CURRICULUM AND SYLLABI

M. Sc. CHEMISTRY

DEPARTMENT OF CHEMISTRY

NATIONAL INSTITUTE OF TECHNOLOGY CALICUT

November 2011

CURRICULUM

Name of Degree	**Name of Specialization**	**Intake**	**Year of Starting proposed**	**Duration**	**Name of Degree and Branch Eligible for Admission**
M.Sc.	Chemistry	20	2012	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]

Semester I

Sl. No	Code	Title	L	T	P/S	C
1	CY6201	Basic Concept of Inorganic Chemistry and Main Group Elements	3	-	-	3
2	CY6202	Aromaticity, Stereochemistry and Reaction Mechanism	3	-	-	3
3	CY6203	Chemical and Statistical Thermodynamics	3	-	-	3
4	CY6204	Mathematical and Computational Methods in Chemistry	2	-	2	3
5	CY6205	Analytical Chemistry	3	-	-	3
6	CY6281	Inorganic Chemistry Lab-I	-	-	3	2
7	CY6282	Organic Chemistry Lab-I	-	-	3	2
		Total credits	**14**	**-**	**8**	**19**

Semester II

Sl. No	Code	Title	L	T	P/S	C
1	CY6211	Coordination and Organometallic Chemistry	3	-	-	3
2	CY6212	Organic Chemistry of Multiple Bonds	3	-	-	3
3	CY6213	Chemical Kinetics and Surface Chemistry	3	-	-	3
4	CY6214	Quantum Chemistry	3	-	-	3
5	CY6215	Group Theory and Theoretical Spectroscopy	3	-	-	3
6	CY6291	Inorganic Chemistry Lab-II	-	-	3	2
7	CY6292	Physical Chemistry Lab	-	-	3	2
		Total credits	**15**	**-**	**6**	**19**

Semester III

Sl. No	Code	Title	L	T	P/S	C
1	CY7201	Inorganic Materials and Bioinorganic Chemistry	3	-	-	3
2	CY7202	Synthetic Methodology and Heterocyclic Chemistry	3	-	-	3
3	CY7203	Electrochemistry	3	-	-	3
4	CY7204	Solid State Chemistry	3	-	-	3
5	CY7205	Application of Spectroscopic Techniques	3	-	-	3
6	CY7281	Organic Chemistry Lab-II	-	-	3	2
7.	CY7282	Instrumentation Lab	-	-	3	2
6.	CY7291	Seminar	-	-	1	1
		Total credits	**15**	-	**7**	**20**

Semester IV

Sl. No	Code	Title	L	T	P/S	C
1	CYxxxx	Elective I	3	-	-	3
2	CYxxxx	Elective II	3	-	-	3
3	CY7292	Project	-	-	9	6
		Total	**9**	-	-	**12**

Total Credits = 70

List of Electives

1. CY7251 Metal Based Drugs
2. CY7252 Porphyrins and Metalloporphyrins
3. CY7253 Introduction to Computational Chemistry
4. CY7254 Advanced Materials
5. CY7255 Lubricant Technology
6. CYxxxx Supramolecular Chemistry
7. CYxxxx Art of Total Synthesis
8. CYxxxx Polymer Chemistry
9. CYxxxx Liquid Crystals
10. CYxxxx Surfactants and Their Interfacial Phenomena
11. CYxxxx Introduction to Green Chemistry
12. CYxxxx Chemical Binding
13. CYxxxx Advanced Quantum Mechanics
14. CYxxxx Introduction to Medicinal Chemistry
15. CYxxxx Basic Biochemistry
16. CYxxxx Stereoselective Synthesis

Brief Syllabus

Semester I

CY6201: Basic Concept of Inorganic Chemistry and Main Group Elements

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Introduction to chemical bonding, VSEPR theory, valence bond theory, hybridization, hypervalency, multiple bonding in polyatomic molecules, limitations of VB theory, molecular orbital theory, applications of MOs for homo and heteronuclear diatomic molecules, bond properties, symmetry of molecular orbitals, bonding in metals and theories, Acid-base concepts, Bronsted-Lowry definition, solvent system definitions, Lux-Flood definition, Lewis definition, Usanovich definition, Hard and Soft Acids and Bases concept (HSAB), symbiosis, General discussion on the properties of group 1, 2, 13, 14, 15, 16, 17 and 18 elements, inorganic chains, rings, cages, clusters and its applications, boranes and carboranes, styx notation, Wade's rule, isolobal analogy, synthesis, properties and structure of boron and silicon compounds, sulphur nitrogen compounds, oxyacids of nitrogen, phosphorus, sulphur and halogens, phosphazenes, selenium biochemistry, interhalogens, polyhalogen ions, psuedohalides and noble gas compounds, allotropes and polymers of main group elements, sources and extraction of lanthanides and actinides, electronic structure and oxidation states, lanthanide and actinide contractions, actinide hypothesis, optical spectra and magnetic properties of lanthanide ion compounds, comparison with transition elements, applications of lanthanide complexes, trans actinide elements, nuclear chemistry, radioactivity, nuclear reactions, nuclear reactors, artificial radioactivity, nuclear waste management.

CY6202: Aromaticity, Stereochemistry and Reaction Mechanism

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Concept of aromaticity and various aromatic systems, electrophilic and nucleophilic aromatic substitutions, Stereochemistry: topicity and prostereoisomerism, CIP rules, symmetry elements, Conformational analysis of acyclic and cyclic systems, conformation and reactivity, quantitative correlation between conformation and reactivity, selectivity in organic reactions, reaction intermediates, reaction mechanism: basic mechanistic concepts, linear free energy relations, isotope effects, catalysis, neighbouring group participation, nonclassical cabcations, rearrangement reactions.

CY6203: Chemical and Statistical Thermodynamics

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Laws of thermodynamics, Cp and Cv; enthalpies, entropy, Gibbs-Helmholtz equation, calculation of entropy. Chemical Equilibrium, . Ideal and Non-ideal solutions,Gibbs Duhem equation, heat capacities, Statistical Thermodynamics, probability, distribution laws, different ensembles and partition functions. Irreversible thermodynamics

CY6204: Mathematical and Computational Methods in Chemistry

L	T	P	C
2	-	2	3

Pre-requisites: Nil **Total Hrs: 56 [28 (T) + 28(P)]**

Basics of Scalar, vectors, matrix, operators, coordinate systems, functions, polynomial, series, statistics, mathematical group, differential and integral calculus, differential equations, special polynomial solutions of differential equations, partial differential equations. Fundamental of Fortran programming and its applications in chemistry.

CY6205: Analytical Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Titrimetric, gravimetric and electro analytical methods. Adsorption partition, exclusion electrochromatography, Solvent extraction and ion exchange, methods. Application of atomic and molecular absorption and emission spectroscopy in quantitative analysis Light scattering techniques including nephelometry and Raman spectroscopy. Electroanalytical techniques: voltammetry, cyclic voltammetry, polarography, amperometry, coulometry and conductometry ion-elective electrodes. Anodic stripping voltammetry; TGA, DTA, DSC and online analyzers.

CY6281: Inorganic Chemistry Lab-I

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Estimation of metals by complexometric, cerimetric and iodometric titrations, Qualitative analysis of less familiar elements from mixtures, colorimetric estimation of metals, synthesis of metal complexes and characterization by instrumental techniques.

CY6282: Organic Chemistry Lab-I

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Introduction to basic laboratory techniques, qualitative and quantitative analysis, single stage preparation and natural product extractions.

Semester II

CY6211: Coordination and Organometallic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Structure of coordination complexes, Coordination Number and geometry, Nomenclature, isomerism in coordination compounds, Reactions of metal complexes, Valence Bond Theory, Crystal field theory, Jahn Teller effect, Molecular orbital Theory, Magnetism of transition metal complexes, Electronic absorption spectra of transition metal complexes, Tanabe-Sugano diagrams, organometallic compounds, synthesis and reactivity of organometallics, general characteristics of carbonyls, nitrosyls, carbenes and metal alkyls, Organometallic compounds of lanthanides and actinides.

CY6212: Organic Chemistry of Multiple Bonds

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Reactions of carbonyl compounds, addition of nucleophiles, enolates: generation and reactions, aldol reactions, Michael additions, stereoselective aldol reactions, addition elimination reactions of carbonyl compounds, synthetic methods for generation of C-C multiple bonds, pyrolytic syn eliminations, reactions of alkenes, stereoselective hydroborations, hydrogenation and hydroxylations, epoxidations, pericyclic reactions, electrocyclic, sigmatropic, cycloadditions, Woodward Hoffmann rules, FMO and orbital correlation approaches, examples f pericyclic reactions in synthesis, photochemistry of excited molecules.

CY6213: Chemical Kinetics and Surface Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Theories of reaction rates – uni and bimolecular reactions , Methods of determining rate laws. Reactions in flow systems, kinetics, flow methods, pulse methods, Adsorption, isotherms-types and derivation, unimolecular and bimolecular surface reactions. Preparation, and purification of colloids, general properties- electrical and electrokinetic, surfactants, HLB , micelle formation- mass action model, phase separation model, CMC , krafft point, solubilization, Adsorption isotherms, catalysis- types, mechanism and kinetics, Michaelis Menten equation, surface reactions, auto catalysis, oscillatory reactions, Experimental techniques for investigation of surfaces

CY6214: Quantum Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

History quantum mechanics, postulates of quantum mechanics and Schrödinger equation; free particle, particle in a box, degeneracy, harmonic oscillator, rigid rotator and the hydrogen atom. Angular momentum, the variation method and perturbation theory : Application to the helium atom, Terms symbols and spectroscopic states. Born – Oppenheimer approximation, Hydrogen molecule ion. Huckel pl-electron theory and its applications to ethylene, butadiene and benzene.

CY6215: Group Theory and Theoretical Spectroscopy

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Molecular symmetry, point groups, reducible and irreducible representation, character table, symmetry aspects of molecular vibrations, complementary character of IR and Raman spectra,
Symmetry versus polarity and chirality. SALC, hybrid and molecular orbitals. Interaction of matter with radiation**,** Energy levels and transition probabilities. Rigid rotaor, 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. Introduction to ESCA and Mossbauer spectroscopy.

CY6291: Inorganic Chemistry Lab-II

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Separation and estimation of the two and / or three components and preparation of simple inorganic complexes and their identification by spectroscopic methods.

CY6292: Physical Chemistry Lab

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Experiments in thermodynamics, kinetics, electrochemistry, spectroscopy, crystal structure analysis and photophysical Chemistry

Semester III

CY7201: Inorganic Materials and Bioinorganic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Inorganic materials, molecular magnetism, metal clusters and complexes with magnetic behavior, non linear optics, NLO active coordination compounds, inorganic polymers, Electronic materials, dielectric resonators, metal oxides and metal nanocomposites, Organometallic reagents, synthetic reagents, Grignard reagents, Ziegler-Natta catalysts, homogeneous and heterogeneous catalysis, hydroformylation, alkene polymerization and isomerisation, Wacker process, Organometallic reagents as gasoline additives and for environmental speciation. Transition elements in biology, beneficial and toxic effects of metal ions and their role, metal deficiency, toxicity, metal based drugs, MRI agents and therapeutic applications, electron carriers, iron-sulphur proteins, blue copper proteins, vitamin B_{12} and cytochrome P_{450} and their mechanisms of action, chlorophyll, siderophores, phytosiderophores, transferrin, ferritin, hemosiderin, water-oxidation reactions, O_2 binding properties of heme and non-heme proteins, 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, monooxygenases.

CY7202: Synthetic Methodology and Heterocyclic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

C-C bond forming reactions: organometallic reagents, ylides of S and N, Pd-catalyzed reactions, C-N bnd forming reactions, protection of functional groups, retrosynthetic analysis, umpolung, steps in planning a synthesis and choice of synthetic methods, organic transformations, methods of oxidations and reductions, asymmetric synthesis, chiral auxiliaries, methods of asymmetric induction, synthesis and reactions of heterocycles like furan, thiophene, pyrrole, pyridine, quinoline, isoquiniline.

CY7203: Electrochemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Electrochemistry- Galvanic cells: standard potentials, reversible cell, representation of electrodes and cells, concentration cells, cells with and without transference, liquid junction potential and its determination, theory of strong electrolytes - Debye-Huckel-Onsager equation - Electrodics Voltametry, current-voltage curves - reversible and irreversible electrode processes -factors contributing to the decomposition voltage - different kinds of overvoltage -hydrogen and oxygen overvoltage. Polarography , corrosion, various theories ,mechanisms and forms of corrosion

CY7204: Solid State Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Crystal Structure**:** Crystalline solids, crystal systems point groups: methods of characterizing crystal structure**.** Preparative methods**:** Thermal analysis**,** microscopy and spectroscopy as tools of characterization**.** Electrical properties**,** Magnetic properties**,** Superconductivity**,** Ionic conductivity and optical properties**.** Amorphous materials - glasses and refractories**.**New Materials - zeolites, fullerenes. Defects - colour centers - reactivity**.**

CY7205: Application of Spectroscopic Techniques

L	T	P	C
3	-	-	3

Pre-requisites: CY6215 Group Theory and Theoretical Spectroscopy **Total Hrs: 42**

Infrared and Raman spectroscopy: vibrational spectra of ionic, coordination and metal carbonyl compounds. Mass spectrometry**:** introduction to soft ionization techniques and illustrative examples in macromolecular and supramolecular chemistry. Electronic spectroscopy**,** Nuclear Magnetic Resonance Spectroscopy: NMR phenomenon, spin 1/2 nuclei, 1H, 13C, 19F and 31P, 1H-NMR, chemical shift, anisotropic effects, chemical and magnetic equivalence, coupling constants. Karplus relationship of J on dihedral angle, Introduction to 31P and 19F NMR. ESR spectroscopy, introduction to the ESR spectra of organic free radicals and ion radicals, transition metal complexes, application of spin traps.

CY7281: Organic Chemistry Lab-II

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Multistep synthesis and mixture analysis.

CY7282: Instrumentation Lab

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Characterization and analysis by using IR, UV-vis, TGA, DSC, Turbidimetry, flame photometry, fluorescence spectroscopy

CY7291: Seminar

L	T	P	C
-	-	1	1

Pre-requisites: Nil **Total Hrs: 14**

Seminar on the current research topic in chemistry

Semester IV

CY7292: Project

L	T	P	C
-	-	9	6

Pre-requisites: Nil **Total Hrs: 42**

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

Electives

CY 7251: Metal Based Drugs

L	T	P	Cr.
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Target specific binding, DNA as drug targets, Types of DNA-drug binding, active binding sites, DNA supercoiling, Proteins as drug targets, synthesis of proteins and structure determination, metal binding sites on proteins, proteins as biomarkers, cytotoxic, antitumor, antibacterial and antiviral drugs, cisplatin, toxicity of cisplatin, use of ruthenium, titanium, copper, zinc and gold in medicine, application of vanadium as insulin mimics for treatment of diabetes, Metal compounds as MRI contrast agents, radionucleides for cancer treatment, Chemical exchange saturation transfer (CEST), Organometallics in medicine, Salvarsan, neosalvarsan and stibamine, nanomedicine, molecular organic frameworks, mesoporous silica and encapsulation, gold nanoparticles in biomedicines, drug delivery by nanoparticles.

CY 7252: Porphyrins and Metalloporphyrins

L	T	P	Cr.
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

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.

CY7253: Introduction to Computational Chemistry

L	T	P	C
2	-	2	3

Pre-requisites: Nil **Total Hrs: 56 (28 (T) + 28 (P))**

Electronic structure methods - Molecular Mechanics - Molecular dynamics- Hartree-Fock theory - Electron correlation – Basis sets- Post-Hartree Fock methods – Basis sets - Calculations using Gaussian 09 program – molecular and thermodynamics properties -

Geometry – Transition state – Vibrational frequencies – Molecular orbitals - Reaction energetic – Potential energy surface - Reaction mechanism

CY7254: Advanced Materials

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Molecular orbital theory, metallic bonding, free electron model, band theory, quantum mechanical tunneling, Fermi energy, Semiconductor materials liquid crystals in display and thermography, porous and nonporous membranes, hierarchical zeolites, super conductors chalcogen photoconductors, polymers for biomedical applications, Materials for biomimetics, biosensors, biomembranes, organic electronics materials. Nanostructures-classification, fabrication methods. Templating the growth of nanomaterials, self assembly and self-organization of nanomaterials, semiconductor nanostructures: quantum wells, quantum wires, quantum dots, carbon nanotubes, functionalized nanoparticles and metal nanoparticles for biomedical applications. Materials for targeted drug delivery, magnetic drug carriers, chemical structure and composition of drug carriers, micelles, vesicles, dentrimers, nanocapsules, multifunctional nanoparticles, hydrogels, polymer drug conjugates.

CY7255: Lubricant Technology

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Surface structure and properties, Surface integrity, Surface texture, Surface roughness-Theories of friction, Measurement of friction, Friction in plastics and ceramics, Theories of wear, Adhesive wear in sliding, Surface treatments, Shot peening, Laser peening, Surface rolling, Explosive hardening, Action of lubricants on surfaces, Theories of lubrication, Structural lubricants, Mechanical lubricants, Chemically active lubricants, Refractories, Mechanism of lubrication- Hydrodynamic, boundary and extreme pressure lubrication,, Classification of lubricants, Properties of lubricants, Detailed study including instrumentation, with industrial significance, Formulation optimization.

Semester I

CY6201: Basic Concept of Inorganic Chemistry and Main Group Elements

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Molecular structure and bonding (10 hrs)

Introduction to chemical bonding, Lewis structures including octet rule and VSEPR theory, isoelectronic molecules, valence bond theory, hybridization (involving d orbitals), resonance and conjugated molecules, hypervalency, multiple bonding in polyatomic molecules, limitations of VB theory, molecular orbital theory, wave mechanical description of orbitals, applications of MOs for homo and heteronuclear diatomic molecules, bond properties, symmetry of molecular orbitals, bonding in metals, free electron, valence bond, zone and band theories.

Module II Acid base chemistry (8 hrs)

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

Module III Main group elements (16 hrs)

General discussion on the properties of group 1, 2, 13, 14, 15, 16, 17 and 18 elements, diagonal relationship between Li and Mg, and between Be and Al, chemistry of main group homo and hetero clusters, inorganic chains, rings, cages and its applications, boron cage compounds, structure and bonding in polyhedral boranes and carboranes, styx notation, Wade's rule, electron count in polyhedral boranes, synthesis of polyhedral boranes, isolobal analogy, carboranes, boron halides, boron heterocycles, metal borides, synthesis, properties and structure of silanes, silicon halides, silicones, silanols, silicates and aluminosilicates, sulphur nitrogen compounds, oxyacids of nitrogen, phosphorus, sulphur and halogens, phosphazenes, selenium biochemistry, interhalogens, polyhalogen ions, psuedohalides and noble gas compounds of Xe, Kr and Rn, allotropes and polymers of main group elements, reduction potentials, Latimer and Frost diagrams.

Module IV Inner transition elements (8 hrs)

Introduction to lanthanides and actinides, sources and extraction of lanthanides and actinides, physical properties including electronic structure and oxidation states, lanthanide and actinide contractions, position of lanthanides in periodic table, actinide hypothesis, optical spectra and magnetic properties of lanthanide ion compounds, differences between

4f and 5f orbitals absorption spectra, comparison with transition elements, applications of lanthanide complexes, trans actinide elements.
Nuclear chemistry: Introduction, radioactivity and measurement, radioactive disintegration and series, half life, nuclear decay, Bethe's notation of nuclear process, types of nuclear reactions, nuclear fission, nuclear reactors, radioactive tracers, artificial radioactivity, nuclear waste management.

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. S. Cotton, *Lanthanide and Actinide Chemistry, Inorganic Chemistry: A Wiley Textbook Series*, John Wiley & Sons Ltd, 2006.
8. G. Choppin, J. Rydberg and J. O. Liljenzin, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 3rd Edition, 2002.
9. W. D. Loveland, D. Morrissey and G. T. Seaborg, Modern Nuclear Chemistry, John Wiley & Sons, 2006.

CY6202: Aromaticity, Stereochemistry and Reaction Mechanism

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Aromaticity **(10 hrs)**

The concept of aromaticity, Huckel's rule, aromatic and antiaromatic compounds, the annulenes, aromaticity in charged rings, homoaromaticity, fused ring systems, heterocyclic rings, aromatic electrophilic substitution, intermediates and orientation, electrophiles, structure – reactivity relationships, reactivity and selectivity, nucleophilic aromatic substitution.

Module II Principles of stereochemistry **(16 hrs)**

Topicity and prostereoisomerism, nomenclature of stereotopic ligands and faces, stereoheterotopic ligands, centre of chirality, assignment of absolute stereochemistry, CIP rules, axial chirality, planar chirality and helicity, descriptors for absolute stereochemistry.
conformational analysis: acyclic systems, cyclic systems, cyclohexane and decalins.conformation and reactivity with examples from molecular rearrangements, neighbouring group participation, elimination reactions, formation and cleavage of epoxides, quantitative correlation between conformation and reactivity, Winstein-Eliel equation, Curtin-Hammett principle.
Selectivity in organic reactions with examples: regioselectivity, chemoselectivity, enantioselectivity and diastereoselectivity, enantiomeric and diastereomeric excess.

Module III Reaction intermediates **(6 hrs)**

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

Module IV Study and description of reaction mechanisms **(10 hrs)**

Definition of reaction mechanism, thermodynamic data, kinetics, substituent effects, linear free energy relationships, Hammett equation and related modifications, basic mechanistic concepts like kinetic vs thermodynamic control, Hammond postulate, isotope effects, acid-base catalysis, and nucleophilic catalysis, nucleophilicity and basicity, leaving group effect, steric effects in substitution reactions, neighbouring group participation, non-classical carbocations. Rearrangement reactions: nucleophilic and electrophilic rearrangements.

References

1. T.W. Graham Solomon and Craig B. Fryhle, O*rganic Chemistry***,**Wiley International, New York, 2004.
2. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry PART A Structure and Mechanisms***,** fourth edition, Kluwer Acdemic and Plenum Publishers , New York, 2000.
3. R.T Morrison and R.N.Boyd, *Organic Chemistry***,** PrenticeHall-Inc., New Jersey, 1992.
4. E.L. Eliel, S.H. Wilen, *Stereochemistry of Organic Compounds***,** Wiley-Interscience, New York, 1994.
5. Peter Sykes, *Advanced Organic Chemistry; Reaction Mechanisms***,** Longman and Scientific Technical, New York, 1985.
6. J. March, *Advanced Organic Chemistry*, 4th edition, Wiley Interscience, 1994.
7. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd edition, Harper and Row Publishers, New York, 1981.
8. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, Wiley Eastern Limited, New Delhi, 1991.
9. Roc Norman and J.M. Coxon, *Principles of Organic Synthesis*, Nelson Thornes, UK, 1993.

CY6203: Chemical and Statistical Thermodynamics

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module 1 Thermodynamics I **(10 hrs)**

First law 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, 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.

Module 1I Thermodynamics of open systems **(8 hrs)**

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

Module III Thermodynamics of solutions **(8 hrs)**

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.

Module IV Statistical Thermodynamics of independeant particles **(8 hrs)**

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,

Module V Thermodynamics of irreversible processes: **(8 hrs)**

Simple examples of irreversible processes. General theory of nonequilibrium processes. Entropy production. The phenomenological relations. Onsager reciprocal relationsand it's application. law of equipartition of energy, heat capacity, anomalous heat capacity of hydrogen, Ortho and para hydrogen.

References

1. S. Glasstone, *Thermodynamics for Chemists*, East-West, 1973.
2. Rajaram and Kuriokose, *Themodynamics* , East-West, 1986.
3. R.P. Rastogi and R.R. Misra, *An introduction to Chemical thermodynamics*, New Age International.
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. Pigoggine, *An introduction to Thermodynamics of irreversible processes*, Interscience.
7. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn, Prentice Hall of India
8. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India.
9. Physical Chemistry by R.S. Berry, S. A. Rice and J. Ross, Oxford University Press, 2nd Ed. 2000.
10. Fundamental of Statistical and Thermal Physics by F. Reif, McGraw Hill, International edition 1985.
11. Statistical Mechanics by R. K. Pathria, Butterworth-Heinemann, 2nd Ed. 1999.

CY6204: Mathematical and Computational Methods in Chemistry

L	T	P	C
2	-	2	3

Pre-requisites: Nil **Total Hrs: 56 [28 (T) + 28 (P)]**

Module I Basic Mathematics-I (8 hrs)

Scalars and vectors. Matrix algebra, solutions of linear equations, secular equations. Operators, linear, Hermitian, unitary operators. Eigen value problems. Cartesian, cylindrical polar and spherical polar co-ordinates. Functions and graphs, polynomials and polynomial equations. Complex numbers, complex functions. Logarithms and general properties.

Module II Basic Mathematics-II (8 hrs)

Infinite series, test for convergence and divergence, power series, Maclaurin and Taylor series, Fourier series and Fourier transforms.
Statistical concepts, probability, classification and minimization of errors, mean and standard deviation, comparison of results: Student's t-test, F-test, analysis of variance (ANOVA), sampling procedure and statistics.
Mathematical group, finite and infinite, cyclic and abelian, group multiplication table, classes in a group, similarity transformation.

Module III Differential and Integral Calculus (12 hrs)

Differential calculus, functions of single and several variables, geometric properties of derivatives, maxima and minima. Integral calculus, line integrals, double and triple integrals. Differential equations, first and second order differential equations, real, imaginary, complex and double roots. Power series methods of solution, Hermite's equation, Laugerre's equation, Legendres's equation, exact and inexact differentials, integrating factors, partial differential equations.

Module IV Fortran Programming (28 hrs)

Types of constants and variables in Fortran, arithmetic expressions, various types of I/O statements, conditional statements, logical expressions, function and subroutine, arrays, library functions. Formatting and file handling.
Application of Fortran programming in chemistry. Roots of polynomials, Newton–Raphson method, solution of linear simultaneous equations, matrix multiplication and inversion. Numerical integration, Least square curve fitting.

References

1. J. R. Barrante, A*pplied Mathematics for Physical Chemistry*, 2nd edition, Prentice Hall, 1997.
2. V. Rajaraman, Computer programming in Fortran 90 and 95, Prentice Hall (India), New Delhi, 2004.
3. S. D. Conte and C. deBoor, *Elementary Numerical Analysis,* McGraw-Hill (Intl. Edition), 1987.
4. K. V. Raman, *Computers in Chemistry,* Tata McGraw Hill, 1993.
5. R. G. Mortimer, *Mathematics for Physical Chemistry, A*cademic Press, 3rd edition, 2005.

CY6205: Analytical Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Titrimetric, gravimetric and electro analytical methods (10 hrs)

Titrimetric Analysis:acid-base titrations, complexometric titrations**,** precipitation titrations**,** oxidation - reduction titrations, radiometric titrations, iodometric titrations, Theory of gravimetric analysis: solubility product, common ion effect, precipitation methods, condition of precipitation, purity of precipitates, precipitation reagents.

Module II Separation techniques (12 hrs)

Solvent extraction: theory and applications, uses of dithiocarbomates, crown ethers, dithiozone and oxine in extraction, electrophoresis, chromatography: mechanisms, retention volume, retention time, chromatographic performance, column chromatography, ion exchange chromatography: action of ion exchange resins, size exclusion chromatography, super critical fluid chromatography, theory and instrumentation of paper, thin layer, liquid and gas chromatography, gel permeation chromatography (GPC), HPLC.

Module III Instrumental methods of analysis (12 hrs)

Theory, instrumentation and applications of spectrophotometry, flame photometry, nephelometry and turbidimetry, fluorimetry, phosphorimetry, atomic absorption spectroscopy, Scanning electron microscopy (SEM), scanning tunneling electron microscopy (STEM), atomic force microscopy (AFM). Thermal, radiochemical and electro analytical methods, theory, instrumentation and applications of TG, DTA, and DSC, theory instrumentation and applications of electrogravimetry, coulometry, amperometry, cyclic voltametry, polarography, chromopotentiometry and stripping analysis.

Module IV Biomedical, chemical pollutants and food analysis (8 hrs)

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, Soil, and Solid Wastes, Food adulteration analysis, analysis of fats and oil, saponification values-significance and determination

References

1. 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
2. H.H. Williard, L.L. Merrit, J.A. Dean and F.A. Settle, *Instrumental Methods of Analysis*, Wadsworth Publishing Company, Belmont, California, 1986.
3. Skoog, West and Holler, *Fundamentals of Analytical Chemistry*, Thomson and Brookes, New York, 2004.
4. D. Harvey, *Modern Analytical Chemistry*, McGraw Hill Higher Education, New York, 2000

CY6281: Inorganic Chemistry Lab-I

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

i) Volumetric determinations using **(18 hrs)**

a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)
b) Cerimetry (Fe^{2+}, nitrite)
c) Potassium Iodate (Iodide, Sn^{2+})

ii) Mixture analyses : Separation and identification of four metal ions of which two are less familiar elements like W, Se, Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present). Confirmation by spot tests. **(15 hrs)**

iii) Colorimetric determination of copper, iron and titanium using photoelectric colorimeter. **(9 hrs)**

References

1. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, Bath Press, Avon, 1989.
2. D A Skoog and D M West, *Analytical Chemistry*, *An Introduction*, Academic Press Inc., New York, 1986.
3. E.J. Meehan, S. Bruckenstein and I. M. Kolthoff and E B Sandell, *Quantitative Chemical Analysis*, Macmillan, London, 1969.

CY6282: Organic Chemistry Lab-I

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Introduction to basic laboratory techniques: Isolation and purification processes: filtration, recrystallization, solvent extraction, distillation, vacuum distillation, chromatography, purification of organic solvents.
Quantitative and qualitative analysis of organic compounds.
Single stage organic preparations.

Natural products extraction and characterization

References

1. Brian S. Furniss et al., *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

Semester II

CY 6211: Coordination and Organometallic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Fundamentals of coordination chemistry (10 hrs)

General structure of coordination complexes, Types of ligands and denticity, Effective atomic numbers, Coordination Number and geometry, Nomenclature of coordination complexes, Geometric, optical and positional isomerism in coordination compounds, Reactions of metal complexes, Electron transfer reactions, Fluxional molecules, Formation constants and stability of metal complexes, chelateand macrocyclic effects

Module II Transition metal chemistry (10 hrs)

First, second and third row transition metals, oxidation state and stability, Valence Bond Theory, High spin- low spin configurations, Crystal Field Theory, Crystal field stabilization energy, Effects of crystal field splitting, Calculation of CFSE, Spectrochemical series, Orgel diagrams showing splittings in octahedral, tetrahedral and square planar complexes, Jahn Teller effect, teteragonal distortions, Molecular orbital Theory, π-acceptors and π-donors

Module III Advanced coordination chemistry (10 hrs)

Magnetism of transition metal complexes, Ferro and antiferromagnetic metal complexes, measurement of magnetic susceptibility by Guoy and VSM method, Variation of magnetic properties of complexes with temperature, Histerisis curves, Electronic absorption spectra of transition metal complexes, Tanabe-Sugano diagrams, Charge transfer spectra, Isopoly and heteropoly anions, Quadrapole bonds

Module IV Organometallic chemistry (12 hrs)

Classification and types of organometallic compounds, 18 electron rule, synthesis and reactivity of organometallics, oxidative addition, substitution , reductive elimination and insertion reactions, general characteristics of carbonyls, nitrosyls, carbenes and metal alkyls, Ferrocenes, σ- and π- bonded complexes, Organometallic compounds of lanthanides and actinides.

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. R. C. Mehrotra and A. Singh, Organometallic Chemistry-A Unified Approach, New Age Interntional Publishers, New Delhi, 2011.

CY6212: Organic Chemistry of Multiple Bonds

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Reactions of carbonyl compounds (12 hrs)

Reactions of carbonyl compounds, addition of C, N, O, and S nuclophiles, formation of enols and enamines, kinetic and thermodynamic enolates, lithium and boron enolates in aldol and Michael reactions, stereoselective aldol condensations, alkylation and acylation of enolates, condensation reactions, Claisen, Dieckman, Knoevenegal, Stobbe and Darzen glycidic ester, acyloin, emphasis on synthetic utility of these reactions, addition-elimination reactions of ketones and aldehydes.

Module II Chemistry of C-C multiple bonds (14hrs)

Synthesis of alkenes, Wittig and related reactions, modern methods of synthesis, Peterson, McMurry, Shapiro reactions, stereo-selective synthesis of tri and tetra substituted alkenes, synthesis from 1,2-diols, pyrolytic elimination of sulfoxides and selenoxides, synthesis of alkynes, allenes and cumulenes, reactions of alkenes and alkynes, stereo and enantioselective hydroboration, hydrogenation, hydroxylation: Woodward and Provost hydroxylation, osmium tetroxide, epoxidation,asymmetric epoxidation and dihydroxylation, ozonolysis, oxymercuration, halolactonisation. Preparation and synthetic uses of lithium and copper acetylides.

Module III Concerted pericyclic reaction (12 hrs)

Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, Woodward-Hoffmann rules, frontier orbital and orbital symmetry correlation approaches, examples highlighting pericyclic reactions in organic synthesis, Claisen, Cope and Diels-Alder reactions in synthesis, stereochemical aspects.

Module IV Photochemistry (6 hrs)

Photochemistry of excited molecules: Photochemistry of alkenes and alkyne: E–Z isomerization, electrocyclic and sigmatropic photorearrangement, di-p-methane and lumiketone rearrangement; carbonyl compounds: photoreduction, Paterno`–Buchi reaction, Norrish type I and II reaction, Photoenolization.

.

References

1. Reinhard 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. Ian Fleming, *Pericyclic Reactions,* Oxford science publications, Cambridge, 1999.
4. Jerry March, *Advanced Organic Chemistry*, *Reactions, Mechanisms and Structure*, John-Wiley and Sons Inc., New York, 1992.
5. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis,* Cambridge University Press, UK, 2000.
6. John D Koyle, *Introduction to Organic Photochemistry*, John Wiley and Sons, 1986.
7. Petr Klan and Jakob Wirz, *Photochemistry of Organic Compounds: From Concepts to Practice*, John Wiley and Sons, 2009.
8. Roc Norman and J.M. Coxon, *Principles of Organic Synthesis*, Nelson Thornes, UK, 1993

CY6213: Chemical Kinetics and Surface Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Chemical kinetics **(10 hrs)**

Rate equations,integration of rate expressions, order and molecularity of reactions, half life time,experimental methods- for studying kinetics of reactions,order of the reaction. Colloisions and encounters,Arrhenius equation, collision theory,activated complex theory, Lindemann theory.

Module II Kinetics of reactions in solutions **(10 hrs)**

Theories of unimolecular gaseous reaction- Hinshelwood theory, RRRK theory,Diffusion controlled reactions, Debye- smoluchowski equation, influence of ionic strength, solvent on reaction rates, fast reactions- kinetics, flow methods. Pulse methods, flash photolysis,pulse radiolysis

Module III Adsorption **(10 hrs)**

Adsorption, factors influencing, isotherms-types and derivation, adsorption from solutions, Gibbs adsorption isotherm, acid – base and enzyme catalysis - mechanism and kinetics. Effect of temperature, unimolecular and bimolecular surface reactions.

Module IV Colloidal state **(10 hrs)**

Colloidal systems- classification, preparation,purification,properties- electrical, electrokinetic. Surfactants- micelle formation,shape and structure,CMC, factors affecting CMC, krafft point, solubilisation,emulsification, gels and their preparation, applications of colloids.

References

1. K.J. Laidler, *Chemical kinetics*, *Vol. I and II*, McGraw Hill.*
2. A.A. Frost and R.J. Pearson, *Kinetics and Mechanism*, Wiley Eastern.*
3. F. Daniels and R.A. Alberty, *Physical Chemistry*, 5th Edition, Wiley Eastern, 1980.
4. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India, *
5. D.A. McQuarrie and J.D. Simon, *Physical Chemistry, A Molecular Approach*, University Science Books, 1997.
6. K.J.Laidler, J.H.Meiser and B.C.Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
7. B.R.Puri, L.R. Sharma and M.S.Pathania, Principles of Physical Chemistry, Vishal Publishing Co., NDelhi

CY6214: Quantum Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Introduction to quantum mechanics (8 hrs)

A brief history of evolution of quantum mechanics, applications of quantum mechanics. Basic postulates of quantum mechanics, State function postulates, operator postulate, Eigen value postulate, expectation value postulate, time dependant Schrodinger equation postulate, time independent Schrodinger equation. Heisenberg and Schrödinger representations of quantum mechanics.

Module II Quantum mechanics of basic movements (12 hrs)

Translational motion, particle in a one dimensional box, symmetry of the wave functions, rectangular and cubical boxes, degeneracy, quantum mechanical tunneling, utility of particle in a box model.
Harmonic oscillator, vibrational motion, classical and quantum mechanical treatment, Hermite polynomials, physical interpretation of ψ and ψ^2, 3D oscillator.
Rotational motion, rigid rotor; planar and non-planar, Legendre and associated Legendre polynomials, spherical harmonics, polar diagrams, quantization of energy
Angular momentum - commutation rules, ladder operators.

Module III Hydrogen-like atoms and many electron atoms (12 hrs)

Hydrogen like systems, complete wave equation, radial and angular plots, hydrogen spectra, spin angular momentum, hydrogen like wave functions. 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- Hartree and Hartree-Fock's SCF.

Module IV Chemical bonding (10 hrs)

The 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, VB theory; H_2^+ and H_2 molecule, MO and VB treatment of diatomic

molecules, polyatomic molecules-Walsh's rules; conjugated π systems, HMO theory, charge on an atom.

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 (2000), Pearson Educ., Inc., New Delhi.

CY6215: Group Theory and Theoretical Spectroscopy

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Molecular symmetry and Point Group (10 hrs)

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

Module II Applications of Group Theory (10 hrs)

Molecular vibrations- symmetry aspects of molecular vibrations- selection rules for vibrational absorption- complementary character of IR and Raman spectra- determination of the number of active IR and Raman lines (H_2O, NH_3, CH_4, SF_6).
Polar versus non-polar molecules - Chirality - Symmetry adapted linear combinations (SALC), projection operator, overlap integrals - construction of hybrid orbitals-BF_3, CH_4, $PC1_5$ as examples. Transformation properties of atomic orbitals. Application to MO theory of H_2O, NH_3 and octahedral complexes.

Module III Rotational and vibrational spectroscopy (12 hrs)

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, CARS.

Module IV Electronic spectroscopy **(10 hrs)**

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, EELS, Mossbauer spectroscopy, surface analysis using spectroscopy.

References

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

CY6291: Inorganic Chemistry Lab-II

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Module I Quantitative analysis of two component mixture (24 hrs)

Separation and estimation of the following mixtures containing two and / or three components – the first by volumetric and the other by gravimetric methods.

(i) Cu^{2+} and Ni^{2+} (ii) Cu^{2+} and Ba^{2+} (iii) Cu^{2+} and Zn^{2+} (iv) Fe^{2+} and Ni^{2+} (v) Fe^{2+}, Cu^{2+} and Zn^{2+} and (vi) others (if any)

Module II Preparative inorganic chemistry (18 hrs)

Preparation of simple inorganic complexes and their identification by spectroscopic methods.
(i) Preparation of tetramminecopper(II) sulphate (ii) Preparation of tris(ethylenediamine) nickel(II) chloride (iii) Preparation of trithioueracopper(I) sulphate (iv) Preparation of potassium trioxaltoaluminate(III) and / or ferrate(III) and / or chromate(III) (v) Preparation of ammonium diamminetetrathiocyanato chromate(III). (vi) others (if any)

References

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

CY6292: Physical Chemistry Lab

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

1. Determination of equivalent conductance of strong electrolytes and verification of onsagar equation.
2. Conductometric titration of (a) strong acid vs. strong base
   (b) weak acidvs strong base
   (c) mixture of (weak acid+ strong acid)vs strong base
3. Potentiometric titration of (a) strong acid vs. strong base
   (b) weak acid vs. strong base and then find out the K_a of weak acid
4. Determination of unknown composition of binary liquid mixtures (e.g., benzene-
   nitrobenzene, water-glyceol) by viscosity measurements
5. Determination of molar refractions of pure liquids (e.g., water, methanol, ethanol,
   chloroform, carbon tetrachloride, glycerol)
6. Determination of refractive index of alcohol-water, glycerol-water mixture. Find
   out the unknown composition from the plot.
7. Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$ using spectrophotometry.
8. Determination of rate constant of saponification of methyl or ethyl acetate using NaOH.
9. Determination of unknown composition of simple, two component with compound formation and three component eutectic systems
10. Determination of molecular mass of biphenyl/amines, by Rast method.
11. Determination of equilibrium constant of the reaction $HgI_2 + 2KI \leftrightarrow K_2HgI_4$ by cryoscopy.
12. Determination of partition coefficient of I_2 between CCl_4 and water.
13. Determination of adsorption coefficient from the isotherm of acetic acid/ oxalic acid by activated charcoal .
14. Computational quantum mechanics of chemical reactions

References

1. Vogel, *Text Book of Quantitative Chemical Analysis*, Longman Scientific and Technical, Harlow, 1989.
2. A. Finlay, *Practical Physical Chemistry*, Longman's Green & Co., London, 1955.
3. A.M. James, *Practical Physical Chemistry*, Longman's Green & Co., London, 1961.
4. F. Daniel, J.W. Williams, P. Bender, R.A. Alberty, C.D. Cornwell and J.E. Harriman, *Experimental Physical Chemistry*, McGraw Hill, 1970.
5. W.G. Palmer, *Experimental Physical Chemistry*, Cambridge University Press, Cambridge, 1962.
6. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry*, McGraw Hill, Boston,1996.
7. Yadav, *Advanced Practical Physical Chemistry,* Geol Publisher House, Meenet, 1989.

Semester III

CY7201: Inorganic Materials and Bioinorganic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Inorganic Materials (11 hrs)

Magnetic materials, molecular magnetism, mono and multinuclear compounds, metal clusters with magnetic behavior, magnetic long-range ordering, non linear optics, NLO active coordination compounds, inorganic polymers, polysiloxanes and polyphosphazenes, Electronic materials, dielectric resonators, metal oxides and metal nanocomposites

Module II Organometallic reagents (10 hrs)

Main group organometallics as synthetic reagents, Grignard reagents, Ziegler-Natta catalysts, catalytic processes, homogeneous and heterogeneous catalysis, hydroformylation reactions, alkene polymerization and isomerisation, Wacker process, Organometallic reagents as gasoline additives, environmental speciation by organometallic compounds.

Module III Trace elements, Electron transfer and iron transport proteins (12 hrs)

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 carriers, iron-sulphur proteins, blue copper proteins, vitamin B_{12} and cytochrome P_{450} and their mechanisms of action, chlorophyll, siderophores, phytosiderophores, transferrin, ferritin, hemosiderin, water-oxidation reactions.

Module IV Oxygen uptake, transport and storage (10 hrs)

Molecular and chemical properties of oxygen, biochemistry of iron and copper, O_2 binding properties of heme (haemoglobin and myoglobin) and non-heme proteins (hemocyanin and hemerythrin), 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, monooxygenases.

References

1. D.W. Bruce, D. O'Hare, *Inorganic Materials*-John Wiley and Sons, New York, 1997
2. U. Schubert, N. Husing, *Synthesis of Inorganic Materials*, Wiley-VCH, Germany, 2005.
3. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry – Principles of Structure and Reactivity*, Pearson India Ltd., 2009.
4. F. A. cotton C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, Inc., India, 2010.
5. R. C. Mehrotra and A. Singh, Organometallic Chemistry-A Unified Approach, New Age Interntional Publishers, India, 2011.
6. R. M. Roat-Malone, *Bioinorganic Chemistry – A Short Course*, John Wiley & Sons, Inc., Hoboken, New Jersey, 2007.
7. H.-B. Kraatz, N. Metzler-Nolte, *Concepts and Models in Bioinorganic Chemistry*, Wiley-VCH Verlag GmbH & Co, KGaA, 2006.
8. S. J. Lippard, and J. M. Berg, *Principles of Bioinorganic Chemistry*, Univ. Science Books, 1994.
9. W. Kaim and B. Schwederski, *Bioinorganic chemistry: Inorganic Elements in the Chemistry of Life – An Introduction and Guide*, John Wiley & Sons, 1994.
10. D. E. Fenton, *Biocoordination Chemistry* (Chemistry Primer 26), Oxford Univ. Press, 1996.
11. L. Bertini, H. B. Gray, S. J. Lippard, and J. S. Valentine, *Bioinorganic Chemistry*, Univ. Science Books, 1994.
12. H. Siegel and T. G. Spiro, *Metal ions of Biological Systems*, Marcel-Dekker, 1980.

CY7202: Synthetic Methodology and Heterocyclic Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I C-C and C-N bond forming reactions (12 hrs)

Nucleophilic C-C bond forming reactions: Organometallic reagents of lithium, magnesium, zinc, copper, chromium and iron, ylides of sulfur and nitrogen, Pd catalyzed coupling, C-C bond formation via free radicals and carbenes,. C-C bond formation using tin reagents.

Nucleophilic nitrogen and electrophilic carbon, electrophilic nitrogen and nucleophilic carbon, rearrangements leading C-N bond formation.

Module II Protection of functional groups and basic retrosynthetic analysis (12 hrs)

Protecting groups, protection of hydroxyl, carboxyl, carbonyl, amino groups. Protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

Retrosynthetic analysis, reversal of carbonyl group polarity, steps in planning a synthesis, choice of synthetic methods and domino reactions.

Module III Organic transformations and asymmetric synthesis (12 hrs)

Reduction: methods of reduction- hydride transfer reagents, catalytic hydrogenations, homogeneous hydrogenation, dissolving metal reductions, borane and its derivatives, Wolff-Kishner, diimide and enzymatic reductions.
Oxidation: transition metal oxidants (Cr and Mn compounds), Swern and related oxidations, nonmetal based oxidants like DMP, TEMPO, allylic oxidation, oxidative decarboxylation.
Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination

Module IV Heterocyclic chemistry (6 hrs)

Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline, and indole. Skraup synthesis, Fischer indole synthesis, Chichibabin reaction.

References

1. F.A. Carey, R.J. Sunburg, *Advanced Organic Chemistry, Part B: Reactions and*
2. *Synthesis*, Kluwer Academic/Plenum Publishers, New York, 2001.
3. J. March, *Advanced Organic Chemistry*, Wiley Interscience Publication, New York, 1992.
4. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis,* Cambridge University Press, UK, 2000.
5. I.L. Finar, *Organic Chemistry* Volume II, ELBS and Longmans, London, 1975.
6. T. Lindberg, Strtegies and Tactics in Organic Synthesis, Academic Press, London, 1989.
7. Roc Norman and J.M. Coxon, *Principles of Organic Synthesis*, Nelson Thornes, UK, 1993.
8. G.S Zweifel, M.H. Nantz, Modern Organic Synthesis: An Introduction, W.H. Freeman and Company, Newyork, 2007.
9. Reinhard Brukner, *Advanced Organic Chemistry, Reaction Mechanisms*, Academic Press, 2002

CY7203: Electrochemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Emf of galvanic cells **(10 hrs)**

Electrochemical cells, Nernst equation ,standard electrode potentials, emf , activity and mean ionic activity of electrolytes, concentration cells, liquid junction potentials, fuel cells,applications of emf measurements.

Module II Applied Electrochemistry. **(10 hrs)**

Corrosion : Introduction to corrosion, Various theories and mechanisms of corrosion, forms of corrosion, Corrosion monitoring and prevention methods. Conversion and storage of electrochemical energy , Electrocatalysis, influence of various parameters

Module III Bio electrochemistry **(10 hrs)**

Debye-Huckel theory of electrolytic conduction - derivation of Debye-Huckel-Onsager equation. Deviation from Debye-Huckel-Onsager equation and corrections. Limiting law, Conductance ratio. Debye-Falkenhagen effect, Wein effect. electrocapillary phenomena; structure of electrified interfaces

Module IV Electrode kinetics **(12 hrs)**

Butler Volmer equation and its implications, irreversible electrode process-overvoltage, polarography, IIkovic equation and its derivation, Ficks laws of diffusion, applications

References

1. S. Glasstone, *Introduction to Electrochemistry,* East-West Press Pvt. Ltd., 1965
2. L.I Anthropov, Theoretical Electrochemistry.Mir Publications, Moscow
3. J.O.M. Bockris and A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic Plenum Publishers, 2000 .
4. A.J.Bard and Faulkner, Electrochemical methods: Fundamentals and Applications.Wiley-India Edition,2006.
5. Ralph. E.White, *Comprehensive Treatise in Electrochemistry.*

CY7204: Solid State Chemistry

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Crystal Structure (12 hrs)

Crystalline solids, crystal systems point groups, metheds of characterising crystal structure – powder x-ray diffraction, electron and neutron diffration; 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. Imprefections in solids.

Module II Preparative methods (10 hrs)

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 as tools of characterization. Amorphous materials - glasses and refractories. New materials-zeolites, fullerenes. Defects - colour centers - reactivity.

Module III Electrical properties (10 hrs)

Development of free electron theory to band theory of solids -metals and their properties,semiconductors - extrinsic and intrinsic, Hall effect, insulators - dielectric, ferroelectric, pyroelectric and piezoelectric properties and the relationship between them.

Module IV Magnetic properties (10 hrs)

Dia, para, ferro, ferri, and antiferro magnetic types -selected magnetic materials such as spinels, garnets and perovskites. Magnetoresistance and spintronics, superconductivity theory, discovery and recent high Tc materials. Ionic conductivity, batteries and fuels cells and optical properties.

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.

CY7205: Application of Spectroscopic Techniques

L	T	P	C
3	-	-	3

Pre-requisites: CY7204 Group Theory and Theoretical Spectroscopy Total Hrs: 42

Module I Vibrational Spectroscopy (8 hrs)

Infrared and Raman 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.

Module II Electronic Spectroscopy (8 hrs)

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.

Module III Mass Spectrometry (12 hrs)

Basic principle, 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 IV Magnetic and Spin Resonance Spectroscopy (14 hrs)

NMR phenomenon, spin 1/2 nuclei, ^{1}H, ^{13}C, ^{19}F and ^{31}P, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution. ^{1}H-NMR, chemical shift, anisotropic effects, chemical and magnetic equivalence, coupling constants. Karplus relationship of J on dihedral angle, first order splitting patterns and structure correlation. Second order effects on the spectrum, AB, AMX, ABX, AA'BB' spin systems, simplification of second order spectra. High field NMR, Relaxation phenomena, double irradiation, NOE effects, selective decoupling, chemical shift reagents, ^{13}C-NMR, natural abundance, sensitivity, ^{13}C chemical shifts to structure correlations, off-resonance spectrum, Dynamic processes by NMR, restricted rotation, examples from few organometallic systems, Structure elucidation of organic molecules.

ESR phenomenon, introduction to the ESR spectra of organic free radicals and ion radicals, EPR spectroscopy of inorganic compounds with unpaired electrons, determination of electronic structure, g-values, hyperfine and superhyperfine coupling constants, application of spin traps, McConnell relation.

References

1. William Kemp, *Organic Spectroscopy* 3rd edition, Palgrave, New York, 2005.
2. 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.
3. Kazuo Nakamoto, *Infrared and Raman Spectra of Inorganic and Co-ordination Compounds*, John-Wiley and sons, New York, 1985
4. D.L.Pavia, G.M.Lampman, G.S.Kriz nd J.R.Vyvyan, *Spectroscopy, Brooks/Cole Cengage Learning,* 2007
5. A.K. Brisdon, *Inorganic Spectroscopic methods* , Oxford university Primers-62, 1998
6. R.S. Drago, *Physical methods for chemist,* Saunders, 1992.

CY7281: Organic Chemistry Lab-II

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

Multistage organic preparations, purification and characterization, qualitative analysis of two component mixtures.

References

1. Brian S. Furniss et al., *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

CY7282: Instrumentation Lab

L	T	P	C
-	-	3	2

Pre-requisites: Nil **Total Hrs: 42**

1. Identification of an organic compound by measuring and analysing its IR and UV-Vis spectrum.
2. Determination of isosbetic point of the given compound by UV-Visible absorption spectra
3. Determination of unknown concentration of a protein by absorption spectroscopy
4. Analysis of hydrated calcium oxalate and Magnesium oxalate by TGA.
5. Determination of glass transition temperature and melting point of a polymer by DSC.
6. Determination of Ba and sulphate ions in solution by turbidimetry.
7. Estimation of potassium in NPK mixture by flame photometry.
8. Determination of refractive index of mixtures and there by their concentrations by refractometer.
9. Synthesis of a luminescent compound and analysis of its fluorescent spectrum.

References

1. Research articles

2. A.B. Viswanath , *Practical Physical Chemistry* , Viva Books Private Limited, New Delhi, 2009 .

3. F. Rouessac and A. Roussac, *Chemical Analysis: Modern Instrumentation Methods and Techniques*, John Wiley and Sons, New York, 2007.

CY7291: Seminar

L	T	P	C
-	-	1	1

Pre-requisites: Nil **Total Hrs: 14**

Identify a current research topic and collect literature from peer reviewed journal. Prepare an abstract on the topic of presentation in the specified format. Each student shall present seminar for about 45 minutes duration on the selected topic. The abstract and presentation shall be evaluated by a team of experts based on the style of presentation, scientific and technical content, communication skills, depth of knowledge, ability to handle question and answer session etc.

Semester IV

CY7292: Project

L	T	P	C
-	-	10	6

Pre-requisites: Nil **Total Hrs: 42**

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.

Electives

CY 7251: Metal Based Drugs

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Targets in metal-drug action (12 hrs)

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

Module II Metal complexes as drugs (10 hrs)

Different kinds of drug action – 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

Module III Metal based diagonostic tools (10 hrs)

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.

Module IV Organometallics and nanomedicine (10 hrs)

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.

CY 7252: Porphyrins and Metalloporphyrins

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hrs: 42**

Module I Nomenclature and Synthesis (10 hrs)

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 II Purification and separation (10 hrs)

Chromatographic methods: Basic analytical methods including paper, thin layer (including preparative TLC), column, flash, gas chromatography and high performance liquid chromatography. Non-chromatographic: Extraction, precipitation, crystallization and sublimation.

Module III Characterization (12 hrs)

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 IV Biomimetic porphyrins (10 hrs)

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. (i) P. Rothemund, *J. Am. Chem. Soc.,* 1936, 58, 625; (ii) E. B. Fleischer, *Inorg. Chem.,* 1962, 1, 493; (iii) P. Rothemund and A. R. Menotti, *J. Am. Chem. Soc.,* 1948, 70, 1808; (iv) A. D. Adler, *J. Org. Chem.,* 1967, 32, 476; (v) A. D. Adler, F. R. Longo, F. Kampas and J. Kim, *J. Inorg. Nucl. Chem.,* 1970, 32, 2443; (vi) J. S. Lindsey, I. C. Schreiman, H. C. Hsu, P. C. Kearney and A. M. Marguerettaz, *J. Org. Chem.,* 1987, 52, 827; (vii) G. M. Badger, R. A. Jones and R. L. Laslett, *Aust. J. Chem.,* 1964, 17, 1028..
5. (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.

CY7253: Introduction to Computational Chemistry

L	T	P	C
2	-	2	3

Pre-requisites: Nil **Total Hours: 56 (28 (T) + 28 (P))**

Module 1 Electronic Structure Methods (14(T) hrs)

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. The Roothan – Hall equations, Koopmans theorem, HF limit - Electron correlation,

Module II Post- Hartree Fock Methods and Basis Sets (14 (T) hrs)

Semi empirical methods - Perturbation theory - Coupled-cluster theory – Configuration Interaction -Density functional theory.
Basis set approximation- Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – Minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets- Correlation-consistent basis sets.

Module III Computing Thermodynamics and Molecular Properties-I (14 (P) hrs)

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 -NMR spectra.

Module 1V Computing Thermodynamics and Molecular Properties-II (14 (P) hrs)

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 & 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 edn.*, Springer 2011.

CY7254: Advanced Materials

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hours: 42**

Module I Chemical bonding (8 hrs)

Molecular orbital theory, MO theory for the ground state and excited state of H_2^+. Hydrogen molecule; MO treatment and calculation of energy, polyatomic molecules-Walsh's rules; conjugated π systems, hybridization, metallic bonding, free electron model, band theory, quantum mechanical tunneling, Fermi energy.

Module II Different advanced materials (14 hrs)

Semiconductor materials (classification and preparation), hard and soft magnetic materials, liquid crystals in display and thermography, polymeric liquid crystals, porous and nonporous membranes, hierarchical zeolites, super conductors (types, properties, applications) chalcogen photoconductors, polymers for biomedical applications (tissue engineering, bioseparations, contact lenses, orthopedic implants, dental materials), materials for biomimetics, biosensors, biomembranes, organic electronics materials.

Module III Nanomaterials (12 hrs)

Nanostructures-classification, fabrication methods: top-down processes-milling, lithographic processes, Bottom –up processes: vapour phase deposition methods, plasma assisted deposition processes, MBE, colloidal methods, sol-gel method, electrodeposition, templating the growth of nanomaterials, self assembly and self-organization of nanomaterials, semiconductor nanostructures: quantum wells, quantum wires, quantum dots. Carbon nanotubes: synthesis, properties and applications, functionalized nanoparticles and metal nanoparticles for biomedical applications.

Module IV Drug delivery systems (8 hrs)

Introduction, materials for targeted drug delivery, magnetic drug carriers, chemical structure and composition of drug carriers, micelles, vesicles, dendrimers, nanocapsules, multifunctional nanoparticles, hydrogels, polymer drug conjugates.

References

1. L. Pauling, *The Nature of the Chemical Bond*, Cornell University Press, Ithaca, New York, 1960.
2. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1994.

3. L. V. Azaroff, *Introduction to Solids*, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1977.
4. J.M.G. Cowie, 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, M. Geoghegan, *Nanoscale Science and Technology*, John Wiley & Sons, New York, 2005.
7. I.F. Uchegbu, A.G. Schatzlein, *Polymers in Drug Delivery*, Taylor & Fransis, Boca Raton, 2006.

CY7255: Lubricant Technology

L	T	P	C
3	-	-	3

Pre-requisites: Nil **Total Hours: 42**

Module I Surface structure and properties (10 hrs)

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

Module II Surface treatments (9 hrs)

Lubricants 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. Cleaning of surfaces, surface morphology- scanning electron and atomic force microscopes. Lubricant-surface compatibility.

Module III Mechanism and classification (12hrs)

Theories of lubrication, structural lubricants, mechanical lubricants, chemically active lubricants, refractories. Mechanism of lubrication- hydrodynamic, boundary and extreme pressure lubrication. Classification of lubricants, solid lubricants, semi-solid lubricants, vegetable oils, mineral oils, blended oils, synthetic lubricants, lubricating emulsions. Criteria for the selection of lubricants, optimization of formulations.

Module IV Lubricant analysis (11 hrs)

Properties of lubricants, detailed study including instrumentation, with industrial significance, on: viscosity index, flash and fire points, colud and pour points, aniline point, steam emulsion number, neutralization number, saponification number, Iodine value , carbon residue. Grease: calcium based greases, lithium based greases, axle greases, mechanical stability, penetration number, dropping point. Cutting fluids.

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.