-Fundamentals and Aplications*, Wiley, 2nd Edition, 2006
5. Peter Atkins, Julio De Paula, *Elements of Physical Chemistry*, Oxford University Press, 5th Edition, 2009.

CY7304E SOLID STATE AND MATERIALS CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the basics of various crystalline solids and their characteristics.
CO2: Apply innovative ideas for the fabrication of novel crystalline materials for various applications.
CO3: Apply the basic solid-state concepts to tune the physico-chemical properties of nanomaterials for novel applications.

Band Theory of Solids - Crystal, Glass, Amorphous Solid, Long-Range Order - Bravais Lattice, Crystal System, Crystal Basis - Unit Cell, Face-Centered Cubic, Simple Cubic, Body-Centered Cubic, Hexagonal Close-Packed - Rock Salt Structure - Diamond Cubic – Birefringence – Crystallography - Methods of Characterizing Crystal Structure -Powder X-ray Diffraction, Electron and Neutron Diffraction - Electron Microscopy, EDAX, AFM - Imperfections in Solids.

Solid State Reaction - Precipitate Reactions, Sol-Gel Route, Precursor Method, Ion Exchange Reactions – Intercalation/de-intercalation Reactions – Defects - Colour Centers, F-centres - Reactivity, Zeolites – Catalysis, Magnetic Materials, Spinels, Garnets and Perovskites, Hexaferrites – Magnetoresistance and Spintronics.

Techniques of Polymerization - Bulk, Precipitation, Suspension and Emulsion Polymerization - Stereoregular Polymers, Polymer Molecular Weight and its Determination, Crystallinity, Glass Transition Temperature - Stress-Strain Properties, Plastics, Elastomers, Fibres, Polymer Blends and Composites, Conducting Polymers - Polymers for Biomedical Applications, Biodegradable Polymers, Polymer Biodegradation.

Extrinsic and Intrinsic Semiconductors - Hall Effect, Insulators - Dielectric, Ferroelectric, Pyroelectric and Piezoelectric Properties and their Relationships, Superconductivity Theory, High Tc Materials.
Introduction to Nanomaterials - Band Gap, Optical and Electronic Properties, Self-Assembly, Lithography, Targeted Drug Delivery, Fullerenes, Mesoporous Materials, Carbon Nanotubes, Quantum Dots-Quantum Confinement, Biological Applications

References:

1. A. R. West, *Solid state Chemistry and its Applications*, Wiley India, 2003
2. L. E. Smart, E. A. Moore, *Solid State Chemistry- an introduction*, Taylor &Fransis, 2005
3. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, *Polymer Chemistry*, New Age, 2015
4. W. D. Callister Jr., *Materials Science and Engineering-An Introduction*, Wiley India, New Delhi, 2006.
5. T. Pradeep, *A Text Book of Nano Science & Technology*, Tata McGraw-Hill Education India, 2008

CY7305E APPLICATIONS OF MOLECULAR SPECTROSCOPY

Pre-requisites: NIL

L	T	P	O	C
3	1	0	8	4

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply spectroscopic methods for the structural elucidation of molecules.
CO2: Choose spectroscopic methods for studying various chemical and physical properties of the molecules.
CO3: Apply spectroscopic methods for the elucidation of reaction mechanisms.

NMR spectroscopy-nuclei in a static magnetic field, basic principles of NMR experiment, resonance; spectral parameters-chemical shift, nuclear shielding, spin-spin coupling, origin of coupling, coupling constants, two bond, three bond, and long-range coupling, first-order splitting patterns and structure correlation, relationship between spectrum and molecular structure – equivalence, symmetry and chirality, homotopic, enantiotopic and diastereotopic groups, second-order effects on the spectrum- AB, AX, AMX, ABX spin systems, simplification of second order spectra.
^{13}C NMR: chemical shifts, proton coupled and decoupled ^{13}C NMR, NOE, DEPT, coupling of ^{13}C to ^{19}F and ^{31}P
Protons on oxygen and nitrogen, tautomerism, variable temperature NMR measurements, chiral shift and chiral resolving agents, multinuclear NMR of B, Al, Si, F and P nuclei; Determination of Magnetism for transition metal complexes, Dia- and paramagnetic NMR spectra of transition metal complexes
Two dimensional NMR spectroscopy: two-dimensional *J*-resolved spectroscopy-homonuclear and heteronuclear two dimensional *J* resolved spectroscopy, two-dimensional correlated spectroscopy – C,H-COSY, H,H-COSY.

Mass Spectrometry- Basic principles, ionization methods, isotope abundance, molecular ions, fragmentation processes of organic molecules and deduction of structural information, high resolution MS, introduction to soft ionization techniques, ESI-MS and MALDI–MS, quadrupole, tandem mass, ion scattering methods, SIMS, TOF, studies of inorganic/coordination and organometallic representative compounds.

EPR Spectroscopy-Introduction to EPR/ESR, comparison between NMR and EPR, g factor, electron-nuclear interactions, hyperfine and super hyperfine interactions, spin-spin and spin-lattice relaxations, hyperfine and g anisotropy, interpretation of EPR parameters for inorganic complexes and organic radicals, application of EPR to biological systems.

Mössbauer Spectroscopy-Mössbauer effect, recoil energy loss, thermal broadening of transition lines, electric and magnetic hyperfine interactions, Mössbauer spectrometers, detectors, isomer shift, quadrupole splitting, Mössbauer as a structural probe for iron complexes and other Mössbauer active transition metals– ^{61}Ni, ^{67}Zn, ^{99}Ru, applications to biological systems.

References:

1. H. Friebolin, *Basic One- and Two- Dimensional NMR Spectroscopy*, 5th Edition, Wiley-VCH, 2011.
2. D. L. Pavia, G. M. Lampman, G.S.Kriz and J.R.Vyvyan, *Spectroscopy, Brooks/ColeCengage Learning*, 2007.
3. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Tata McGraw Hill, 1988.
4. R. M. Silverstein, F. X. Webster and D. J. Kiemle, *Spectrometric Identification of Organic* Compounds**,** 7th Edition**,** John-Wiley and sons, New York, 2005.
5. S. K. Dewan, *Organic Spectroscopy*, 1st edition, CBS Publishers and Distributers Pvt. Ltd., 2010.
6. I. Bertini, C. Luchinat and G. Parigi, *Solution NMR of Paramagenetic Molecules-Applications to Metallo-biomolecules and Models*, Elsevier, 2001.
7. J. A. Weil and J. R. Bolton, *Electron Paramagnetic Resonance: Elementary Theory and Practical Applications*, John- Wiley and Sons, Inc, New Jersey, 2007
8. G. R. Eaton, S. S. Eaton and K. M. Salikhov, *Foundations of Modern EPR*, World Scientific Publishing Co., Singapore, 1999.

9. G. Hanson and L. Berliner Eds., *High Resolution EPR – Applications to Metalloenzymes and Metals in Medicine*, Springer, New York, 2009.
10. N. N. Greenwood and T. C. Gibb, *Mössbauer Spectroscopy*, Chapman and Hall Ltd., London, 1971.
11. P. Gütlich, R. Link and A. Trautwein, *Mössbauer Spectroscopy and Transition Metal Chemistry*, Springer-Verlag Berlin Heidelberg, 1978.
12. G. J. Long, Ed., *Mössbauer Spectroscopy Applied to Inorganic Chemistry*, Vol. 1, Springer New York, 1984.
13. D. P. E. Dickson and F. J. Berry Eds., *Mössbauer Spectroscopy,* Cambridge University Press, New York, 2005.

CY7398E PROJECT PHASE I

Pre-requisites: NIL

L	T	P	O	C
0	0	0	9	3

Course Outcomes:

CO1: Investigate contemporary research topics.
CO2: Select and solve chemical problems.
CO3: Explain the research findings and write technical and scientific reports.

Syllabus:

The student under the supervision of a faculty carries out state-of-the-art research in the frontier areas of chemistry. At the end of the semester, the final report/thesis describing the details of the entire project work has to be submitted to the Department, in a prescribed format. Presentation of the entire work and oral defence of the thesis has to be done before an evaluation committee.

CY7399E PROJECT PHASE II/ INTERNSHIP

Pre-requisites: NIL

L	T	P	O	C
0	0	0	18	6

Course Outcomes:

CO1: Do research on a relevant research topic or do internship.
CO2: Propose solutions for research problems or gain experience by internship.
CO3: Explain the research findings or internship experience and write technical and scientific reports.

Syllabus:

The student must carry out a research project under the supervision of a faculty in the contemporary areas of chemistry or do an internship at reputed organisations. The final report/thesis describing the details of the entire project work or internship has to be submitted to the Department at the end of the fourth semester. Evaluation of the work with a presentation at the department would be carried out at the department at the end of the project/internship.

Institute Elective Basket

ZZ6003E RESEARCH METHODOLOGY

Pre-requisites: NIL

L	T	P	O	C
2	0	0	4	2

Total Lecture sessions: 26

Course Outcomes:

CO1: Explain the basic concepts and types of research.
CO2: Develop research designs and techniques of data analysis.
CO3: Execute efficient and optimum methods of data collection and analysis.
CO4: Carry out effective data interpretation and to consolidate research reports.

Exploring Research Inquisitiveness
Philosophy of Scientific Research - Role of Research Guide - Planning the Research Project - Research Process - Research Problem Identification and Formulation – Variables - Framework Development - Research Design: Types of Research, Sampling, Measurement, Validity and Reliability, Survey - Designing Experiments - Research Proposal - Research Communication - Research Publication: Structuring a research paper, structuring thesis/ dissertation.

Systematics and Ethics of Research
Hypothesis-Driven Research: Experiment Design, Improving Experiments - Codes of Ethics: Scientific Misconduct, Plagiarism, Authorship, Regulation of Research - Intellectual Property Rights: Copyright, Patents, Designs – Peer Review – Citation Metrics – Safety Measures: laboratory, Human, Animal and Environment.

Sample Surveys and Test of Hypotheses
Design of Sampling: Introduction, Sample Design, Sampling and Non-sampling Errors, Sample Survey versus Census Survey - Measurement and Scaling: Qualitative and Quantitative Data, Classifications of Measurement Scales - Selection of Appropriate Method for Data Collection - Testing of Hypotheses, P-Value Approach, Test of Independence of Attributes, Test of Goodness of Fit, Chi Square Tests - Correlation and Regression - Simple Regression Analysis.

References:

1. K. N. Krishnaswamy, A. I. Sivakumar and M. Mathirajan, *Management Research Methodology,* Pearson Education, 2006.
2. P. D. Leedy, *Practical Research: Planning and Design*, 12th Edition, Pearson, 2018.
3. M. P. Marder, *Research Methods for Science*, Cambridge University Press, 2011.
4. C. R. Kothari, G. Garg, *Research Methodology: Methods and Techniques*, New Age International, 4th Edition, 2018.
5. R. Kumar, *Research Methodology: A Step-by step Guide for Beginners*, Sage Publications Ltd, 3rd Edition, 2011.
6. W. M. Trochim, *Research Methods: The Concise Knowledge Base*, Atomic Dog Publishing, 2005.

MS6174E TECHNICAL COMMUNICATION AND WRITING

Pre-requisites: NIL

L	T	P	O	C
2	1	0	3	2

Total Lecture sessions: 26

Course Outcomes:

CO1: Apply effective communication strategies for different professional and industry needs.
CO2: Collaborate on various writing projects for academic and technical purposes.
CO3: Combine attributes of critical thinking for improving technical documentation.
CO4: Adapt technical writing styles to different platforms.

Technical Communication

Process(es) and Types of Speaking and Writing for Professional Purposes - Technical Writing: Introduction, Definition, Scope and Characteristics - Audience Analysis - Conciseness and Coherences - Critical Thinking - Accuracy and Reliability - Ethical Consideration in Writing - Presentation Skills - Professional Grooming - Poster Presentations

Grammar, Punctuation and Stylistics

Constituent Structure of Sentences - Functional Roles of Elements in a Sentence - Thematic Structures and Interpretations - Clarity - Verb Tense and Mood - Active and Passive Structures - Reporting Verbs and Reported Tense - Formatting of Technical Documents - Incorporating Visuals Elements - Proofreading

Technical Documentation

Types of Technical Documents: Reports, Proposals, Cover Letters - Manuals and Instructions - Online Documentation - Product Documentation - Collaborative Writing: Tools and Software - Version Control Document Management - Self Editing, Peer Review and Feedback Processes

References:

1. Foley, M., & Hall, D. (2018). *Longman advanced learner's grammar, a self-study reference & practice book with answers*. Pearson Education Limited.
2. Gerson, S. J., & Gerson, S. M. (2009). *Technical writing: Process and product*. Pearson.
3. Kirkwood, H. M. A., & M., M. C. M. I. (2013). *Hallidays introduction to functional grammar* (4th ed.). Hodder Education.
4. Markel, M. (2012). *Technical Communication* (10th ed.). Palgrave Macmillan.
5. Tuhovsky, I. (2019). *Communication skills training: A practical guide to improving your social intelligence, presentation, Persuasion and public speaking skills.* Rupa Publications India.
6. Williams, R. (2014). *The Non-designer's Design Book*. Peachpit Press.

IE6001E ENTREPRENEURSHIP DEVELOPMENT

Pre-requisites: NIL

L	T	P	O	C
2	0	0	4	2

Total Lecture Sessions: 26

Course Outcomes:

CO1: Describe the various strategies and techniques used in business planning and scaling ventures.
CO2: Apply critical thinking and analytical skills to assess the feasibility and viability of business ideas.
CO3: Evaluate and select appropriate business models, financial strategies, marketing approaches, and operational plans for startup ventures.
CO4: Assess the performance and effectiveness of entrepreneurial strategies and actions through the use of relevant metrics and indicators.

Entrepreneurial Mindset and Opportunity Identification

Introduction to Entrepreneurship Development - Evolution of entrepreneurship, Entrepreneurial mindset, Economic development, Opportunity Recognition and Evaluation - Market gaps - Market potential, Feasibility analysis - Innovation and Creativity in Entrepreneurship - Innovation and entrepreneurship, Creativity techniques, Intellectual property management.

Business Planning and Execution

Business Model Development and Validation - Effective business models, Value proposition testing, Lean startup methodologies - Financial Management and Funding Strategies - Marketing and Sales Strategies - Market analysis, Marketing strategies, Sales techniques - Operations and Resource Management - Operational planning and management, Supply chain and logistics, Stream wise Case studies.

Growth and Scaling Strategies

Growth Strategies and Expansion - Sustainable growth strategies, Market expansion, Franchising and partnerships - Managing Entrepreneurial Risks and Challenges - Risk identification and mitigation, Crisis management, Ethical considerations - Leadership and Team Development - Effective communication - Entrepreneurial Ecosystem and Global Perspectives - Entrepreneurial ecosystem, Stream wise Case studies.

References:

1. Kaplan, J. M., Warren, A. C., & Murthy V. (Indian Adoption) (2022). Patterns of entrepreneurship management. John Wiley & Sons.
2. Kuratko, D. F. (2016). Entrepreneurship: Theory, process, and practice. Cengage learning.
3. Barringer, B. R. (2015). Entrepreneurship: Successfully launching new ventures. Pearson Education India
4. Rajiv Shah, Zhijie Gao, Harini Mittal, Innovation, Entrepreneurship, and the Economy in the US, China, and India, 2014, Academic Press
5. Sundar, K. (2022). Entrepreneurship Development, 2nd Ed, Vijaya Nichkol Imprints, Chennai
6. E. Gordon,Dr. K. Natarajan., (2017).Entrepreneurship Development, 6th Ed, Himalya Publishers,Delhi
7. Debasish Biswas, Chanchal Dey, Entrepreneurship Development in India, 2021, Taylor & Francis.

Electives

CY7351E NUCLEAR CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Understand the nuclear structure, radioactivity, radioactive decay and growth, nuclear reactions, artificial radioactivity and applications of nuclear chemistry.
CO2: Identify and understand various nuclear reactions easily with the simple notations.
CO3: Think innovatively and apply the knowledge in useful applications.

Nuclear structure: Composition of the nucleus, nuclear size, shape and density, theories of nuclear composition, magnetic and electric properties of nucleus, nuclear spin and parity, nuclear binding forces.

Measurement of radioactivity, radioactive decay and growth: Measurement of radioactivity, group displacement law, radioactive disintegration series, rate of disintegration, half-life, average life of radioactive elements, unit of radioactivity, nuclear decay, determination of decay constants, decay rates, types of nuclear decay.

Nuclear reactions-Bethe's notation of nuclear process, types of nuclear reactions, nuclear fission, fission products, theory of nuclear fission, nuclear reactors, classification of reactors including power nuclear reactor, breeder reactor, nuclear reactors in India.

Artificial radioactivity and applications of nuclear chemistry-Discovery of artificial radioactivity, synthesis of trans-uranium elements, importance and applications of artificial radioactivity, production and separation of radioactive isotopes, radioactive tracers, applications of tracer element in medical, agriculture and analytical fields, age determination, isotopic dilution analysis, neutron activation analysis, biological effects of radiation, waste disposal and radiation protections.

References:

1. H. I. Arnikar, *Essentials of nuclear chemistry*, 2ndedition, Wiley, New York, 1987.
2. U. N. Dash, Nuclear Chemistry for B.Sc and M.Sc students, S. Chand, 2008.
3. G. Choppin, J. Rydberg and J. O. Liljenzin, *Radiochemistry and Nuclear Chemistry*, Butterworth-Heinemann, 3rd edition, 2002.
4. W. D. Loveland, D. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, John Wiley & Sons, 2006.
5. G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rdedition, John Wiley & Sons, USA, 1981.

CY7352E PORPHYRINS AND METALLOPORPHYRINS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Learn the IUPAC nomenclature of porphyrins and related compounds.
CO2: Study the synthesis, separation, purification and characterization of porphyrins and metalloporphyrins.
CO3: Learn various biomimetic porphyrins and their related compounds.
CO4: Formulate independent research ideas in the field of porphyrin chemistry.

Nomenclature and Synthesis-Introduction to tetrapyrrole pigments in biology, nomenclature in pyrrole, system with two pyrrole rings, porphyrin and related compounds, Fischer and Revised nomenclature; Synthesis of porphyrin (β and *meso*-substituted) ligand from monopyrroles based on Rothemund, Adler and Lindsey methods, mechanistic considerations of porphyrin formation, metallation of porphyrins in different reaction conditions.

Purification and separation-Physical methods for separating the components of a mixture, chromatographic methods including paper, thin layer (TLC), preparative TLC, column, flash, gas chromatography and high-performance liquid chromatography. Non-chromatographic methods: Extraction, precipitation, recrystallization and sublimation.

Characterization-Fundamentals of spectroscopic techniques including UV-Visible, IR, NMR, EPR, Mass and Elemental analysis, Raman, Single crystal X-ray diffraction studies of porphyrins and metalloporphyrins.

Biomimetic porphyrins-Porphyrins with appended peptides, chelated hemes: porphyrins having covalently attached imidazole, pyridine, sulphur, quinone and other interactive groups, picket fence porphyrins and related species, capped porphyrins and related species, strapped porphyrins containing bulky and interactive groups.

References:

1. (a) K. M. Kadish, K. M. Smith, R. Guilard, *The Porphyrin Handbook*, Vol. 1-10, Academic Press, San Diego, 1999; (b) K. M. Kadish, K. M. Smith, R. Guilard, *The Porphyrin Handbook*, Vol. 11-20, Academic Press, San Diego, 2003.
2. D. Dolphin, *The Porphyrins,* Volume 1: *Structure and Synthesis, Part A,* Academic Press, New York, 1978.
3. J. E. Merritt, and K. L. Loening, *Pure & Appl. Chem.*, 1979, 51, 2251.
4. (a) T. Kitagawa and Y. Ozaki, *Structure and Bonding*, 1987, Vol. 64, 71; (b) B. Morgan and D. Dolphin, *Structure and Bonding*, 1987, Vol. 64, 115.

CY7353E MEDICINAL CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Deliver the basic principles, terms and definitions of medicinal chemistry
CO2: Convey the types of drug receptors and drug- targets interactions
CO3: Deliver various stages and strategies used in drug discovery, design and development processes
.

Introduction to biological molecules: amino acids, peptides and proteins, nucleotides, DNA and RNA, catalytic antibodies, protein-small molecule interactions, evaluation of enzyme inhibitors.

Drug design and drug action. ADMET - drug absorption, distribution, metabolism (phase 1 and phase II) and toxicity; physicochemical properties that affect ADMET- acid-base properties, water solubility, partition coefficient; introduction to rational approach to drug design**,** physical and chemical factors associated with biological activities and mechanism of drug action, **c**lassification of drugs based on structure or pharmacological basis with examples.

Combinatorial chemistry: introduction, strategies, general techniques, solid phase methods and solid phase anchors, combinatorial synthesis in solution, multi-component reactions, encoding methods, deconvolution, lead discovery, and high-throughput screening.

Structure-activity relationships and lead optimization: introduction, quantitative assessment of stereo-electronic effects - lipophilic parameters, electronic parameters and steric parameters, QSAR, examples.

References:

1. G. Jung (Editor), *Combinatorial Chemistry: Synthesis, Analysis and Screening*, Wiley- VCH, 2001.
2. D. L. Nelson and M. M. Cox, *Lehninger, Principles of Biochemistry, 4th revised edition*, Palgrave Macmillan, 2008.
3. G. L. Patrick, *An Introduction to Medicinal Chemistry*, 3rd Edition, Oxford University Press, 2005.
4. J. M. Berg, J. L. Timoczko, and L. Stryer, *Biochemistry*, 6th Edition, WH Freeman, 2007.
5. G. Thomas, *Fundamentals of Medicinal Chemistry*, John Wiley, 2003.
6. R. K. Murray, D. K. Granner, P. A. Mayes, and V. W. Rodwell, *Harper's Illustrated Biochemistry*, 26th Edition, The McGraw Hill Companies, 2003.

CY7354E PRINCIPLES OF BIOCHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Deliver the basic principles, terms, and definitions of biochemistry.
CO2: Demonstrate an understanding of biochemical processes.
CO3: Demonstrate the link between chemical reactions and biological processes.

Protein structure and functions: amino acids, peptides and proteins; primary, secondary and tertiary structure of proteins- Enzymes: basic concepts, kinetics, structure, function and catalysis.

Carbohydrates and lipids of physiological significance, an overview of metabolism and metabolic pathways: glycolysis, gluconeogenesis, pentose phosphate pathway, citric acid cycle, fatty acid catabolism, amino acid oxidation, oxidative phosphorylation and photophosphorylation.

Structure and functions of nucleic acids, the basic structure of DNA and RNA, DNA, replication, recombination and repair, RNA synthesis, processing and modification.

The flow of genetic information: from genes to proteins, transcription, translation, splicing and post-translational modifications.

References:

1. R. H. Garrett and C. M. Grisham, *Biochemistry, 4th Edition*, Brooks and Cole, 2010.
2. D. L. Nelson and M. M. Cox, *Lehninger*, *Principles of Biochemistry, 4th revised edition*, Palgrave Macmillan, 2008.
3. J. M. Berg, J. L. Timoczko and L. Stryer, *Biochemistry*, 6th Edition, WH Freeman, 2007.
4. R. K. Murray, D. K. Granner, P. A. Mayes and V. W. Rodwell, Eds. *Harper's Illustrated Biochemistry* 26th Edition, McGraw Hill, 2003

CY7355E ORBITAL INTERACTIONS IN CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Construct molecular orbitals from fragment orbitals.
CO2: Explain the stability, geometrical shape, and reactivity
CO3: Apply the orbital concept to understand the structure-activity relationship.

Concepts of bonding – Atomic orbitals, Molecular orbitals, Orbital interaction energy, Molecular orbital coefficients, Electron density distribution, Perturbational molecular orbital theory - Linear H_3, HF, and the Three-orbital problem
.
Molecular orbital construction from fragment orbitals – Linear and triangular H_3, Rectangular and square planar H_4, Tetrahedral and linear H_4, Pentagonal H_5, Hexagonal H_6. Molecular orbitals of diatomic molecules - Electronegativity perturbation, Geometrical perturbation. Molecular orbitals of AH_2, Walsh diagrams, Jahn–Teller distortions. Molecular orbitals of small building blocks - AH system, AH_3 systems, π-bonding effects of ligands, AH_4 system, Molecules with two heavy atoms - A_2H_6 and A_2H_4 systems. Orbital interactions through space and through bonds

Polyenes and conjugated systems - Acyclic polyenes, Hückel Theory, cyclic systems, conjugation in three dimensions, Solids - energy bands. Hypervalent molecules

Transition metal complexes - Octahedral ML_6, π-effects in an octahedron, Distortions from an octahedral geometry, Square planar and tetrahedral ML_4 complexes, Five coordination, Transition metal fragments - Square pyramidal ML_5, ML_3, ML_2, ML_4, CpM and Cp_2M. Isolobal analogy

.
References:

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, *Orbital Interactions in Chemistry*, 2nd Edition, John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, *Molecular Orbitals and Organic Chemical Reactions*, Students Edition, Wiley, 2009.
3. A. Rauk, *Orbital Interaction Theory of Organic Chemistry*, 2nd Edition, Wiley-Blackwell, 2000.
4. W. L. Jorgensen, L. Salem, *The Organic Chemist's Book of Orbitals*, Academic Press, 1973.

CY7356E ADVANCED MATERIALS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the synthetic procedures and practical application of nanomaterials.
CO2: Identify new type of materials for application in required fields.
CO3: Identify the suitable material characterization techniques.

Physical and chemical basis and principles of nanotechnology, Industrial applications of nanoparticles, Implications of nanotechnology for environmental health research. Synthesis of noble metal nanoparticles, functionalized nanoparticles and metal nanoparticles for biomedical applications, self-assembly and self-organization of nanomaterials, semiconductor quantum dots, Syntheses of water soluble QDs, Optical properties of QDs, Dynamic optical properties of Au and Ag NPs, Synthesis of magnetic nanoparticles, Synthesis of Carbon nanotubes, Protein and DNA based nano structures, Polymer nanoparticles and thin films.

Principles of biomimetics, materials for biomimetics, biosensors, bio membranes, antimicrobial coatings, super hydrophobic materials, contact angle, self-cleaning materials, super adsorbents, Dyes for imaging, Liquid crystals in display and thermography, polymeric liquid crystals, hierarchical zeolites, polymer supported catalysts.

Plastic degradation, biodegradable polymers-structure, mechanism of degradation, biocomposites-fabrication and biodegradation, conducting polymers, organic electronics, shape memory polymers, polymers for biomedical applications (tissue engineering, bioseparations, contact lenses, orthopedic implants, dental materials), polymer nanofibres-electrospinning. porous and nonporous polymer membranes, chemical structure and composition of drug carriers, micelles, vesicles, dendrimers, nanocapsules, multifunctional nanoparticles, hydrogels, polymer drug conjugates.

Material characterisation: TGA, DSC, UTM, SEM, TEM, SPM, AFM, Raman spectroscopy, X-ray, biocompatibility, cytotoxicity, antimicrobial analysis.

References:

1. V. Biju, T. Itoh, A. Anas, A. Sujith, and M. Ishikawa, Semiconductor quantum dots and metal nanoparticles: syntheses, optical properties and biological applications. *Analytical and Bioanalytical Chemistry* 391, 2469-2495 (2008).
2. T. Vo-Dinh, Ed. *Nanotechnology in biology and medicine: methods, devices and applications*, CRC Press; 2006.
3. L. V. Azaroff, *Introduction to Solids*, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1977.
4. J. M. G. Cowie and V. Arrighi, *Polymers: Chemistry and Physics of Modern Materials*, CRC Press, Taylor and Fransis, 2008.
5. G. Heimke, V. Soltesz and A. J. C. Lee, Eds., *Advances in Materials*, Elsevier, Amsterdam, 1990.
6. R. W. Kelsall, I. W. Hamley and M. Geoghegan, *Nanoscale Science and Technology*, John Wiley & Sons, New York, 2005.

CY7357E RAMAN SPECTROSCOPY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the theory of Raman Spectroscopy.
CO2: Demonstrate the basic instrumentation of Raman Spectroscopy.
CO3: Identify the new possibilities of Raman spectroscopy in different fields.

Historical background, Energy units, vibration of diatomic and polyatomic molecules, Rayleigh scattering, Mie scattering, Raman scattering, Resonance Raman scattering, Raman and IR spectroscopy, classical theory of Raman effect: polarizability, quantum theory of Raman scattering, selection rules for Raman spectra, molecular symmetry, character table, fundamental modes of vibration, symmetry selection rules, mutual exclusion principle.

Source, monochromator, detection device, sample handling techniques, fibre coupled Raman spectrometer, FT-Raman spectrometer, Effect of polarisation on Raman spectra, pure rotation Raman spectra: linear, symmetric and asymmetric top molecules, vibration Raman spectra: spherical top molecules, structural determination from IR and Raman spectroscopy.

High pressure Raman Spectroscopy, Raman microscopy and imaging, Raman spectroelectrochemistry, Time resolved Raman spectroscopy, non-linear Raman spectroscopy, Surface enhanced Raman Scattering (SERS): Mechanism: electromagnetic and chemical, SERS substrates: metal films, metal electrodes, metal sol, SERS microscopy and imaging, SERS study of bio molecules, Tip enhanced Raman spectroscopy.

Materials and Applications: phase transitions, electrical conductors: C_{60}, carbon nanotubes, Raman dyes, biomolecules: proteins, DNA, bacteria and virus, cells, polymers, drug delivery, food, petroleum industry, water analysis, forensic and pharmaceutical analysis, archaeology, Raman sensors

References:

1. J. R. Ferraro, K. Nakamoto and C. W. Brown, *Introductory Raman Spectroscopy*, Academic Press, San Diego, 2003
2. E. Smith and G. Dent, *Modern Raman Spectroscopy A Practical Approach*, Wiley, England, 2005.
3. S. -L. Zhang, *Raman Spectroscopy and its application in nanostructures*, Wiley, 2012
4. J. Laane, Ed., *Frontiers of Molecular spectroscopy*, Elsevier, 2009
5. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, McGraw Hill Education, New Delhi, 2013.

CY7358E METAL BASED DRUGS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the use of metal complexes as drug candidates
CO2: Detail different possible metal complex-drug interactions
CO3: Predict possible mechanisms of drug action

DNA as drug targets, Structure and conformations of DNA, coiling, replication and transcription mechanism, Types of DNA-drug binding, active binding sites, DNA supercoiling, telomeres and G-quadruplexes, Genomes, DNA-protein interactions, Proteins as drug targets, synthesis of proteins and structure determination, protein purification, metal binding sites on proteins, proteins as biomarkers.

Action of different drugs – cytotoxic, antitumor, antibacterial and antiviral drugs, cisplatin development and its drug action, DNA-base recognition by cisplatin, intracellular hydrolysis, toxicity of cisplatin, other platinum based anticancer drugs, use of ruthenium, titanium, copper, zinc and gold in medicine, application of vanadium as insulin mimics for treatment of diabetes.

Metal compounds as MRI contrast agents, radionucleides for cancer treatment, use of technetium as imaging agents, Lanthanides as shift reagents, Chemical exchange saturation transfer (CEST), Cellular imaging, Integrated micro- and nano- imaging techniques for analysis of metalloproteomics.

Organomercury and organosilicon compounds in medicine, Salvarsan, neosalvarsan and stibamine, organotin and organogermanium compounds as anticancer agents, nanomedicine, molecular organic frameworks, mesoporous silica and encapsulation, gold nanoparticles in biomedicines, drug delivery by nanoparticles, cytotoxic nanoparticles, health risks of nanoparticles.

References:

1. J. C. Dabrowiak, *Metals in medicine*, John Wiley & Sons, Inc., New York, 2009.
2. M. Gielen, E. R. T. Tiekink, *Metallotherapeutic drugs and metal-based diagnostic agents*, John Wiley & Sons, Inc., New York, 2005.
3. N. Farrell, *Uses of inorganic chemistry in medicine*, Royal Society of Chemistry, UK, 1999.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry – Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
5. R. C. Mehrotra and A. Singh, *Organometallic Chemistry-A Unified Approach*, New Age International Publishers, India, 2011.
6. C. Elschenbroich, *Organometallics*, Wiley-VCH, Germany, 2006.

CY7359E METAL COMPLEXES IN MOLECULAR SYSTEMS AND DEVICES

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Describe the photochemical or photophysical and optical properties of complexes
CO2: Predict electrochemical activities of transition metal complexes
CO3: Propose new coordination complexes in molecular systems and devices

Photochemistry and photophysics of transition metal complexes – excited states and electron transitions, absorption and emission bands, Jablonski Diagrams, photophysical parameters in solution, Photochemical reactivity, polynuclear metal complexes.

Luminescent lanthanide complexes- triplet mediated energy transfer, designing the complex, selection of lanthanides and antennae, macrocyclic and bicyclic ligands, modulating the luminescence, lanthanide luminescent sensors and switches.

Linear and Nonlinear Optical activity, Theory of NLO, second and third harmonic generation, Difference frequency generation, Optical parameter amplification, N Wave mixing, NLO active metal complexes, HOMO – LUMO band gaps, Polymers and Third Order NLO, Donor –pi- Acceptor complexes, Complexes with macrocyclic ligands, Bimetallic Complexes.

Transition metal complexes in photovoltaic cells and light emitting diodes – Dye sensitized solar cells, principles, molecular sensitizers, photovoltaic properties of metal complexes, complexes as triplet emitters in organic light emitting diodes, controlling quantum yields, Applications of metal complexes in OLEDs.

References:

1. M. Montalti, *Handbook of Photochemistry*, 3rd Edition, Taylor and Francis, Florida, 2006.
2. A. S. Abd-El-Aziz, C. E. Carraher, C. U. Pittman, M. Zeldin, *Inorganic and Organometallic Macromolecules*, Springer LLC., USA, 2008.
3. V. W. W. Yam Eds. *Photofunctional Transition Metal Complexes*, Springer- Verlag Berline Heidelberg, 2007.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry – Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
5. R. van Eldik, C. D. Hubbard, *Advances in Inorganic Chemistry*, Academic Press, USA, 2003.
6. D. W. Bruce, D. O’Hare, *Inorganic Materials*-John Wiley and Sons, New York, 1997

CY7360E APPLIED COORDINATION CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Explain the versatile applications of coordination and organometallic complexes
CO2: Predict the structures of different coordination compounds
CO3: Apply the theory and concept to contemporary research on transition metal complexes

Transition and non-transition metal complexes, tetragonal and rhombic distortions and their effects on structural properties, mononuclear and multinuclear complexes with polydentate ligands, fluxional compounds, geometrical and optical isomers in coordination complexes, air-sensitive complexes of lanthanides and actinides.

One-dimensional and two-dimensional coordination polymers, applications, magnetic metal complexes, variations in magnetic moment with temperature, luminescent inorganic metal complexes, their potential applications in biological and optical fields, catalysis by transition metal complexes, homogenous and heterogeneous catalysis, chiral and asymmetric catalysis.

Types of organometallic compounds, synthesis, carbocyclic groups, polynuclear carbonyl complexes, substitution reactions in carbonyls, oxidative addition and elimination, metal alkyls, carbene, carbyne and carbide complexes, their synthesis and applications, alkene and alkyne complexes, ferrocenes, cyclopentadienyl complexes, cyclooctatetraene and cyclobutadiene complexes.

Inorganic complexes in biological systems, action of cisplatin and its cell toxicity, metal complexes as antiproliferative agents, metalloporphyrins, non-heme proteins, cytochromes and ferredoxins, structure and stability of proteins, protein folding and synthesis, techniques for isolation, purification and characterization of proteins, Protein crystallography, ligand-protein interactions, protein biomarkers, metalloenzymes, enzyme catalysis.

References:

1. (a) K. M. Kadish, K. M. Smith, R. Guilard, *The Porphyrin Handbook*, Vol. 1-10, Academic Press, San Diego, 1999; (b) K. M. Kadish, K. M. Smith, R. Guilard, *The Porphyrin Handbook*, Vol. 11-20, Academic Press, San Diego, 2003.
2. D. Dolphin, *The Porphyrins*, Volume 1: *Structure and Synthesis, Part A,* Academic Press, New York, 1978.
3. J. E. Merritt, and K. L. Loening, *Pure & Appl. Chem.*, 1979, 51, 2251.
4. (a) T. Kitagawa and Y. Ozaki, *Structure and Bonding*, 1987, Vol. 64, 71; (b) B. Morgan and D. Dolphin, *Structure and Bonding*, 1987, Vol. 64, 115.

CY7361E CHEMISTRY OF MACROMOLECULES

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the basic aspects of polymeric materials to the product fabrication.
CO2: Do polymer compounding and curing.
CO3: Carry out testing of polymeric materials for characterization.
CO4: Apply the concepts and methods of rheology.

Basic concepts: Classification- mechanisms and methods of polymerization- polymers through coupling reactions- molecular weights: methods of determination, molecular weight distribution, viscosity and molecular weight, mechanical properties and molecular weight-- glass transition determination-degree of crystallinity- morphology- viscoelasticity models.
Biomacromolecules: cellulose based systems-structure, characterization, properties, surface modification chemistry

Molecular motions (self-diffusion, hydrodynamic radius, Rouse Model, Zimm Model, entangled polymer dynamics and de Gennes reptation model)- thermodynamics of polymer solutions- behaviour in solvents: swelling, entropy, enthalpy and free energy of mixing- solubility parameter- casting of solutions.

Difference between macromolecular flow and small-molecular flow, evaluation of degradation of polymers in terms of tensile strength, tear strength, modulus, hardness, compression set, creep, stress- relaxation- molecular interpretations- thermal evaluations- degradation examination, combustion calculations- plastic utilization and environment.

Basic principles in processing- plastic processing: injection moulding, extrusion, blow moulding, calendaring- rubber processing- chemistry of vulcanization- compression moulding- latex processing-
Making of plastic, dry rubber and latex based products- application in opto-electronic and biomedical fields.

References:

1. R. J. Young and P. A. Lovell, Introduction to Polymers, 2nd Edition, Chapman and Hall, 2002.
2. F. W. Billmeyer, Textbook of Polymer Science, 3rd Edition, John Wiley, 1994.
3. V. R. Gowariker, N. V. Viswanathan, Jayadev Sreedhar, New Age International (P) Ltd, 2005.
4. G. Odian, Principles of Polymerization, Fourth edition, Wiley-Interscience, 2004.
5. L. H. Sperling, Introduction to Physical Polymer Science, Wiley- Interscience, 1986.
6. M. Rubinstein and R. A. Colby, Polymer Physics, Oxford University Press, 2003.
7. C. M. Blow, C. Hepburn, Rubber Technology and Manufacture, Elsevier Science & Technology Books, 1982.
8. J. Brydson, Plastics Materials, 7th Edition, Butterworth-Heinemann,1999.
9. George Wypych, Handbook of Polymers, Chem Tec Publishing, 2012.
10. U. W. Gedde and M. S. Hedenqvist, *Fundamental Polymer Science*, Springer International Publishing, 2019.

CY7362E LUBRICANT CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Evaluate surfaces critically for the identification of suitable lubrication strategy.
CO2: Examine and quantify lubricant formulations.
CO3: Propose appropriate vegetable oil lubricant formulations for various applications.
CO4: Develop and characterize lubricants for specific applications.

Surface structures-chemistry and properties of different substrates: metals, ceramics and polymers- surface characterization protocols- surface roughness- hardness- morphology- alloys- theories of friction- -friction in plastics and ceramics- theories of wear – surface treatments

Necessity for lubrications- lubricant identification-mechanism of lubrication- synthetic and natural base oils- compositions- solid, liquid and semi-solid lubricant formulations- additives- antioxidants- viscosity improvers- thermal stabilisers -vegetable oil modifications- transesterification- polymer modifications

Characterization of lubricants- chemical modifications to alter viscosity and viscosity index- flash point and fire point- cloud and pour posits- acid value- saponification value- aniline point- steam emulsion number- carbon residues evaluation

Industrial formulations- structure-property relationships, performance evaluation, degradation, emission calculations, environmental impacts, environment- friendly additives, scope of biopolymers for lubricant applications.

References:

1. R. G. Bruce, W. K. Dalton, J. E. Neely and R. R. Kibbe, *Modern Materials and Manufacturing Processes*, Prentice Hall, 2004.
2. R. M. Mortier, M. F. Fox, M. M. Roy, F. F. Malcolm, S.T. Orszulik (Eds.) *Chemistry and Technology of Lubricants*, Springer, 2010.
3. V. Stepina and V. Vesely, *Lubricants and Special Fluids*, Elsevier, 1992.
4. C. M. Mate and R. W. Carpick, *Tribology on the Small Scale: A Modern Textbook on Friction, Lubrication and Wear (Second Edition)*, Oxford University Press, 2019.
5. A. Rudawska, *Surface Treatment in Bonding Technology*, Academic Press, 2019.
6. S. P. Athavale, *Hand Book of Adhesive Formulations: Adhesive Technology*, Notion Press, 2018.

CY7363E HETEROCYCLIC CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the principles of nomenclatures to any heterocyclic molecules.
CO2: Categorize the aromatic and nonaromatic heterocyclic compounds.
CO3: Deliver the reactivity of various heterocyclic compounds.
CO4: Design the synthesis of numerous heterocyclic compounds.

Introduction, nomenclature – Hantzsch Widman system, trivial system, fusion system, replacement system – monocyclic, fused, spiro and bridged systems, and heterocyclic ring assemblies, chemical behavior of aromatic heterocycles, criteria of aromaticity, selectivity and reactivity.

Three membered heterocycles: aziridines – synthesis using Gabriel method, Wenker method and Hassner methods, nucleophilic, electrophilic, electrocyclic ring opening reactions, fragmentation and rearrangement reactions; oxiranes – synthesis *via* epoxidation of alkenes, nucleophilic alkylation of carbonyl compounds, intramolecular cyclization and condensation reactions, nucleophilic, electrophilic ring opening reactions, thermal and rearrangement reactions; thiiranes – synthesis from oxiranes, using intramolecular cyclization reactions, methylene insertion reactions, ring opening reactions; four membered heterocycles: azetidines, oxetanes and thietanes synthesis, ring opening reactions, rearrangement reactions and photochemical reactions.

Structure, stability, synthesis and reactions with electrophiles, nucleophiles, free radicals, electron deficient species, oxidizing agents, reducing agents, cycloaddition reactions and photochemical reactions of five membered heterocycles with one heteroatom – pyrroles, furans, thiophenes, five membered heterocycles with two heteroatoms – imidazoles, oxazoles, thiazoles, pyrazoles, isoxazoles and isothiazoles; benzo fused five membered heterocycles with one heteroatom – indoles, isoindoles, indolizines, carbazoles, benzofurans, and benzothiophenes; five membered heterocycles with more than two heteroatoms – triazoles, tetrazoles, oxadiazoles, thiadiazoles; six membered heterocycles – pyridine and benzo fused six membered heterocycles – quinolines and isoquinolines; Applications of heterocycles in the field of medicinal chemistry as antibacterial agents, anticancer agents, vaccine adjuvants and kinase inhibitors.

References:

1. J. A. Joule and K. Mills, *Heterocyclic Chemistry*, 5th Edition, John Wiley & Sons, Ltd., UK, 2010.
2. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry*, 2 volume set, Springer (India) Pvt. Ltd., 2009.
3. J. Alvarez-Builla, J. J. Vaquero and J. Barluenga, *Modern Heterocyclic Chemistry*, Volume 4, Wiley-VCH, Weinheim, Germany, 2011.
4. T. L. Gilchrist, *Heterocyclic Chemistry* 3rd Edition, Pearson education, New Delhi, India, 2005.
5. A. Atritzky, C. Ramsden, J. Joule and V. Zhdankin, *Handbook of Heterocyclic Chemistry*, 3rd Edition, Elsevier, 2010.
6. R. M. Acheson, *An Introduction to the Chemistry of Heterocyclic Compounds*, 3rd Edition, Wiley India Pvt. Ltd., 2008.

7. T. Eicher, S. Hauptmann and A. Speicher, *The Chemistry of Heterocycles: Structure, Reactions, Syntheses, and Applications*, 3rd Edition, completely revised and enlarged edition, Wiley-VCH, Weinheim, Germany, 2012.
8. L. D. Quin and J. Tyrell, *Fundamentals of Heterocyclic Chemistry: Importance in Nature and in the Synthesis of Pharmaceuticals,* 1st Edition, John Wiley & Sons, Inc., New Jersey, USA, 2010.
9. R. J. Anderson, P. W. Groundwater, A. Todd and A. J. Worsley, *Antibacterial Agents: Chemistry, Mode of Action, Mechanisms of Resistance and Clinical Applications,* 1st Edition, Wiley, 2012.
10. C. Avendaño and J. C. Menéndez, *Medicinal Chemistry of Anticancer Drugs*, 2nd Edition, ScienceDirect, 2015.
11. V. E. J. C. Schijns and D. T. O'Hagan, *Immunopotentiators in Modern Vaccines.* 2nd Edition, Science Direct, 2017.
12. R. Li and J. A. Stafford, *Kinase Inhibitor Drugs*. Wiley, 2009.

CY7364E CHEMISTRY AT INTERFACES

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Comprehend fundamental aspects of interfaces formed between two immiscible surfaces, and their electrical, thermodynamic & mechanical properties
CO2: Apply potentials of interfaces in controlling the morphology and the properties of nanomaterials
CO3: Design the synthesis of various nanostructures and apply for various industrial processes

Liquid Surfaces, Microscopic Picture of the Liquid Surface, Surface Tension, Curved Liquid Surfaces, Derivation of Young-Laplace Equations, Capillary Condensation, Techniques of Surface Tension Measurements - Thermodynamics of Interfaces - Surface Excess, Internal Energy and Helmholtz Energy, Free Surface Energy, Interfacial Enthalpy and Gibbs Surface Energy - Gibbs Adsorption Isotherm, Two Component Systems, Location of the Interface.

Surface Forces, Van der Waals Forces Between Molecules, Electrostatic Interaction Between Two Identical Surfaces, Steric Interaction - Properties of Polymers, Polymer Coated Surfaces - Contact Angle Phenomena and Wetting, Hysteresis in Contact Angle Measurements, Young's Equation - Particles in the Liquid Gas Interface, Surface Roughness and Heterogeneity - Dynamics of Wetting and Dewetting - Applications, Flotation, Detergency, Microfluidics.

The Electric Double Layer, Helmholtz and Gouy-Chapman Model, the Poisson–Boltzmann Equation, the Stern Layer, Free Energy of Electric Double Layers, Measuring Surface Charge Densities - Interfaces of Solid Surfaces, Substrate Structure, Adsorbate Structures - Determination of Surface Energy, Classification of Adsorption Isotherms - Surface Modifications, Chemical Vapor Deposition - Self-assembled Monolayers - Physisorption of Polymers, Polymerization on Surfaces - Etching Techniques, Mechanical Properties of Surfaces.

Thin film Lubrication, Lubricants, Thin Films on Surfaces of Liquids, Monomolecular Films, Evolution of Forms, Experimental Techniques to Study Monolayers, Thermodynamics of Spreading of Layers, Synthesis of Two-dimensional Materials at Solid-Liquid, Solid-Gas and Liquid-Liquid Interfaces, Grapheme, Polymers, Metal Oxides - Catalysis by Surfaces, Kinetic Expressions, NH_3 Synthesis, Hydrogenation of CO, Catalyst Poisoning.

References:

1. H. J. Butt, K. Graf, M. Kappl, *Physics and Chemistry of Interfaces,*2nd Edition, Wiley India, 2003.
2. M.A. Rolando, R. Malherbe, *Adsorption and Diffusion in Nanoporous Materials*, 2nd Edition, Taylor & Francis Group, 2018.
3. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6th Edition, Wiley, 2011.
4. G. A. Somorjai and Y. Li, *Introduction to Surface Chemistry and Catalysis*, 2nd Edition, Wiley 2010.

CY7365E GREEN CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the principles of green chemistry in chemical transformation
CO2: Design the chemical reaction in a safer and environment-friendly way
CO3: Deliver various green strategies in industrially relevant chemical processes

Introduction to green chemistry, principles of green chemistry, introduction to green synthesis, life cycle assessment, methods to minimize waste/ by-products, avoiding the stoichiometric reagents, atom economic reaction, and E-factors in the chemical process. Prevention of chemical accidents by designing greener processes, minimizing the generation of hazardous substances in chemical processes.

Green solvents in synthesis– supercritical fluids, ionic liquids, fluorous biphasic system, PEGs as solvents, immobilized solvents, water as a benign reaction medium, solvent-less processes and solid phase reactions.
Green strategies and techniques in organic synthesis- microwave chemistry, ball milling technique, sonochemistry, and electrochemical reactions.

Examples of green synthesis in: homogeneous catalysis, heterogeneous catalysis, bio-catalysis, asymmetric catalysis, catalysis with non-toxic metals, solid-supported catalysis, nano-catalysis, single atom catalysis, metal-free synthesis, and visible light catalysis

Green chemistry for sustainable development and climate change, CO_2 capture, transformation of CO_2 into valuables chemicals, and polyolefins into light hydrocarbons.

References:

1. P. T. Anastas and J. C. Warner, *Green Chemistry-Theory and Practical*, Oxford University Press, 1998
2. V.K. Ahluwalia, and M. R. Kidwai, *New Trends in Green Chemistry*, Anamalaya Publishers, 2005
3. A. S. Matlack, *Introduction to Green Chemistry*, CRC Press 2nd Edition, 2016
4. M.C. Cann, and M.E. Connely, *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
5. M.A. Ryan, and M. Tinnesand, *Introduction to Green Chemistry*, American Chemical Society Washington, 2002
6. M. Lancaster, *Green Chemistry an Introductory Text*, 3rd Edition, RSC 2016
7. R. Sanghi and M.M. Srivastava, *Green Chemistry: Environment Friendly Alternatives*, Alpha Science International Ltd, 2003.
8. V. K. Ahulwalia, *Strategies for Green Organic Synthesis*, Ane Books Pvt. Ltd. 2012.

CY7366E ORGANOMETALLIC CHEMISTRY OF MAIN GROUP ELEMENTS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Understand the basic principles to synthesis of various main group organometallic compounds.
CO2: Comprehend the bonding nature in main group organometallic compounds and compare that with the transition metal complexes.
CO3: Understand the sensitivity as well as reactivity of various main group organometallic compounds.
CO4: Design the synthesis of various main group organometallic compounds applicable in material, biological and catalysis field of research.

Introduction, fundamental properties of main group elements, heteroatom effect, and stabilization of α carbocation by resonance: stereoelectronic effect, coordination with Lewis acids; synthesis, bonding, structures, reactivity, dynamics, low-valent and catalysis of s-block organometallics.

Organometallic chemistry of boron, gallium and aluminium: synthesis, structure and nature of bonding, reactivity and applications in the field of material and biological chemistry aspects; Synthesis and structural aspects of organosilanes, organogermanium, organotin, organolead compounds; applications in display technology, material chemistry, anti-viral and anti-bacterial; Hypervalent carbon compounds, synthesis and reactivity; synthesis and reactivity of organophosphorous, antimony, bismuth compounds; Tertiary phosphine and its nucleophilic reaction, optically active organophosphine and their importance in catalysis.

Synthesis, structure and reactivity of organometallic compounds of sulfur, selenium and tellurium; structure and reactivity of hypervalent organosulfur compounds; synthesis, structural, bonding aspects and reactivity of organo fluoro, chloro, bromo and iodo compounds; Synthesis and reactivity of hypervalent organoiodide compounds. Unsaturated compounds of main group organometallic compounds, boron, gallium, silicon, germanium, phosphorous and heavier elements; aromatic compounds of group 14 and 15 elements; ligand coupling reactions of phosphorous, antimony, bismuth, sulfur, selenium, tellurium and iodide; selectivity of ligand coupling reaction; catalytical activity of main group organometallic compounds.

References:

1. K-. Y. Akiba, *Organo Main Group Chemistry* by John Wiley & Sons, Inc., Hoboken, New Jersey 2011.
2. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, Pergamon (1985).
3. P Simpson, *Organometallic Chemistry of the Main Group Elements (Concepts in Chemistry S.)* Longman Group Ltd.; First Edition, Prentice Hall Press (1970)
4. J. J. Eisch, *The Chemistry Of Organometallic Compounds: The Main Group Elements* 1967, ASIN : B0000COA9T ;Publisher : The Macmillan Company (1967)
5. C. E. Housecroft, A. G. Sharpe, *Inorganic chemistry,* 3rd edn., London, Pearson-Prentice Hall; 2008, Chapters 6. 9 and 7. 13.
6. F. A. Carey, R. J. Sundberg, *Advanced Organic Chemistry: Part B Reactions and Synthesis.* 5th Edition, Springer, New York; 2007.
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CY7367E METAL CATALYSED ASYMMETRIC SYNTHESIS

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Understand the general features of chirality and apply them to medicinal chemistry aspects.
CO2: Classify the chiral and non-chiral metal catalysts and understand their importance.
CO3: Comprehend the reactivity of various chiral metal complexes.
CO4: Design the synthesis of numerous chiral metal complexes for various applications.

Introduction, Asymmetric synthesis: Importance, classification and principle; modes of asymmetric induction; Stereoselective reactions: Classification, importance and advantages; concepts of prochirality, diastereoselective and enatioselective reactions; Kinetic resolution, parallel kinetic resolution, dynamic kinetic resolution and dynamic thermodynamic resolution.

Concepts of chiral ligands and introduction of chiral ligands phosphine, oxazoline, N-heterocyclic, diamine, binapthyl, ferrocene, chiral spiro ligands; introduction to mono, bi and poly dentated ligands; chiral pincer type ligands; structure, stability, synthesis and reactions of chiral ligand and earth abundant metals such as Iron, Cobalt, Nickel, Manganese and Copper; Controlling the electronic and steric factors for stabilisation metal complexes; asymmetric Friedel-Crafts, intramolecular Friedel-Crafts reaction, Heck reaction including asymmetric Heck reaction, intramolecular Heck reaction; asymmetric hydro functionalisation reactions such as hydrogenation, hydrosilylation, hydroborylation, cyanation, hydroxylation; selective asymmetric epoxidation reactions.

Synthesis of air stable metal catalyst from precious metals such as Iridium, Rhodium, Gold, Platinum, Ruthenium, Palladium; Fujiwara–Moritani reaction, Catellani reaction, Enantioselective reductions and Noyori asymmetric hydrogenation; Hydrosilylation: platinum catalyst, Asymmetric palladium catalyst, Rhodium Catalysts for asymmetric ketone reduction; Wilkinson's catalyst; Asymmetric hydrogenation (Enantio-selective hydrogenation); Metal catalyzed asymmetric enantioselective oxidation, C-C bond forming reactions, allylic substitution, cyclization, and other important reactions; very important reactions on lanthanide based asymmetric catalysis. Determination of optical purity using NMR, GC and HPLC techniques including principles, determination of absolute configuration by NMR and X-Ray crystallography. Application of asymmetric synthesis in the industrially relevant molecules such as L-DOPA, (S)-metolachlor, carbapenem, menthol, (-) PGE2, (-) shikimic acid.

References:

1. A. Berkessel and H. Groger., *Asymmetric Organocatalysis – From Biomimetic Concepts to Applications in Asymmetric Synthesis* Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2005.
2. G. Shang, W. Li, X. Zhang, *Catalytic Asymmetric Synthesis*, 3rd Edition, Wiley−VCH, New York, 2010.
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6. E. N. Jacobsen, A. Pfaltz, H. Yamamoto, *Comprehensive Asymmetric Catalysis I-III*, Springer-Verlag Berlin Heidelberg, Germany, 1999.
7. M. Christmann and S. Brase, *Asymmetric Synthesis – The Essentials*, Wiley-VCH Verlag GmbH, Weinheim, 2007.

CY7368E SUPRAMOLECULAR CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Account for the fundamental concepts, methods and theories of supramolecular chemistry.
CO2: Understand and account for current problems and research in the field.
CO3: Acquire special competence in the supramolecular association within the life sciences and life science technologies.
CO4: Experience in analytical methods for characterization of supramolecular systems.
CO5: Design of artificial molecular receptors for selective recognition of biologically important molecules.

Introduction to supramolecular chemistry, Fundamentals of Supramolecular Chemistry Terminology and definitions in supramolecular chemistry; Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-π, anion-π, π-π interactions, Van der Waal forces, halogen bonding, N-H-π interactions, Sulfur-aromatic interactions.

Host-guest chemistry, Definition, Development, Classification, Receptors, Coordination and the "Lock and Key" Analogy; Chelate, Conformational and Macrocyclic Effects; Pre-organisation and complementarity; introduction to molecular hosts
(a) Cation Binding Hosts - crown ether, cryptand, spherand; nomenclature, selectivity and solution behaviour; alkalides, electrides, calixarenes and siderophores;
(b) Anion binding hosts - challenges and concepts, biological receptors, conversion of cation hosts to anion hosts, neutral receptors, metal-containing receptors, cholapods;
(c) Ion Pair Receptors - contact ion pairs, cascade complexes, remote anion and cation binding sites, symport and metals extraction;
(d) Hosts for Neutral Receptors -clathrates, inclusion compounds, zeolites, intercalates, coordination polymers, guest binding by cavitands and cyclodextrins, cucurbituril;
Solvent and solution properties, solvation and hydrophobic effect; Binding constants; definition and use, determination of binding constant by physical methods. Thermodynamic and kinetic selectivity, molecular recognition and design principles for molecular receptors.

Molecular switches and machines; Use of supramolecular forces to assemble components that respond (on-off) to external stimuli; Molecular shuttles, abacus and muscles; Assembling such components into surfaces for molecular electronics. Crystal Engineering: supramolecular synthons, structure-property correlation, design of solids, design of properties, phase transformations, stimuli responsive solids; topochemical 2+2 cycloadditions in cinnamic acids under light; topochemical photopolymerization in crystals. Applications: Supramolecular reactivity, homogeneous and heterogeneous catalysis, electronic devices (switches, wires and rectifiers) and non-linear optical materials; concepts and applications, role of strong and weak hydrogen bonds in biological systems.

References:

1. F. Diederich, P. J. Stang, R. T. Tykwinski, M*odern Supramolecular Chemistry: Strategies for Macrocycle Synthesis*, Wiley, New York., 2008. https://doi.org/10.1002/9783527621484.
2. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons Ltd, West Sussex, 2000.
3. J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, Wiley VCH, Weinheim 1995.
4. L. De Cola and V. Balzani, *Supramolecular Chemistry*, L. De Cola, Kluwer Academic Publishers, USA, 1992.
5. Y. Murakami, *Supramolecular Assemblies*, Mita Press, Tokyo, 1990.
6. G. W. Gokel, *Advances in Supramolecular Chemistry*, Vol 1 (1990), Vol 2 (1992), Vol 3 (1993), JAI Press, Greenwich.
7. G.R. Desiraju, *Crystal Engineering, The Design of Organic Solids*, Elsevier, 1989.

CY7369E BIOINORGANIC CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Analyze the various roles of metal ions in biology including bioactive ligands.
CO2: Corroborate the relationship between metal ion properties in structural and functional roles.
CO3: Evaluate the spectroscopic properties of metal complexes to understand the electronic structure and to relate structure to function.
CO4: Formulate independent research ideas in the field of bioinorganic chemistry.
CO5: Critically read, analyze and present the research from the bioinorganic chemistry literature to others.

Essential and trace metal ions in biology and their distribution with function, thermodynamic and kinetic factors for the presence of selected metal ions; bioligands- amino acids, proteins, nucleic acids, nucleotides and their potential metal-binding sites; special ligands-porphyrins, chlorin, corrin and corrole.
Oxygen binding properties of heme (hemoglobin & myoglobin) and non-heme proteins (hemocyanin & hemerythrin), their coordination geometry and electronic structure, cooperativity effect, Hill coefficient and Bohr Effect; characterization of O_2 bound species by Raman and infrared spectroscopic methods; typical synthetic models of heme and non-heme systems.

Transport of ions and small molecules through the membrane. Iron transport and storage proteins in bacterial and mammalian systems-siderophores, transferrin, ferritin.
Electron transport proteins–redox properties, organic- redox protein cofactors–FAD, NAD, FMN, ubiquinone; blue copper proteins-plastocyanin, amicyanin, stellacyanin, rusticyanin, azurin; iron-sulfur proteins–rubredoxin, ferridoxins, HIPIP; electron transport chain in respiration, cytochromes, nitrogen-fixation and photosynthesis.

Enzymes-Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts kinetics of enzyme catalyzed reactions Michaelis-Menten constant- effect of pH, temperature on enzyme reactions, factors contributing to the catalytic efficiency of enzymes.
Iron enzymes-Catalase, peroxidase, cytochrome P450 and cytochrome *c* oxidase.
Cobalt enzyme-Cobalamin.
Nickel enzymes-Urease and Hydrogenases.
Copper proteins-tyrosinase, dopamine *β*-monooxygenase and Peptidylglycine alpha-hydroxylating monooxygenase, phenoxazinone synthase, catechol oxidase etc.,
Zinc enzymes-Carboxypeptidase, carbonic anhydrase, alcohol dehydrogenases, phosphatase and its mechanism of action.
Superoxide dismutase (Cu/Zn,Cu/Mn) and mechanism of dissimulation of superoxide ion.

Manganese in photosynthesis and O_2 evolution from water: Photosystem I and II–chlorophyll, oxygen-evolving complex (OEC) and their related biomimetic model compounds.

References:

1. I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, *Bioinorganic Chemistry*, University Science Books, 1994.
2. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, 1994.
3. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life – An Introduction and Guide*, John Wiley & Sons, 1994.
4. L. Que, *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism*, Univ. Science Books, 2000.
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6. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry – Principles of Structure and Reactivity*, Pearson India Ltd., 2009.

CY7370E ADVANCED QUANTUM CHEMISTRY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the theories and concepts of quantum mechanics to simple chemical systems.
CO2: Deliver the basis of density functional methods.
CO3: Use the appropriate functional depending on the chemical problems.

Hartree-Fock equations and solution, interpretations of the solution - Restricted Closed-shell and Unrestricted Open-Shell Hartree-Fock - Roothan`s equations - Koopmans' theorem - Limitations of HF theory - Post HF method - Variation based and Perturbation based method, Møller-Plesset Perturbation theory - CI method, Multi-configuration wave function, full CI matrix, singly and doubly excited CI, illustrations of CI calculations on small atoms/molecules - Natural orbitals - Truncated CI and size consistency.

Coupled Cluster Approximation (CCA), Couple Cluster Operator, CASSCF, Truncation and size consistency in multi-configurational CASSCF, Semi empirical methods.

Density Functional Theory: Electron density in DFT, Hohenberg-Kohn Theorems, Kohn-Sham approach, Kohn-Sham equations: Kinetic, External, Hartree and Exchange-correlation energy, Functional derivatives, KS orbitals, KS eigenvalues.

Correlation hole, Exchange-correlation hole), Local density approximation (Homogeneous electron gas, Exchange, Correlation, and XC energy), Generalized Gradient approximation (PW91, PBE), meta GGA and hyper GGA functionals.

References:

1. R. K. Prasad, *Quantum Chemistry*, 5th Edition, New Age International publishers, 2022.
2. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Edition, McGraw Hill Education, 2017.
3. F. Jensen, *Introduction to Computational Chemistry*, 3rd Edition, Wiley, New York, 2017.
4. J. B. Foresman and Æ Frisch, *Exploring Chemistry with Electronic Structure Methods*, 3rd Edition, Gaussian, Inc.: Wallingford, CT, 2015.
5. I. N. Levine, *Quantum Chemistry*, 7th Edition, Pearson Education India, 2013.
6. E. Engel, R. M. Dreizler, *Density Functional Theory, An Advanced Course*, Springer 2011.
7. P. W. Atkins, *Molecular Quantum Mechanics*, 5th Edition, Oxford University Press, New York, 2010.
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9. Kieron Burke, et al., *The ABC of Density Functional Theory*, University of California, Irvine 2007.
10. C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition, John Wiley & Sons Ltd, 2004.
11. W. Koch and M. C. Holthause, *A Chemist's Guide to Density Functional Theory*, 2nd Edition, 2001.
12. D. C. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, Inc. 2001.
13. D. S. Sholl, *Density Functional Theory: A practical Introduction*, 1st Edition, Wiley-Interscience, 2001.
14. A. Szabo, N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications, Inc., Mineola, New York, 1996.
15. M. W. Hanna, *Quantum mechanics in chemistry*, 2nd Edition, W. A. Benjamin Inc. New York, 1969.

CY7371E POLYMER SCIENCE AND TECHNOLOGY

Pre-requisites: NIL

L	T	P	O	C
3	0	0	6	3

Total Lecture Sessions: 39

Course Outcomes:

CO1: Apply the basic aspects of polymeric materials for product fabrication.
CO2: Do polymer compounding and curing.
CO3: Carry out testing of polymeric materials for characterization.
CO4: Apply the concepts and methods of rheology.

Basic concepts: Characteristic features of polymers-texture of polymers- molecular forces and chemical bonding-secondary bond forces- tacticity in polymers- stereoisomerism in polymers- basic determinants of polymer properties- polymer chain flexibility- factors affecting chain flexibility-glass transition temperature and crystalline melting points- variation and structures- molecular interpretation of glassy state of polymers- new polymerization strategies- multicomponent polymer systems

Additives for compounding plastics- additives for compounding rubbers- mastication, two roll milling, internal mixing, compounding ingredients, pigments, processing aids- processing methods for manufacture of products: blending, calendaring, extrusion and moulding- different elastomer curing systems: efficient, semi efficient, conventional and sulphurless cure mechanism of vulcanization, sulphur vulcanizing systems, non-sulphur vulcanizing systems for olefin rubbers- batch vulcanization: autoclave, gas curing, oven curing, water curing, cold curing- continuous vulcanization – high performance steam, hot air tunnel, molten salt bed, fluidized bed, continuous drum cure, microwave curing- product development.

Importance of standards and standard organizations- processability and performance- testing of plastics and rubbers-material characterization tests such as hardness, tensile stress/strain, compression stress/strain, shear stress/strain, flexurai stress/strain, tear tests, rebound resilience, friction, creep, fatigue, melt flow index, capillary rheometer test, viscosity test, gel permeation chromatography, thermal analysis using TGA, TMA and DSC.

Introduction to polymer melt rheology- viscosity-types of fluid flow- time dependent fluids- viscoelastic fluids-complex rheological fluids- time-independent fluids- Newtonian fluids- non-Newtonian fluids: Bingham plastics, pseudo plastics- rheopectic and thixotropic behavior- rheological measurements- capillary rheology- cone and plate viscometer- elastic effects in polymer melt flow: die swell, flow turbulence, melt fracture, shark skin effect.

References:

1. V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, *Polymer Science,*3rd Edition, New Age International Publishers, 2019.
2. F.W. Billmayer, *Text Book of Polymer Science*, 3rd Edition, John Wiley, 2002.
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5. C.A. Harper, *Handbook of Plastic Technologies*, Mc Graw-Hill Publishers, 2006.
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