DEPARTMENT OF CHEMISTRY
NATIONAL INSTITUTE OF TECHNOLOGY CALICUT

M.Sc. Chemistry

Curriculum & Syllabi (2016)

CURRICULUM FOR POST-GRADUATE PROGRAM LEADING TO MASTER OF SCIENCE (M.Sc.) DEGREE IN CHEMISTRY

I. PROGRAM DETAILS

Name of Degree	Name of Specialization	Intake (Full-time)	Year of Starting Proposed	Duration	Name of Degree &Eligibility for Admission
M.Sc.	CHEMISTRY	20	2016	2 years	Bachelors’ degree with **Chemistry** as main subject and **Mathematics** as one subsidiary course or Bachelors degree through **Chemistry and Mathematics** among the main subjects, with 60% mark or CGPA 6.5/10 or equivalent. [For SC/ST candidates, minimum marks is 50% or CGPA 5.5/10]

II. PROGRAM EDUCATIONAL OBJECTIVES

PEO1	To develop in-depth understanding on the fundamental concepts in chemistry and its relevance to science, society and technology
PEO2	To give adequate exposure to laboratory practices and experimental protocols to make ‘research-ready’ students
PEO3	To instill critical thinking and problem solving abilities along with good communication and interpersonal skills in students
PEO4	To develop human resources for scientific research and education in the area of chemical science

III. PROGRAM OUTCOMES

PO1	The students should be able to deliver the fundamental theoretical concepts and propose experiments to support the concept.
PO2	The students should be able to identify research problems, propose and execute methodologies, collect and analyze the data, and draw conclusions with future outlooks.
PO3	The students should be able to demonstrate competence in assignments they take and should be able to perform individually and in a team.
PO4	The students should be able to apply the scientific knowledge for the betterment of society.

IV. PROGRAM STRUCTURE

I SEMESTER

Sl. No	Code	Title	L	T	P/S	C
1	CY6301	Basic Concept of Inorganic Chemistry and Main Group Elements	3	-	-	3
2	CY6302	Concepts of Organic Chemistry and Introductory Biochemistry	3	-	-	3
3	CY6303	Chemical and Statistical Thermodynamics	3	-	-	3
4	CY6304	Group Theory and Principles of Quantum Mechanics	4	-	-	4
5	CY6305	Analytical Chemistry	3	-	-	3
6	CY6391	Inorganic Chemistry Laboratory	-	-	5	3
		Total credits	**16**	**-**	**5**	**19**

II SEMESTER

Sl. No	Code	Title	L	T	P/S	C
1	CY6311	Chemistry of Coordination Compounds	3	-	-	3
2	CY6312	Chemistry of Multiple Bonds and Rearrangement Reactions	3	-	-	3
3	CY6313	Chemical Kinetics and Surface Chemistry	3	-	-	3
4	CY6314	Molecular Quantum Mechanics and Computational Chemistry	3	-	-	3
5	CY6315	Molecular Spectroscopy - I	3	-	-	3
6	CY6392	Organic Chemistry Laboratory	-	-	5	3
		Total credits	**15**	**-**	**5**	**18**

III SEMESTER

Sl. No	Code	Title	L	T	P/S	C
1	CY7301	Organometallic and Bioinorganic Chemistry	3	-	-	3
2	CY7302	Synthetic Methodologies in Organic Chemistry	3	-	-	3
3	CY7303	Electrochemistry	3	-	-	3
4	CY7304	Solid State Chemistry	3	-	-	3
5	CY7305	Molecular Spectroscopy - II	4	-	-	4
6	CY7391	Physical Chemistry Laboratory	-	-	5	3
7	CY7392	Computational Chemistry Laboratory	-	-	3	2
		Total credits	**16**	**-**	**8**	**21**

IV SEMESTER

Sl. No	Code	Title	L	T	P/S	C
1	CYxxxx	Elective I	3	-	-	3
2	CYxxxx	Elective II	3	-	-	3
3	CY7399	Project	-	-	-	6
		Total	**6**	**-**	**-**	**12**

TOTAL CREDITS = 19+18+21+12 = 70; AVERAGE CREDITS PER SEMESTER = 17.5

ELECTIVES

The department may offer electives based on student's choice, provided at least 5 students opt for a particular elective and also based on faculty availability. Courses at level of M. Tech. or any other M. Sc program in NIT Calicut may be chosen as elective based on student's interest after discussing with the faculty advisor.

LIST OF ELECTIVES

Sl. No	Code	Title	L	T	P/S	C
1	CY7351	Nuclear Chemistry	3	-	-	3
2	CY7352	Porphyrins and Metalloporphyrins	3	-	-	3
3	CY7353	Medicinal Chemistry	3	-	-	3
4	CY7354	Principles of Biochemistry	3	-	-	3
5	CY7355	Introduction to Computational Chemistry	2	-	2	3
6	CY7356	Advanced Materials	3	-	-	3
7	CY7357	Raman Spectroscopy	3	-	-	3
8	CY7358	Metal Based Drugs	3	-	-	3
9	CY7359	Complexes in Molecular Systems and Devices	3	-	-	3
10	CY7360	Applied Coordination Chemistry	3	-	-	3
11	CY7361	Chemistry of Macromolecules	3	-	-	3
12	CY7362	Lubricant Chemistry	3	-	-	3

Brief Syllabus

Semester I

CY6301 BASIC CONCEPT OF INORGANIC CHEMISTRY AND MAIN GROUP ELEMENTS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Introduction to chemical bonding, valence bond theory, hybridization, molecular orbital theory, applications of MOs for homo and heteronuclear diatomic molecules, symmetry of molecular orbitals, theories of bonding in metals, Bronsted-Lowry definition, solvent system definitions, Lux-Flood definition, Lewis definition, Hard and Soft Acids and Bases concept (HSAB), General discussion on the properties of main group elements, boranes and carboranes, styx notation, Wade's rule, synthesis, properties and structure of boranes and carboranes, halogens, phosphazenes, interhalogens, pseudohalogens, noble gas compounds, allotropes of carbon, lanthanides and actinides, 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, radioactivity, nuclear reactions, nuclear reactors, artificial radioactivity, radio-analytical techniques, activation analysis.

CY6302 CONCEPTS OF ORGANIC CHEMISTRY AND INTRODUCTORY BIOCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Symmetry in molecules, prostereoisomerism, stereoisomerism of molecules with axial, planar, and helical chirality, cis-trans isomerism, conformational analysis – acyclic and cyclic molecules, reaction mechanism, kinetic/thermodynamic control, linear free energy relationships, catalysis, isotope effects, solvent effects, concept of aromaticity, different classes of aromatic compounds and their reactions, introduction to biochemistry, important biomolecules, building blocks, conformations, flow of genetic information and enzymes.

CY6303 CHEMICAL AND STATISTICAL THERMODYNAMICS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

First and second laws of thermodynamics, enthalpies, entropy, Gibbs-Helmholtz equation, calculation of entropy, partial molar quantities and their significances,determination of these quantities, chemical potential, Gibbs-Duhem equation, heat capacities, third law of thermodynamics, need for the third law, Nernst heat theorem, irreversible thermodynamics, statistical thermodynamics, probability, distribution laws, different ensembles and partition functions.

CY6304 GROUP THEORY AND PRINCIPLES OF QUANTUM MECHANICS

L	T	P	C
4	0	0	4

Pre-requisites: NIL

Mathematical group, classes in a group, similarity transformation. symmetry elements and operations, point groups, group multiplication table, matrix representation of symmetry operations, construction of irreducible representation, great orthoganality theorem (GOT),construction of character tables (C_{2v}, C_{3v}, C_{2h} and C_{4v}), Mülliken symbols, reduction formula,chemical applications of group theory, wave particle duality, postulates of quantum mechanics, solution for Schrödinger equation for different types of motion, hydrogen atom and Zeeman effect, approximation methods, Slater type orbitals, SCF methods,Hartree and Hartree-Fock's SCF.

CY6305 ANALYTICAL CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Theory of gravimetric analysis, gravimetric factor and calculations, solubility product, common ion effect, solvent extraction - theory and applications, electrophoretic methods, chromatography - mechanisms, retention volume, retention time, theory and instrumentation of paper, thin layer, column, liquid and gas chromatography, GC and HPLC, instrumentation and applications of atomic absorption spectroscopy, scanning electron microscopy (SEM), atomic force microscopy (AFM), thermal, radiochemical and electro analytical methods, radiochemical methods, estimation of biological fluids - hemoglobin, cholesterol and blood sugar, chemical pollutants analysis in air, water, and soil, food adulteration analysis and saponification values.

CY6391 INORGANIC CHEMISTRY LABORATORY

L	T	P	C
0	0	5	3

Pre-requisites: NIL

Separation and identification of four metal ions.Separation and estimation of the metal cation mixtures.Preparation of simple inorganic complexes and their identification by spectroscopic methods.

Semester II

CY6311 CHEMISTRY OF COORDINATION COMPOUNDS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Theories of chemical bonding, VB theory, crystal field theory, calculation of crystal field stabilization energy, spectrochemical series, molecular orbital theory of octahedral, tetrahedral and square planar complexes, substitution reactions of square planar and octahedral metal complexes, trans effect, associative, dissociative and interchange mechanisms, kinetics of octahedral substitution, redox reactions, electron transfer reactions, electronic absorption spectra of transition metal complexes, term symbols, correlation diagrams, Orgel diagrams, Tanabe-Sugano diagrams and Jahn Teller effect.

CY6312 CHEMISTRY OF MULTIPLE BONDS AND REARRANGEMENT REACTIONS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Formation and selected reactions of C-C double bond: β-Elimination reactions, stereoselective and regioselective eliminations, β-eliminations via cyclic transition states, major C-C double bond forming reactions, selected reactions of alkenes, carbonyl chemistry, reactions with nucleophiles, C-C bond formation using enolates and enamines, prediction of sterochemical outcome of reactions using transition state models, concerted pericyclic reactions and their classifications, FMO analysis, orbital correlation diagrams and transition state aromaticity methods, pericyclic reactions in synthesis and rearrangement reactions.

CY6313 CHEMICAL KINETICS AND SURFACE CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Empirical reaction kinetics, reaction rates and their temperature dependence, reaction schemes, mechanisms, reactions on surfaces, enzyme catalysis, theories of unimolecular gaseous reactions, kinetics of reactions in solution, adsorption, adsorption isotherms, experimental methods for studying surfaces, dispersions, surfactants, emulsions, colloids, vesicles, lipid bilayer membrane, structure and properties.

CY6314 MOLECULAR QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

MO theory, LCAO approximation, VB theory, conjugated π systems, HMO theory, molecular mechanics and force fields, potential energy surfaces, ab initio MO calculations, basis sets, semi-empirical SCF methods,electron correlations, post-Hartree-Fock methods and density functional theory.

CY6315 MOLECULAR SPECTROSCOPY-I

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Interaction of matter with radiation**, e**nergy levels and transition probabilities, rigid rotor, harmonic oscillator model, potential energy surfaces in the ground and excited electronic states, Franck-Condon principle, spectroscopy of diatomic molecules (rotational, vibrational and electronic), rotational and vibrational spectroscopy of polyatomic molecules, Raman spectroscopy, Applications of IR, Raman and electronic spectroscopy.

CY6392ORGANIC CHEMISTRY LABORATORY

L	T	P	C
0	0	5	3

Pre-requisites: NIL

Introduction to laboratory techniques, separation of mixtures and analysis, organic synthesis, purification and characterization, natural product extraction and characterization

Semester III

CY7301 ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Structure of organometallic compounds, MOT and 18 electron rule, metal carbonyl and nitrosyl complexes – preparation and properties, isolobal fragments, Fischer and Schrock carbenes, ferrocenes, main group organometallics – preparation and use as synthetic reagents, substitution, oxidative addition, reductive elimination and insertion reactions, preparation and properties of transition metal alkyl and aryl compounds, catalytic processes, homogeneous and heterogeneous catalysis, carbon – heteroatom coupling, transition elements in biology, metalloproteins and enzymes, metal based drugs, electron transfer reactions, chlorophyll, water-oxidation reactions, nitrogen fixation, O_2 binding properties of heme and non-heme proteins, co-cooperativity effect, Hill coefficient and Bohr effect; characterization of O_2 bound species by spectroscopic methods, synthetic models for oxygen binding

CY7302 SYNTHETIC METHODOLOGIES IN ORGANIC CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Methods for oxidation and reduction: reagents, mechanism and application in synthesis, organometallic reagents of transition and non-transition metals in C-C bond formation, illustrative examples, stereoselective synthesis: importance, strategies and examples, protection/deprotection of functional groups and its relevance in synthesis with examples and retrosynthesis – from concept to practice.

CY7303 ELECTROCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Electrolytic conductance, applications, electromotive force of galvanic cell, applications, electrified interface and electroanalytical techniques.

CY7304 SOLID STATE CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Introduction to crystal systems, point groups, hcp and ccp, packing efficiency, radius ratios, structure types-NaCl, ZnS, Na_2O, $CdCl_2$, wurtzite, nickel arsenide, CsCl, CdI_2, rutile and Cs_2O, perovskite ABO_3, K_2NiF_4, spinels, imperfections in solids, solid state reaction, precipitative reactions, sol-gel route, precursor method, ion exchange reactions, intercalation / deintercalation reactions, glasses and thin film preparation, thermal analysis, microscopy and spectroscopy, amorphous materials - glasses and refractories, zeolites, fullerenes, mesoporous materials and carbon nanotubes, defects - colour centers-reactivity, band theory of solids, semiconductors-extrinsic and intrinsic, Hall effect, insulators-dielectric, ferroelectric, pyroelectric and piezoelectric properties, selected magnetic materials, magnetoresistance and spintronics, superconductivity theory, discovery and recent high Tc materials. Ionic conductivity, batteries and fuels cells and optical properties

CY7305 MOLECULAR SPECTROSCOPY- II

L	T	P	C
4	0	0	4

Pre-requisites: NIL

Physical basis of NMR spectroscopy, spectral parameter, spin-spin coupling, first order splitting patterns and structure correlation, relationship between spectrum and molecular structure,second order effects on the spectrum, ^{13}C NMR: chemical shifts, NOE, DEPT, coupling of ^{13}C to ^{19}F and ^{31}P, applications, multinuclear NMR of B, Al, Si, F and P nuclei; application of NMR- metal complexes. Two dimensional NMR spectroscopy: two dimensional *J*-resolved spectroscopy, two dimensional correlated spectroscopy – C,H-COSY, H,H-COSY, long range COSY, HSQC, HMQC, two dimensional INADEQUATE, NOESY and ROESY. Comparison between NMR and EPR, sensitivity and g factor, hyperfine and super hyperfine interactions, spin-spin and spin-lattice relaxations. Applications to inorganic and organic radicals and biological systems, basics of Continuous Wave ENDOR, mass spectrometry, basic principle, ionization methods, isotope abundance, fragmentation processes of organic molecules and deduction of structural information, introduction to soft ionization techniques, studies of inorganic/coordination and organometallic representative compounds, Mössbauer effect, electric and magnetic hyperfine interactions, Mössbauer spectrometers, Quadrupole splitting, Mössbauer as a structural probe for inorganic and biological systems, other Mössbauer active transition metals – ^{61}Ni, ^{67}Zn, ^{99}Ru and applications

CY7391 PHYSICAL CHEMISTRY LABORATORY

L	T	P	C
0	0	5	3

Pre-requisites: NIL

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

CY7392 COMPUTATIONAL CHEMISTRY LABORATORY

L	T	P	C
0	0	3	2

Pre-requisites: NIL

C programming and its applications in chemistry. Introduction to basic techniques in computational chemistry.

Semester IV

CY7399 PROJECT

L	T	P	C
0	0	12	6

Pre-requisites: NIL

The student under the supervision a faculty carries out state of the art research in the frontier areas of chemistry

Electives

CY7351 NUCLEAR CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Nuclear structure, magnetic and electric properties of nucleus, nuclear models, measurement of radioactivity, decay and growth, disintegration series, nuclear decay, decay constants, nuclear reactions, Bethe's notation of nuclear process, nuclear fission and theory, nuclear reactors, artificial radioactivity, trans-uranium elements, production and separation of radioactive isotopes, radioactive tracers and their applications in medical, agriculture and analytical fields, age determination, biological effects of radiation, waste disposal and radiation protections.

CY7352 PORPHYRINS AND METALLOPORPHYRINS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Tetrapyrrole pigments in biology, nomenclature in pyrrole, system with two pyrrole rings, porphyrin and related compounds: Fischer and Revised nomenclature, synthesis of porphyrin ligand; Rothemund, Adler and Lindsey methods, mechanism of porphyrin formation, metallation of porphyrins, chromatographic and non-chromatographic methods of purification and separation of porphyrins, characterization of porphyrins and metalloporphyrins, biomimetic porphyrins.

CY7353 MEDICINAL CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Elucidation of enzyme structure and mechanism, catalytic antibodies, protein-small molecule interactions, enzyme inhibitors, drug design and drug action, ADMET - introduction to rational approach to drug design, factors associated with biological activities and mechanism of drug action, classification of drugs, combinatorial chemistry: strategies, general techniques, solid and solution phase methods, multi-component reactions, encoding methods, deconvolution, lead discovery, and high-throughput screening, structure-activity relationships and lead optimization, QSAR, examples.

CY7354 PRINCIPLES OF BIOCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Protein structure and functions, enzymes: basic concepts, kinetics, structure, function and catalysis. Carbohydrates and lipids, 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, basic structure and functions of DNA and RNA, Flow of genetic information: from genes to proteins, post translational modifications.

CY7355 INTRODUCTION TO COMPUTATIONAL CHEMISTRY

L	T	P	C
2	0	2	3

Pre-requisites: NIL

Electronic structure methods, molecular mechanics, molecular dynamics, Hartree-Fock theory,electron correlation, basis sets, post-HartreeFock methods, calculations using Gaussian 09 program, molecular and thermodynamics properties, geometry, transition state, vibrational frequencies, molecular orbitals, reaction energetics, potential energy surface and reaction mechanism

CY7356 ADVANCED MATERIALS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Principles of nanomaterials, metal nanoparticles, quantum dots, synthesis of carbon nanotubes, biomimetics, super hydrophobic materials, liquid crystals, biocomposites, shape memory polymers, polymers for biomedical applications, chemical structure and composition of drug carriers, TGA, DSC, UTM, SEM, TEM, SPM and AFM.

CY7357 RAMAN SPECTROSCOY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Classical and quantum theory of Raman scattering, molecular symmetry, pure rotation and vibration Raman spectra, Surface enhanced Raman Scattering (SERS), SERS substrates, Raman Imaging, nanobioanalysis, materials and applications.

CY7358 METAL BASED DRUGS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

DNA as drug targets, Types of DNA-drug binding, DNA supercoiling, telomeres and G-quadruplexes, Genomes, Proteins as drug targets, synthesis, structure determination, purification of proteins, proteins as biomarkers, cytotoxic, antitumor, antibacterial and antiviral drugs, cisplatin development and its drug action, toxicity of cisplatin, anticancer drugs, use of ruthenium, titanium, copper, zinc and gold in medicine, vanadium drugs as insulin mimics, Metal compounds as MRI contrast agents, radionucleides for cancer treatment, use of technetium as imaging agents, Chemical exchange saturation transfer (CEST), Cellular imaging, Integrated micro- and nano- imaging techniques for analysis of metalloproteomics, Salvarsan, neosalvarsan and stibamine, organotin and organogermanium compounds as anticancer agents, molecular organic frameworks, nanomedicine, gold nanoparticles in biomedicines, drug delivery by nanoparticles, cytotoxic nanoparticles, health risks of nanoparticles.

CY7359 COMPLEXES IN MOLECULAR SYSTEMS AND DEVICES

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Photochemistry and photophysics of transition metal complexes – excited states and electron transitions, Jablonski Diagrams, photophysial parameters and 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, Theory of NLO, second and third harmonic generation, Difference frequency generation, Optical parameter amplification, N Wave mixing, NLO active metal complexes, Polymers and Third Order NLO, Donor –pi- Acceptor complexes, Transition metal complexes in photovoltaic cells and light emitting diodes – Dye sensitized solar cells, molecular sensitizers, metal complexes as triplet emitters in organic light emitting diodes, quantum yields, Applications of metal complexes in OLEDs.

CY7360 APPLIED COORDINATION CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Structure of coordination compounds, polydentate ligands and complexes, isomerism, lanthanide and actinide complexes, Magnetism in complexes, variations in magnetic moment with temperature, coordination polymers, applications, luminescent complexes, catalysis by transition metal complexes, chiral and asymmetric catalysis. Organometallic compounds, carbocyclic groups, polynuclear carbonyl complexes, substitution reactions in carbonyls, oxidative addition and elimination, metal alkyls, carbene, carbyne and carbide complexes, alkene and alkyne complexes, ferrocenes, cyclopentadienyl complexes, Inorganic complexes in biological systems, cisplatin and cell toxicity, other metal complexes, metalloporphyrins, non-heme proteins, cytochromes and ferredoxins, structure and stability of proteins, isolation, purification and characterization of proteins, Protein crystallography, ligand-protein interactions, protein biomarkers, enzyme catalysis.

CY7361 CHEMISTRY OF MACROMOLECULES

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Basic concepts - classification, biomacromolecules, mechanisms and methods of polymerization, molecular motion. Thermodynamics of polymer solutions, testing of polymers, thermal characterization, melt flow, rheological features, Non-newtonian flow, degradation examination, applications: basic principles in processing, chemistry of vulcanisation, compression moulding, latex processing, making of plastic, dry rubber and latex based products

CY7362 Lubricant Chemistry

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Surface structure, chemistry, and properties- iron, aluminium, copper, surface modification chemistry, alloys, Hume-Rothery rules, Chemistry of lubricant- surface interactions, surface tension, viscosity calculations, lubricant formulations, chemistry of vegetable oils, mineral oils, blended oils, synthetic lubricants, lubricating emulsions, criteria for the selection of lubricants, optimization of formulations, macromolecules in lubricant formulations, physic-chemical aspects of lubricants, steam emulsion number, neutralization number, saponification number, iodine value, carbon residue.

CY6301 BASIC CONCEPT OF INORGANIC CHEMISTRY AND MAIN GROUP ELEMENTS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[7 (L) Hours]**

Chemical bonding: valence bond theory, hybridization, 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.

Module 2 **[7 (L) Hours]**

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.

Module 3 **[14 (L) Hours]**

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.

Module 4 **[14 (L) Hours]**

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, nuclear fusion, nuclear reactors, radioactive tracers, artificial radioactivity, radio-analytical techniques, activation analysis.

References:

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, *Inorganic Chemistry, Principles of Structure and Reactivity*, Pearson Education, 2004.
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, 2000.
4. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins:Inorganic Chemistry*, Fourth edition, Oxford University Press, Oxford, 2000.
5. F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley Interscience, 2003.

6. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Prentice Hall, 2005.
7. G. Choppin, J. Rydberg and J. O. Liljenzin, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 3rd Edition, 2002.
8. W. D. Loveland, D. Morrissey and G. T. Seaborg, Modern Nuclear Chemistry, John Wiley & Sons, 2006.

Course Outcomes:

1. Students will be learning and they will be able to think innovatively about the basic concept and principles of inorganic chemistry.
2. They also study about various properties of main group elements and its related compounds which make them to synthesis new compounds of inorganic interest.
3. They will know about the importance of nuclear chemistry, its related reactions and their applications.

CY6302 CONCEPTS OF ORGANIC CHEMISTRY AND INTRODUCTORY BIOCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[12 (L) Hours]**

Symmetry in molecules – dissymmetric and non-dissymmetric molecules, 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, 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

Module 2 **[10 (L) Hours]**

Structure and stability of reaction intermediates, 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.

Module 3 **[12 (L) Hours]**

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, VilsmeierHaackformylation, Reimer-Tiemannn reaction, Kolbe-Schmidt carboxylation, Gattermann-Koch Reaction, Gattermannformylation.

Module 4 **[8 (L) Hours]**

Introduction to biomolecules – structure and functions of carbohydrates, lipids, proteins and nucleic acids; flow of genetic information – DNA replication, transcription, translation and post translational modifications, introduction to enzymes, properties and features, enzyme catalysis, enzyme inhibition and allostery.

References:

1. F. A. Carey and R. A. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, Fifth edition, Springer, New York, 2007

2. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Second edition, Harper & Row, New York, 1981
3. N. S. Isaacs, *Physical Organic Chemistry*, ELBS, Longman, UK, 1987.
4. D. Nasipuri, *Stereochemistry of Organic Compounds. Principles and Applications*, Second edition, Wiley Eastern Limited, New Delhi, 1994.
5. D. G. Morris, *Stereochemistry*, RSC Tutorial Chemistry Text 1, 2001
6. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
7. P. Sykes, *Advanced Organic Chemistry; Reaction Mechanisms*, Longman and Scientific Technical, New York, 1985
8. R. Brukner,*Advanced Organic Chemistry, Reaction Mechanisms*, Academic Press, 2002.
9. R. O. C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, CRC Press, UK, 1993.
10. J. M. Berg, J. L. Tymoczko and L. Stryer, *Principles of Biochemistry*, 6th edition, W.H. Freeman & Co, 2006.
11. D. L. Nelson and M. M. Cox. *Lehninger Principles of Biochemistry*, 5th edition, W.H. Freeman & Co, 2008.
12. R. K. Murray, D. K. Granner, P. A. Mayes and V. W. Rodwell, Eds. *Harper's Illustrated Biochemistry* 26th edition, McGraw Hill, 2003

Course Outcomes:

1. Student should be able to apply the principles of stereochemistry to organic reactions
2. Student must be able to deliver the fundamental concepts of reaction mechanism in organic chemistry
3. Student should be able to deliver the chemical aspects of biological processes that sustain life.

CY6303 CHEMICAL AND STATISTICAL THERMODYNAMICS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[9 (L) Hours]**

Laws of thermodynamics, internal energy, enthalpy, heat capacity relation between Cp and Cv,limitations second law, concept of entropy, entropy change in an isothermal expansion of an ideal gas, reversible and irreversible processes and changes of phase, calculation of entropy changes of an ideal gas, entropy of mixing, physical significance, work and free energy functions, Maxwell relations, Gibbs Helmholtz equation, chemical equilibrium and Le chatelier's principle.

Module 2 **[10 (L) Hours]**

Partial molar quantities and their significances. Determination of these quantities, chemical potential, Gibbs-Duhem equation, variation of chemical potential with temperature and pressure, phase rule- one, two and three component systems, Clapeyron – Clausius equation, applications Duhem-Margules equation and its applications. Fugacity and activity, determination.

Module 3 **[10 (L) Hours]**

Third law of thermodynamics, need for the third law, Nernst heat theorem, apparent exceptions to third law, applications and verification of third law, entropies of real gases, entropy changes in chemical reactions, Boltzmann entropy equation, determination of absolute entropies, residual entropy, simple examples of irreversible processes, general theory of nonequilibrium processes, entropy production and phenomenological relations.

Module 4 **[13 (L) Hours]**

Statistical concepts and examples, basic principles, probability distribution of particles in energy states, statistical weight factor (g), most probable distribution, thermodynamic probability and entropy, distribution laws, limit of applicability, partition function, different types, factorization, relation between partition function and thermodynamic functions, anomalous heat capacity of hydrogen, ortho and para hydrogen, heat capacity of solids- Einstein's theory, BE/FD statistics and Bose-Einstein condensation.

References:

1. S. Glasstone, *Thermodynamics for Chemists*, East-West, 1973
2. J. Rajaram and J. C. Kuriokose, *Thermodynamics for Students of Chemistry*, 2nd edition, S.L.N. Chand and Co, Jalandhar, 1986.
3. R.P. Rastogi and R.R. Misra, *An introduction to Chemical thermodynamics*, Vikas Publishing, Pvt., Ltd., New Delhi, 1990.
4. D.A. McQuarrie and J.D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
5. K.J.Laidler, J.H.Meiser and B.C.Sanctuary, *Physical Chemistry*, Houghton Mifflin Company, New York, 2003.

6. I. Pigoggine, *An introduction to Thermodynamics of irreversible processes*, Wiley Interscience, 1968.
7. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd edition, Prentice Hall of India, 1984.
8. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India, 1997.
9. R.S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, 2nd edition, 2000.
10. F. Reif, *Fundamental of Statistical and Thermal Physics*, McGraw Hill, International edition 1985.
11. R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 2nd edition, 1999.
12. M.C. Gupta, *Statistical Thermodynamics*, New Age International, New Delhi, 2015.
13. P. Atkins, *Elements of Physical Chemistry*, Oxford University Press, 2015.

Course Outcomes:

1. Students can understand the fundamentals of chemical thermodynamics
2. Students can solve the problems related to the feasibility of a physical/chemical processes
3. Students can correlate thermodynamics with quantum mechanics

CY6304 GROUP THEORY AND PRINCIPLES OF QUANTUM MECHANICS

L	T	P	C
4	0	0	4

Pre-requisites: NIL

Module 1 **[12 (L) Hours]**

Mathematical group, finite and infinite, cyclic and Abelian, group multiplication table, classes in a group, similarity transformation, symmetry elements and operations, point groups, matrix representation of symmetry operations, representations using different basis, reducible and irreducible representations, construction of irreducible representation, great orthogonality theorem (GOT), construction of character tables (C_{2v}, C_{3v}, C_{2h} and C_{4v}), Mülliken symbols, reduction formula, direct sum and direct products.

Module 2 **[12 (L) Hours]**

Polar versus non-polar molecules, chirality, symmetry adapted linear combinations (SALC), projection operator, overlap integrals, construction of hybrid orbitals-BF_3, CH_4 and $PC1_5$ as examples, transformation properties of atomic orbitals, application to MO theory of H_2O, NH_3 and octahedral complexes.
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).

Module 3 **[16 (L) Hours]**

Wave particle duality, postulates, operators, eigenvalue problem, Heisenberg and Schrödinger representations of quantum mechanics, solution for Schrödinger equation – particle in 1D, 2D, 3D boxes and quantum mechanical tunneling, simple harmonic oscillator, particle in a sphere and spherical harmonics, rigid rotator and angular momentum, hydrogen atom, Zeeman effect and electronic spin.

Module 4 **[16 (L) Hours]**

Many electron atom (He), approximation methods: independent particle method, perturbation method (treatment of ground state of He atom), variation method (treatment of 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. 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. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, New York, 2005.

6. D. A. Mc Quarrie, *Quantum Chemistry*, University Science Books, Mill Valley CA.,1983.
7. M. W. Hanna, *Quantum Mechanics in Chemistry*, Benjamin/Cummings, Melano Park, CA, 1981.
8. R. K. Prasad, *Quantum Chemistry*, Oscar Publications, New Delhi, 2000.
9. I. N. Levine, *Quantum Chemistry*, 5thedition (2000), Pearson Educ., Inc., New Delhi.
10. S. N. Datta, *Lectures on Chemical bonding and quantum chemistry*, Prism Books, Bangalore, 1997.

Course Outcomes:

1. Students should be able to apply the concepts of symmetry and group theory to chemical problems.
2. Students should be able to apply the concepts of quantum mechanics to simple chemical systems.
3. Students should be able to demonstrate the application of fundamental laws to solve chemical problems.

CY6305 ANALYTICAL CHEMISTRY

Pre-requisites: NIL

L	T	P	C
3	0	0	3

<u>Module 1</u> **[10 (L) Hours]**

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

<u>Module 2</u> **[12 (L) Hours]**

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

<u>Module 3</u> **[12 (L) Hours]**

Theory, instrumentation and applications of spectrophotometry, fluorimetry, phosphorimetry, atomic absorption spectroscopy, Scanning electron microscopy (SEM), atomic force microscopy (AFM). Thermal, radiochemical and electro analytical methods, theory, instrumentation and applications of TG, DTA, and DSC, theory, instrumentation and applications of coulometry, amperometry, cyclic voltametry, cathodic and anodic stripping analysis.

<u>Module 4</u> **[8 (L) Hours]**

Radiochemical methods: carbon dating, neutron activation analysis, isotope dilution techniques, modern methods of drug analysis, estimation of biological fluids: hemoglobin, cholesterol and blood sugar, chemical pollutants analysis in air, water and soil, food adulteration analysis, analysis of fats and oil, saponification values-significance and determination

References:

1. D. A. Skoog and D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole, Florence, 2004.
2. G. D. Christian, *Analytical Chemistry*, 6th edition, John Wiley & Sons, Singapore, 2008.
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, 2000
4. H. H. Williard, L. L. Merrit, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis,* Wadsworth Publishing Company, Belmont, California, 1986.
5. D. Harvey, *Modern Analytical Chemistry,* McGraw Hill Higher Education, New York, 2000

Course Outcomes:

1. An overview of the separation, purification and analysis of chemical compounds.
2. Information about the instrumentation of modern sophisticated instruments.
3. Knowledge of the theory and principles of modern analytical methods.

CY 6391 INORGANIC CHEMISTRY LAB

L	T	P	C
0	0	5	3

Pre-requisites: NIL

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).

References:

1. G. H. Jeffery, J. Bassett, J. Mendham and R.C. Denny, *Vogel'sText 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*, Macmillan, London, 1969.

Course Outcomes:

1. Students will be trained to carry out the experiments on their own which helps them to attain more technical / practical skills.
2. They will understand how to estimate / quantify the presence of metal ions in a given mixture.
3. They use the various spectroscopic techniques for the characterization of inorganic and coordination compounds through hands-on-practice with the instruments.

CY6311 CHEMISTRY OF COORDINATION COMPOUNDS

Pre-requisites: NIL

L	T	P	C
3	0	0	3

<u>Module 1</u> **[10 (L) Hours]**

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.

<u>Module 2</u> **[10 (L) Hours]**

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

<u>Module 3</u> **[12 (L) Hours]**

Electronic absorption spectra of transition metal complexes, calculation of number of microstates, term symbols, correlation diagrams, 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

<u>Module 4</u> **[10 (L) Hours]**

Magnetism of transition metal complexes, ferro and antiferromagnetic metal complexes, measurement of magnetic susceptibility, variation of magnetic properties of complexes with temperature, histerisis curves, magnetic anisotropy, hard and soft magnetic materials and magnetic long range ordering

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. J. D. Lee, *Concise Inorganic Chemistry*, Blackwell Science, Oxford, 2011.
4. F. A. Cotton C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley India Ltd., New Delhi, 2010.
5. D. W. Bruce and D. O'Hare, *Inorganic Materials*-John Wiley and Sons, New York, 1997

Course Outcomes:

1. An overview of the theories of bonding in coordination complexes.
2. Knowledge of the reactions and electronic spectral properties of coordination complexes.
3. Introduction to organometallic compounds of carbonyls, nitrosyls and related compounds

CY6312 CHEMISTRY OF MULTIPLE BONDS AND REARRANGEMENT REACTIONS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[11 (L) Hours]**

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 and McMurry coupling and C-C double bond formation via reduction of alkynes.
Selected reactions of alkenes: hydration of alkenes –oxymercuration-demercuration, hydroboration, oxidation; SeO_2 oxidation, halolactonization.

Module 2 **[11 (L) Hours]**

Chemistry of carbonyl group: nucleophilic addition to carbonyl group: 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, explanation of stereochemistry of addition using various models; reactions of enamines – enamines in Aldol and Michael reactions; Claisen, Dieckmann, Knoevenegal, Stobbe, Perkin and Darzen condensations.

Module 3 **[14 (L) Hours]**

Classification, Woodward Hoffmann rules; FMO analysis, orbital symmetry correlations and transition state aromaticity methods for electrocyclic, cycloaddition and sigmatropic reactions; pericylic reaction in organic synthesis – Diels-Alder reactions, 1,3-dipolar additions, Cope, Claisen and Ireland-Claisen reactions; chelotropic, group transfer and ene reactions.
Introduction to photochemistry and selected photochemical reactions of alkenes, alkynes, carbonyl and aromatic compounds.

Module 4 **[6 (L) Hours]**

Types of rearrangement, rearrangement involving carbocations - Wagner Meerwein rearrangement, nonclassical carbocations and neighbouring group participation, 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. Brukner, *Advanced Organic Chemistry, Reaction Mechanisms*, Academic Press, 2002.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, PART B: Structure and*

Mechanisms, Kluwer Acdemic and Plenum publishers, New York, 2000.
3. J. J. Li, *Name reactions*, Springer, 2009.
4. I. Fleming, *Pericyclic Reactions*, Oxford Science Publications, Cambridge, 1999.
5. S. Sankararaman, *Pericyclic reactions – A Textbook*, Wiley-VCH, 2005.
6. J. March, *Advanced Organic Chemistry, Reactions, Mechanisms and Structure,* John-Wiley and Sons Inc, New York, 1992.
7. W. Carruthersand I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge, University Press, UK, 2000.
8. J. D. Koyle, *Introduction to Organic Photochemistry*, John Wiley and Sons, 1986.
9. P. Klan and J. Wirz, *Photochemistry of Organic Compounds: From Concepts to Practice*, John Wiley and Sons, 2009.
10. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, CRC Press, UK, 1993.

Course Outcomes:

1. Student should be able to deliver methods for the synthesis of compounds containing C=C / C=X bonds and their reactions
2. Student should be able to predict the stereochemical outcome of the reactions based on the various transition state models
3. Student should be able to deliver the principles and application of pericyclic reactions

CY6313 CHEMICAL KINETICS AND SURFACE CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

Empirical reaction rates, laws and constants, determination of rate laws, temperature dependence of reaction rates- Arrhenius theory, collision and activated complex theory, Eyring equation, thermodynamic aspects, reaction schemes and mechanisms, formulations of rate laws, steady state approximation, chain reactions and photochemical processes and applications.

Module 2 **[12 (L) Hours]**

Reactions on surfaces, enzyme catalysis- mechanism, analysis and inhibition, theories of unimolecular gaseous reactions – Lindemann, Hinshelwood, RRK and RRKM, kinetics of reactions in solution, encounters, Debye- Smoluchowski equation, role of salt and solvent on the rate of reaction, material balance equations, relaxation methods, stopped flow method, laser flash photolysis, flow tube methods, ultra fast laser techniques, step and chain polymerization kinetics

Module 3 **[10 (L) Hours]**

Adsorption, adsorption isotherms -Langmuir's unimolecular theory of adsorption, statistical derivation of Langmuir isotherm. BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination, experimental methods for studying surfaces, principles of SEM, STM,ESCA and Auger spectroscopy.

Module 4 **[10 (L) Hours]**

Dispersions, types, spontaneous self-organization*;* surfactants - structure of surfactants in solution; critical micellation concentration (CMC); temperature dependence; influence of chain length and salt concentration; surfactant parameter, emulsions*:* macro- and micro-emulsions; aging and stabilization of emulsions; phase behaviour of microemulsions, colloids, vesicles, lipid bilayer membrane - structure and properties, monolayers, liquid crystals, foams and aerosols.

References:

1. P. Atkins, *The Elements of Physical Chemistry*,3rd edition, Oxford University Press, Oxford, 2001.
2. P. Atkins and J.D. Paula, *Physical Chemistry*,8th edition, Oxford University Press, Oxford, 2009.
3. J. I Steinfeld, J.S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics*, 2nd edition Prentice Hall, 1998.
4. K. J. Laidler, *Chemical Kinetics*, 3rd edition, 1997, Benjamin-Cummings, Indian reprint - Pearson, 2009.
5. W. Demtroder, *Laser Spectroscopy- Basic concepts and instrumentation*, 3rd edition, Springer 2004.
6. K. K. Rohatgi-Mukkerjee, *Fundamentals of Photochemistry*, Wiley Eastern Ltd., 1992.
7. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, Wiley, 1997.

8. H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2006.
9. D. K. Chakrabarty and B. Viswanathan, *Heterogeneous Catalysis*, New Age, 2008.
10. H. Kuhn, H. -D. Forsterling and D.H. Waldeck, *Principles of Physical Chemistry*, Wiley, 2009.
11. G. A. Somorjai and Y. Li, *Introduction to Surface Chemistry and Catalysis*,2nd edition, 2010.
12. M. Chanda, *Advanced Polymer Chemistry*, Marcel Dekker, Inc., New York, 2000.
13. J. R. Fried, *Polymer Science and Technology*, Prentice-Hall of India Pvt. Ltd., New Delhi, 1999.

Course Outcomes:

1. To get an overview of the reaction kinetics and surface chemistry in terms of established theories.
2. To predict the possible mechanisms involved in it.
3. To correlate the theory, predictions and mechanisms for day-to-day life activities.

CY6314 MOLECULAR QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[12 (L) Hours]**

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.

Module 2 **[12 (L) Hours]**

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.

Module 3 **[10 (L) Hours]**

Hartree-Fock limit, electron correlation, post Hartree-Fockmethods, qualitative description of configuration interaction, coupled cluster and MøllerPlessetPerturbation theory, semiempirical methods and its basic principles.

Module 4 **8 (L) Hours]**

Introduction to Density Functional Theory (DFT) methods - Hohenberg-Kohntheorems, Kohn-Sham orbitals, exchange correlation functional, local densityapproximation, generalized gradient approximation and hybrid functionals.

References:

1. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, New York, 2005.
2. D. A. Mc Quarrie, *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. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st edition, revised, Dover, 1989.
7. F. Jensen, *Introduction to Computational Chemistry*, Wiley, New York, 1999.
8. C. J. Cramer, *Essentials of computational Chemistry: Theories and models,* John Wiley & Sons, 2002.
9. J. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.

10. E. G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics*, 2nd edition, Springer 2011.

Course Outcomes:

1. Students should be able to apply the theories and models of chemical bonding.
2. Students should be able to deliver the basis of wave function based methods.
3. Students should be able to deliver the basis of density functional methods.

CY6315 MOLECULAR SPECTROSCOPY-I

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[14 (L) Hours]**

Infrared and Raman spectroscopy, 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, SEIRS, ATR, Raman effect, classical and quantum mechanical model, rotational Raman of diatomic molecules, vibrational Raman spectroscopy, vibration-rotation Raman spectroscopy of diatomic molecules, SERS, RRS and CARS.

Module 2 **[10 (L) Hours]**

Application of vibrational spectroscopy- vibrational modes, group frequencies of organic, inorganic and organometallic systems, factors affecting the group frequencies, study of hydrogen bonding effects, vibrational spectra of ionic, coordination and metal carbonyl compounds, analysis of representative spectra of metal complexes with various groups at the coordination sites, applications in isotopic effects; in semiconductor microelectronics, etc.

Module 3 **[10 (L) Hours]**

Electronic spectroscopy: Basic principle, electronic transitions, 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, fluorescence spectroscopy, photoelectron spectroscopy-XPES and UPES theory, Auger electron spectroscopy, XRF and EELS.

Module 4 **[8 (L) Hours]**

Electronic levels and types of electronic transitions in organic, inorganic and organometallic systems, solvent effects, effect of extended conjugation, Woodward-Fieser rules for calculation of absorption maximum, stereochemistry and electronic absorption.

References:

1. C. N. Banwell and Elaine M. McCash, *Fundamentals of Molecular Spectroscopy*, McGraw-Hill, International, UK, 1995.
2. P. F. Bernath, *Spectra of Atoms and Molecules*, Oxford University press, NewYork, 2005.
3. S. Hufner, *Photolectron Spectroscopy*, Springer-Verlag, Berlin, 1995.
4. W. Kemp, *Organic Spectroscopy* 3rd edition, Palgrave, New York, 2005.
5. R. M. Silverstein, F.X. Webster and D. J. Kiemle, *Spectrometric Identification of Organic Compounds*, 7th edition, John-wiley and sons, New York, 2005.
6. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Co-ordination Compounds*, John-Wiley and sons, New York, 1985

7. D. L. Pavia, G. M. Lampman, G. S. Krizand J. R. Vyvyan, *Spectroscopy, Brooks/Cole Cengage Learning*, 2007
8. A. K. Brisdon, *Inorganic Spectroscopic methods*, Oxford university Primers-63, 1998
9. R. S. Drago, *Physical methods for chemist,* Saunders, 1992.

Course Outcomes:

1. Students should be able to predict the allowed transitions between various molecular energy levels.
2. Students should be able to deliver the theoretical basis of rotational, vibrational and Raman spectroscopy.
3. Students should be able to apply vibrational and electronic spectroscopy for the structural elucidation of chemical compounds.

CY6392 ORGANIC CHEMISTRY LABORATORY

L	T	P	C
0	0	5	3

Pre-requisites: NIL

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 and characterization of organic compounds

References:

1. A. I. Vogel and B. S. Furniss, *Vogel's Text Book of Practical Organic Chemistry,* Longman and Scientific Technical, New York, 1989
2. F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, Longman, London, 1983

Course Outcomes:
1. Students should be able to execute basic laboratory techniques.
2. Students should be able to set up and monitor different types of reactions.
3. Students should be able to do purification and structural characterization of products obtained.

CY7301 ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

Pre-requisites: NIL

L	T	P	C
3	0	0	3

Module 1 **[10 (L) Hours]**

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

Module 2 **[12 (L) Hours]**

Main group organometallics – preparation and use as synthetic reagents, substitution reactions, oxidative addition, reductive elimination and insertion reactions, Grignard reagents, organolithium compounds, organoberyllium and magnesium compounds, organoboranes, organometallic compounds of aluminium, silicon and tin, preparation and properties of transition metal – alkyl and aryl compounds

Module 3 **[8 (L) Hours]**

Catalytic processes, homogeneous and heterogeneous catalysis, Ziegler-Natta catalysts, hydroformylation reactions, alkene polymerization and isomerisation, Wacker process, carbon – heteroatom coupling by amination of arenes, hydroamination and hydroboration

Module 4 **[12 (L) Hours]**

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, metal based drugs, MRI agents and therapeutic applications, electron transfer reactions, vitamin B12 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 C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, Inc., India, 2010.
3. R. C. Mehrotra and A. Singh, *Organometallic Chemistry-A Unified Approach*, New Age International Publishers, India, 2011.
4. C. Elschenbroich, *Organometallics*, Wiley-VCH, Germany, 2006.
5. R. M. Roat-Malone, *Bioinorganic Chemistry – A Short Course*, John Wiley & Sons, Inc., Hoboken, New Jersey, 2007.

6. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry*, Univ. 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.

Course Outcomes:

1. An overview structure, bonding, preparation and reactivity of organometallic compounds.
2. Information on the mechanism of the catalytic processes of organometallic complexes.
3. An elaborate content on the biological inorganic processes.

CY7302 SYNTHETIC METHODOLOGIES IN ORGANIC CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[14 (L) Hours]**

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, Corey-Kim oxidation, oxidations of alkenes -hyxroxylation reactions, OsO_4, Sharpless asymmetric dihydroxylation, aminohydroxylation, Woodward and Prevost dihydroxylation reactions; asymmetric epoxidation of alkenesusing peroxy acids and DMDO; epoxidation of allylic alcohols –peroxy acids and transition metal catalyzed, Sharpless asymmetric epoxidation, Jacobsen asymmetric epoxidation, dioxiranes; oxidative cleavage – lead tetraacetate, ruthenium tetroxide.

Reduction - catalytic hydrogenation, heterogeneous and homogeneous catalysts, reduction with metal hydrides – lithium aluminium hydride, alkoxyaluminates, borohydrides-sodium, lithium and Zn borohydrides, alkoxy and alkylborohydrides, cyanoborohydrides, superhydrides, selectrides, boranes, aluminium hydrides and its derivatives, selectivity in the reduction of carbonyl compounds, dissolving metal reductions, reduction with zinc, tin and tin compounds, non-metallic reducing agents.

Module 2 **[6 (L) Hours]**

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.

Module 3 **[12 (L) Hours]**

C-C bond formation - organometallic reagents - organo-lithium, magnesium, titanium, copper, chromium, zinc, boron and silicon reagents, palladium catalyzed coupling reactions; carbenes – structure, stability, addition and insertion reactions; radicals – structure, stability, C-C bond formation reactions, Baldwin rules, acyloin condensation
Radicals as intermediates, selected reactions-defunctionalization with tributylstannane, Barton-Mccombie deoxygenation, Barton nitrile photolysis, Hoffmann-Loffler-Freytag reaction.

Module 4 **[10 (L) Hours]**

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 B: Structure and Mechanisms*, Kluwer Acdemic and Plenum publishers, New York, 2000.
2. J. J. Li, *Name reactions*, Springer, 2009.

3. M. B. Smith, *Organic Synthesis*, 2nd edition, Wavefunction Inc, 2005.
4. S. Warren, *Organic Synthesis, The disconnection Approach*, John Wiley & Sons, 2004.
5. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994
6. J. March, *Advanced Organic Chemistry*, *Reactions*, *Mechanisms and Structure*, John-Wiley and Sons , New York, 1992.
7. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis,* Cambridge, University Press, UK, 2000.
8. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, CRC Press, UK, 1993.

Course Outcomes:

1. Student should be able to recommend reagents and methods for functional group interconversions
2. Student should be able to design synthetic strategies for C-C bond formation.
3. Student should be able to deliver the concepts and methods of stereoselective synthesis and retrosynthesis

CY7303 ELECTROCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

Conductance, variations with dilution, Kohlrausch's law and its application, diffusion and ionic mobility, conductometric and precipitation titrations, Ostwald dilution law,anomalous behavior of strong electrolytes, mechanism of electrolytic conductance, relaxation and electrophoretic effects, Debye-Hückel-Onsager equation, deviation from Debye-Hückel-Onsager equation, degree of dissociation and its determination, conductance ratio, Debye-Falkenhagen effect, Wein effect.

Module 2 **[10 (L) Hours]**

Activity and activity coefficients of electrolytes, ionic strength, variation of activity coefficient with concentration, Debye-Hückel theory and limiting law, its qualitative and quantitative verification.

Module 3 **[12 (L) Hours]**

Nernst equation, origin of EMF of a galvanic cell, polarizable and non-polarizable electrodes, applications of emf and potentiometric measurements, corrosion, types, mechanisms and protection methods.

Module 4 **[10 (L) Hours]**

Bjerrum theory of ion association, electrified interface and their structures, surface excess, kinetics of electrode reactions, Butler Volmer equation, diffusion overpotential, overvoltage, polarography, Ilkovic equations from Ficks law of diffusion, applications, amperometry.

References:

1. S. Glasstone, *Introduction to Electrochemistry*, East-West Press Pvt. Ltd., 1965(Reprint 2008).
2. J. O. M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. I and II, Kluwer, Academic/Plenum Publishers, 2000.
3. B. R .Puri, L. R.Sharma and M. S. Pathania, *Principles of Physical Chemistry,* 46^{th} Ed. Vishal Publishing Co, 1965(Reprint 2012).
4. D. I. Antropov, *Theoretical Electrochemistry*, Mir Publishers, 1972.
5. J. Koryta, J. Dvorak, V. Bohackova, *Electrochemistry*, Methuen & Co. Ltd., 1970.

Course Outcomes:

1. Students can understand the fundamentals of Electrochemistry
2. Students can demonstrate and practically develop different electrochemical cells
3. Students can solve the problems in electrochemistry

CY7304 SOLID STATE CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[14 (L) Hours]**

Crystalline solids, crystal systems point groups, methods of characterizing crystal structure-powder x-ray diffraction, electron and neutron diffraction; Types of close packing-hcp and ccp, packing efficiency, radius ratios, structure types-NaCl, ZnS, Na_2O, $CdCl_2$, wurtzite, nickel arsenide, CsCl, CdI_2, rutile and Cs_2O, perovskite ABO_3, K_2NiF_4, spinels; Imperfections in solids.

Module 2 **[10 (L) Hours]**

Solid state reaction, precipitate reactions, sol-gel route, precursor method, ion exchange reactions, intercalation / deintercalation reactions, glasses and thin film preparation; Thermal analysis, microscopy and spectroscopy as tools of characterization; Amorphous materials-glasses and refractories; New materials-zeolites, fullerenes, mesoporous materials and carbon nanotubes; Defects-colour centers-reactivity.

Module 3 **[9 (L) Hours]**

Band theory of solids -metals and their properties, semiconductors - extrinsic and intrinsic, Hall effect, insulators - dielectric, ferroelectric, pyroelectric and piezoelectric properties and their relationships.

Module 4 **[9 (L) Hours]**

Magnetic materials such as spinels, garnets and perovskites, hexaferrites and lanthanide-transition metal compounds; Magnetoresistance and spintronics, superconductivity theory, discovery and high Tc materials. Ionic conductivity, batteries and fuels cells.

References:

1. L.V. Azaroff, *Introduction to Solids*, Mc Graw Hill, New York, 1960.
2. A. K. Galwey, *Chemistry of Solids*, Chapmann and Hall, London, 1967.
3. N. B. Hanna, *Solid State Chemistry*, Prentice Hall, New Delhi, 1988.
4. A. R. West, *Basic Solid State Chemistry*, John Wiley and Sons, New York, 1984.
5. W. D. Callister Jr., *Materials Science and Engineering-An Introduction*, Wiley India, New Delhi, 2006.

Course Outcomes:

1. Students completing this course will be able to understand the basics of various crystalline solids and their characteristics.
2. They will be trained to get innovative ideas to make the new / unknown solid samples through different methods of preparation of solids with interesting properties which pronounces in many applications.

CY7305 MOLECULAR SPECTROSCOPY- II

L	T	P	C
4	0	0	4

Pre-requisites: NIL

Module 1 **[16 (L) Hours]**

Physical basis of 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, A_2, AB, AX, AB_2….AX_2, A_2B_2….A_2X_2, 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; application of NMR to magnetism and magnetic susceptibility measurements of paramagnetic metal complexes.

Module 2 **[8 (L) Hours]**

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, long range COSY, HSQC, HMQC, two dimensional INADEQUATE, NOESY and ROESY.

Module 3 **[12 (L) Hours]**

Introduction to EPR, comparison between NMR and EPR, scope of EPR technique, measurement of paramagnetic resonance, EPR sensitivity, 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 and organic radicals, application of EPR to biological systems, basics of double resonance technique continuous wave ENDOR.

Module 4 **[10 (L) Hours]**

Basic principle of mass spectrometry, 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.

Module 5 **[10 (L) Hours]**

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 carbonyls, iron phthalocyanines, porphyrins and phenanthroline complexes, applications to biological systems – heme proteins, other Mössbauer active transition metals – ^{61}Ni, ^{67}Zn, ^{99}Ru and applications.

References:

1. H. Friebolin, *Basic One- and Two- Dimensional NMR Spectroscopy*, 5thedition, 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* C*ompounds***,** 7th edition**,** John-wiley and sons, New York, 2005.
5. J. A. Weil and J. R. Bolton, *Electron Paramagnetic Resonance: Elementary Theory and Practical Applications*, John- Wiley and Sons, Inc, New Jersey, 2007
6. G. R. Eaton, S. S. Eaton and K. M. Salikhov, *Foundations of Modern EPR*, World Scientific Publishing Co., Singapore, 1999.
7. G. Hanson and L. Berliner Eds., *High Resolution EPR – Applications to Metalloenzymes and Metals in Medicine*, Springer, New York, 2009.
8. N. N. Greenwood and T. C. Gibb, *Mössbauer Spectroscopy*, Chapman and Hall Ltd., London, 1971.
9. P. Gütlich, R. Link and A. Trautwein, *Mössbauer Spectroscopy and Transition Metal Chemistry*, Springer-Verlag Berlin Heidelberg, 1978.
10. G. J. Long, Ed., *Mössbauer Spectroscopy Applied to Inorganic Chemistry*, Vol. 1, Springer New York, 1984.
11. D. P. E. Dickson and F. J. Berry Eds., *Mössbauer Spectroscopy*, Cambridge University Press, New York, 2005.

Course Outcomes:

1. Students should be able to apply spectroscopic methods for the structural elucidation of molecules.
2. Students should be able to choose spectroscopic methods for studying various chemical and physical properties of the molecules.

CY7391 PHYSICAL CHEMISTRY LABORATORY

L	T	P	C
0	0	5	3

Pre-requisites: NIL

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

References:

1. B .Viswanathan 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.

Course Outcomes:

1. To familiarize students with hands-on experiments in various areas of physical chemistry.

CY7392 COMPUTATIONAL CHEMISTRY LABORATORY

L	T	P	C
0	0	3	2

Pre-requisites: NIL

Application of C programming in chemistry. Roots of polynomials, Newton–Raphson method, solution of linear simultaneous equations, matrix multiplication and inversion. Numerical integration, Least square curve fitting.

Computational calculations using programming package - Building of molecular structure, molecular geometry optimization, conformational analysis, thermodynamic and spectroscopic properties, molecular orbital analysis electron density and electrostatic potential map.

References:

1. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill, 1993.
2. E. Balaguruswamy, *Programming in Ansi C*, Tata McGraw Hill, 2007.
3. C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd edition, Wiley & Sons, New York, 2004.
4. F. Jensen, *Introduction to Computational Chemistry*, 2nd edition, Wiley & Sons, New York, 2006.

Course Outcomes:

1. Students should be able to apply C-programming to solve chemical problems.
2. Students should be able to apply computational methods to study chemical properties of a molecule.

CY7399 PROJECT

L	T	P	C
0	0	12	6

Pre-requisites: NIL

The student under the supervision a faculty carries out state of the art research in the frontier areas of chemistry. At the end of the fourth 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 defense of the thesis are to be done before an evaluation committee.

Course Outcomes:

1. Students should be able to do literature survey in a particular research topic.
2. Students should be able to select and solve a chemical problem.
3. Students should write a scientific report.

Electives

CY7351 NUCLEAR CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[8 (L) Hours]**

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.

Module 2 **[12 (L) Hours]**

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.

Module 3 **[10 (L) Hours]**

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.

Module 4 **[12 (L) Hours]**

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, NewYork, 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.

Course Outcomes:

1. Students come to know about the nuclear structure, radioactivity, radioactive decay and growth, nuclear reactions, artificial radioactivity and applications of nuclear chemistry.
2. They will be able to identify and understand various nuclear reactions easily with the simple notations.
3. Those who are completing this course will be able to think innovatively and in turn to attend many competitive exams with wide scope especially the one conducted by BARC.

CY7352 PORPHYRINS AND METALLOPORPHYRINS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

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.

Module 2 **[10 (L) Hours]**

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.

Module 3 **[12 (L) Hours]**

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.

Module 4 **[10 (L) Hours]**

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.

Course Outcomes:

1. Students will be learning the IUPAC nomenclature of porphyrins and related compounds.
2. They also study about the synthesis, separation, purification and characterization of porphyrins and metalloporphyrins.
3. Various biomimetic porphyrins and its related compounds will also be educated to them.

CY7353 MEDICINAL CHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

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

Module 2 **[12 (L) Hours]**

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.

Module 3 **[10 (L) Hours]**

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.

Module 4 **[10 (L) Hours]**

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, Fourth revised edition*, Palgrave Macmillan, 2008.
3. G. L. Patrick, *An Introduction to Medicinal Chemistry*, Third edition, Oxford University Press, 2005.
4. J. M. Berg, J. L. Timoczko, L. Stryer, *Biochemistry*, 6th edition, WH Freeman, 2007.
5. G .Thomas, *Fundamentals of Medicinal Chemistry*, John Wiley, 2003.
6. *Harper's Illustrated Biochemistry*, 26th edition, The McGraw Hill Companies, 2003.

Course Outcomes:

1. Student should be able to deliver the basic principles, terms and definitions in medicinal chemistry.
2. Student must be able to convey the types of the drug receptors and drug- targets interactions.
3. Student should be able to deliver various stages and strategies used in drug discovery, design and development processes

CY7354 PRINCIPLES OF BIOCHEMISTRY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[12 (L) Hours]**

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

Module 2 **[12 (L) Hours]**

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.

Module 3 **[10 (L) Hours]**

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

Module 4 **[8 (L) Hours]**

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, Fourth 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

Course Outcomes:

1. Student should be able to deliver the basic principles, terms and definitions in medicinal chemistry.
2. Student must be able to convey the types of the drug receptors and drug- targets interactions.
3. Student should be able to deliver various stages and strategies used in drug discovery, design and development processes

CY7355 INTRODUCTION TO COMPUTATIONAL CHEMISTRY

L	T	P	C
2	0	2	3

Pre-requisites: NIL

Module 1 **(14 (L) Hours)**

Scope of computational chemistry, molecular mechanics, molecular dynamics, the fundamental concepts of quantum mechanics - Schrödinger equation, Born-Oppenheimer approximation, variational theory, LCAO, Hartree-Fock theory, restricted HF calculations; open shell systems, ROHF and UHF calculations, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation,

Module II **(14 (L) Hours)**

Semi empirical methods, perturbation theory, coupled-cluster theory, configuration interaction, density functional theory, basis set approximation, hydrogen-like, Slater-type andgaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets andcorrelation-consistent basis sets.

Module III **(14 (P) Hours)**

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.

Module 1V **(14 (P) Hours)**

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. I. N. Levine, *Quantum Chemistry*, 6th edition, Pearson Education Inc., 2009.
2. P. W. Atkins and R. S. Friedman, *Molecular quantum mechanics*, 4th edition, Oxford University Press, 2005.
3. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons, 2002.
4. F. Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons, 1999.
5. J. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.

6. E. G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics*, 2nd edition, Springer 2011.

Course Outcomes:

1. Students should be able to deliver the basic principles of computational chemistry.
2. Students should able to perform simple computational calculations.
3. Students should be analysis the output of simple computational quantum mechanical calculations.

CY7356 ADVANCED MATERIALS

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[12 (L) Hours]**

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.

Module 2 **[8 (L) Hours]**

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.

Module 3 **[15 (L) Hours]**

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.

Module 4 **[7 (L) Hours]**

Material characterisation: TGA, DSC, UTM, SEM, TEM, SPM, AFM, Raman spectroscopy, X-ray, biocompatibility, cyto-toxicity, 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.
7. I. F. Uchegbu and A. G. Schatzlein, *Polymers in Drug Delivery*, Taylor & Fransis, Boca Raton, 2006.

Course Outcomes:

1. Students can understand about the synthetic procedures and practical application of nanomaterials.
2. Students can understand about new type of materials for application in different fields. calculations.
3. Students can understand about the theory of different material characterization techniques.

CY7357 RAMAN SPECTROSCOY

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

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.

Module 2 **[10 (L) Hours]**

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.

Module 3 **[12 (L) Hours]**

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.

Module 4 **[10 (L) Hours]**

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.

Course Outcomes:

1. Students can understand about the theory of Raman Spectroscopy
2. Students can understand about the practical applications of Raman Spectroscopy
3. Students can understand the research possibilities in Raman spectroscopy in different fields.

CY7358 METAL BASED DRUGS

Pre-requisites: NIL

L	T	P	C
3	0	0	3

<u>Module 1</u> **[12 (L) Hours]**

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

<u>Module 2</u> **[10 (L) Hours]**

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

<u>Module 3</u> **[10 (L) Hours]**

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

<u>Module 4</u> **[10 (L) Hours]**

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., Nedw 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 Interntional Publishers, India, 2011.
6. C. Elschenbroich, *Organometallics*, Wiley-VCH, Germany, 2006.

Course Outcomes:
1. An overview the application of metal complexes as drug candidates.
2. Information about the different drug actions.
3. An introduction to possible mechanisms of drug action.

CY7359 METAL COMPLEXES IN MOLECULAR SYSTEMS AND DEVICES

Pre-requisites: NIL

L	T	P	C
3	0	0	3

Module 1 **[10 (L) Hours]**

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

Module 2 **[10 (L) Hours]**

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

Module 3 **[10 (L) Hours]**

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

Module 4 **[12 (L) Hours]**

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 edn., 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

Course Outcomes:
1. An overview of the use of coordination complexes in molecular systems and devices.
2. Information of the photochemical or photophysical and optical properties of complexes.
3. An introduction to electrochemical activities of transition metal complexes.

CY7360 APPLIED COORDINATION CHEMISTRY

Pre-requisites: NIL

L	T	P	C
3	0	0	3

Module 1 **[12 (L) Hours]**

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

Module 2 **[10 (L) Hours]**

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.

Module 3 **[10 (L) Hours]**

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

Module 4 **[12 (L) Hours]**

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. F. Holleman and E. Wiberg, (Nils Wiberg eds.), Inorganic Chemistry, Academic Press, U.S.A.,2001.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry-principles of structure and reactivity, Pearson Education India, 2008.
3. M. M. Cox and G. N. Phillips eds, Handbook of proteins- structure, function and methods, Wiley, England, 2007.
4. S. J. Lippard and J. M. Berg, Principles of bioinorganic chemistry, University science books, CA, 1994.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley India Edition, 2009.
6. H. Siegel and T. G. Spiro, Metal ions of Biological Systems, Marcel-Dekker, New York, 1980.

7. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic elements in the chemistry of Life: An Introduction and Guide, John Wiley and Sons, Chichester UK, 1996.

Course Outcomes:

1. An overview of application of coordination and organometallic complexes.
2. Information of the different structures of coordination compounds.
3. An elaborate introduction to contemporary research on transition metal complexes.

CY7361 CHEMISTRY OF MACROMOLECULES

L	T	P	C
3	0	0	3

Pre-requisites: NIL

Module 1 **[10 (L) Hours]**

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

Module 2 **[10 (L) Hours]**

Molecular motion (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, Flory-Huggins theory, solubility parameter, casting of solutions

Module 3 **[12 (L) Hours]**

Testing of polymers, tensile strength, tear strength, modulus, hardness, compression set, creep, stress-relaxation, molecular interpretations, thermal characterization, melt flow, characterization by TGA and DSC, rheological features- Non-newtonian flow, degradation examination, combustion, plastic utilization in environment

Module 4 **[10 (L) Hours]**

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

Reference:

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.

Course Outcomes:

1. The students shall get a clear idea regarding the chemistry involved in macromolecular formation.
2. The students shall learn the fine tuning of the properties of macromolecules and their characterization logically.
3. The various processes, through which product fabrication is done, based on macromolecules, shall be learnt by the students which shall support them to have a better interfacing with industries/ higher level research.

CY7362 Lubricant Chemistry

L	T	P	C
3	0	0	3

Pre-requisites: NIL

<u>Module 1</u> **[10 (L) Hours]**

Surface structure, chemistry, and properties- iron, aluminium, copper, surface integrity, surface texture, surface roughness, measurement of surface roughness, arithmetic mean value and root mean square average, surface modification chemistry, alloys, Hume-Rothery rules, theories of friction, measurement of friction, friction in plastics and ceramics, theories of wear, adhesive wear in sliding, role of lubricants.

<u>Module 2</u> **[12 (L) Hours]**

Chemistry of lubricant- surface interactions, surface tension, viscosity calculations, lubricant formulations, llubricants on various surfaces, surface treatments, shot peening, laser peening, surface rolling, explosive hardening, cladding, mechanical plating, thermal spraying, diffusion coating, electroplating, electroless plating, organic coatings, surface morphology- scanning electron and atomic force microscopes.

<u>Module 3</u> **[12 (L) Hours]**

Theories of lubrication, structural lubricants, mechanical lubricants, chemically active lubricants, mechanism of lubrication- hydrodynamic, boundary and extreme pressure lubrication, classification of lubricants, solid lubricants, semi-solid lubricants, chemistry of vegetable oils, mineral oils, blended oils, synthetic lubricants, lubricating emulsions, criteria for the selection of lubricants, optimization of formulations, macromolecules in lubricant formulations

<u>Module 4</u> **[8 (L) Hours]**

Properties of lubricants, detailed study including instrumentation, with industrial significance, on: viscosity index, flash and fire points, cloud and pour points, aniline point, steam emulsion number, neutralization number, saponification number, iodine value , carbon residue.

References:

1. S. Kalpakjian and. S. R. Schmid, *Manufacturing Processes for Engineering Materials*, Prentice Hall, New Delhi, 2007.
2. J. Edwards, *Coating and Surface Treatment Systems for Metals: A Comprehensive Guide to Selection*, ASM International, Ohio, 1997.
3. W. A. Glasser, *Materials for Tribology*, Elsevier, Amsterdam, 1992.
4. K. G. Budinski, *Surface Engineering for Wear Resistance*, Prentice Hall, New Jersey, 1998.
5. E. S. Nachtman and S. Kalpakjian, *Lubricants and Lubrication in Metal-working Operations*, Marcel Dekker, New York, 1985.

Course Outcomes:

1. The students shall get a clear idea regarding the role of chemistry in a major industrial product, lubricant and its formulations.
2. The students shall learn to examine the chemical and physical properties of lubricants, and the level of contamination in lubricants, which shall support them to perform well in industries/ academia.
3. The students shall learn the major characterization strategies of lubricants and similar chemical entities.