Master of Science

In

Chemistry

Course Structure & Syllabus

Department of Chemistry

National Institute of Technology Hamirpur

Hamirpur (HP) – 177005, India

Course Structure of M. Sc. Chemistry

SEMESTER-I

Sr. No	Course No.	Course Name	Teaching Schedule			Hours /week	Credit
			L	T	P		
1	CY-611	Inorganic Chemistry-I	4	0	0	4	4
2	CY-612	Organic Chemistry-I	4	0	0	4	4
3	CY-613	Physical Chemistry-I	4	0	0	4	4
4	CY-614	Molecular Spectroscopy	4	0	0	4	4
5	CY-615	Solid State & Colloidal Chemistry	4	0	0	4	4
6	CY-616	Inorganic Lab-I	0	0	4	4	2
7	CY-617	Organic Lab-I	0	0	4	4	2
8	CY-618	Physical Lab-I	0	0	2	2	1
	Total		**20**	**0**	**10**	**30**	**25**

SEMESTER-II

Sr. No	Course No.	Course Name	Teaching Schedule			Hours /week	Credit
			L	T	P		
1	CY-621	Inorganic Chemistry-II	4	0	0	4	4
2	CY-622	Organic Chemistry-II	4	0	0	4	4
3	CY-623	Physical Chemistry-II	4	0	0	4	4
4	CY-624	Organic Synthetic Methodology	4	0	0	4	4
5	CY-7MN	Programme Elective – I	4	0	0	4	4
6	CY-625	Inorganic Lab-II	0	0	4	4	2
7	CY-626	Physical Lab-II	0	0	4	4	2
8	CY-627	Organic Lab-II	0	0	2	2	1
	Total		**20**	**0**	**10**	**30**	**25**

SEMESTER-III

Sr. No	Course No.	Course Name	Teaching Schedule			Hours /week	Credit
			L	T	P		
1	CY-631	Organometallics	4	0	0	4	4
2	CY-632	Interpretative Molecular Spectroscopy	4	0	0	4	4
3	CY-7MN	Programme Elective-II	4	0	0	4	4
4	XY-8MN	Open elective-I	4	0	0	4	4
5	CY-633	Physical Lab-III	0	0	4	4	2
6	CY-634	Organic Lab-III	0	0	4	4	2
7	CY-635	Inorganic Lab-III	0	0	2	2	1
	Total		**16**	**0**	**10**	**26**	**21**

SEMESTER-IV

Sr. No	Course No.	Course Name	Teaching Schedule			Hours /week	Credit
			L	T	P		
1	CY-7MN	Programme Elective - III	4	0	0	4	4
2	CY-7MN	Programme Elective - IV	4	0	0	4	4
3	XY-8MN	Open elective-II	4	0	0	4	4
4	CY-851	Seminar	-	-	-	-	1
5	CY- 699	M. Sc. Project	-	-	-	-	6
	Total		**12**	**0**	**0**	**12**	**19**

Programme Elective - I, II, III & IV: Any course listed in Annexure (List of Electives)
Total Credit of the Programme = 25+25+21+19 = 90

Annexure

List of Programme Electives and Open Electives

Semester-II (Programme Elective-I)

CY-701	Natural Products and Medicinal Chemistry
CY-702	Biochemistry
CY-703	Computational Chemistry

Semetser-III (Programme Elective-II)

CY-704	Polymer Chemistry
CY-705	Advanced Physical Chemistry
CY-706	Supramolecular Chemistry

Semester-IV (Programme Elective-III)

CY-707	Molecular Energetics and Dynamics
CY-708	Green Chemistry

Semester-IV (Programme Elective-IV)

CY-709	Bioinorganic Chemistry
CY-710	Heterocyclic Chemistry

List of Open Electives

CY- 881	Polymer and Polymer Composites
CY- 882	Nanomaterials

Course Name: **Inorganic Chemistry -I**
Course Code: **CY-611**
Course Type: **Core**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- To make the students conversant with bonding theories of co ordination complexes.
- To impart knowledge of reaction mechanisms of transition metal complexes.
- To enable the students to understand various analytical techniques and their applications

Course Content

Stereochemistry and Bonding in Main Group Compounds and Metal Ligand BondingVSEPR, Walsh diagrams (tri and tetra-molecules), d π-p π bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. Limitations of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π bonding and molecular orbital theory. Reaction Mechanism of Transition Metal Complexes-I Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valance bond and crystal field theories, kinetics of octahedral substitution reactions. Reaction Mechanism of Transition Metal Complexes –II Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, reactions without metal-ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of substitution reaction, Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross-reactions and Marcus Hush Theory, inner sphere type reactions. Analytical techniques (Instrumentation and Applications) Polarography (DC, AC and pulse), cyclic voltammetry, coulometry and anode stripping voltammetry, X-ray photoelectron spectroscopy (XPS), Auger Electron Spectroscopy (AES), Atomic absorption and emission spectroscopy, GC-Mass Spectroscopy , Separation Methods: Theory and applications of separation methods in analytical chemistry: solvent extraction, ion exchangers including liquid ion exchangers and chromatographic methods for identification and estimation of multicomponent systems (such as TLC, GC, HPLC, etc.)

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Demonstrate an understanding of bonding in coordination complexes

CO2: Understand the substitution reactions in transition metal complexes.

CO3: Able to explain various analytical techniques and their applications in various fields

Books and References

1. Wilkinson Advanced Inorganic Chemistry by Cotton, F.A., John Wiley& Sons.
2. Inorganic Chemistry: Principles of Structure and Reactivity by Huheey, James E., Harper Collins College Publishers.
3. Chemistry of the Elements by Greenwood, N.N. and Earnshaw, A., Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Inorganic Electronic Spectroscopy by Lever, A.B.P, Elsevier Science Publishers B.V.
5. Inorganic Chemistry by Shriver, D.F.; Atkins, P.W., Oxford University Press.
6. Physical Methods for Chemists by Drago, Russell S, Saunders College Publishing.
7. Analytical Chemistry by Christian, G. D, John Wiley & Sons, Inc.
8. Principles of Instrumental Analysis by Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A, Saunders Golden Sunburst Series.
9. Instrumental Methods of Analysis by Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A., Wadsworth Publishing.

Course Name: **Organic Chemistry-I**
Course Code: **CY-612**
Course Type: **Core**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- The objective of this course is to impart understanding of the reactive intermediates and their structure and reactivity through various organic reactions.
- To introduce the fundamental concepts of the principles of stereochemistry and their application in organic chemistry.

Course Content

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.Free Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radicalanions, SRN1 mechanisms.Carbenes: Formation and structure, reactions involving carbenes and carbenoids. Nitrenes: Generation, structure and reactions of nitrenes. Arynes: Generation and reactivity of arynes, nucleophilic aromatic substitution reactions, SNAr mechanism; Ipso effect. Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number. Stereoisomerism: Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.Simple chemical correlation of configurations with examples, quasiracemates.Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones. Asymmetric induction: Cram's, Prelog's and Felkin-Ahn model; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle. Molecular dissymmetry and chiroptical properties: Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Comprehend the structure-reactivity pattern of reactive intermediates involved in organic reactions.

CO2: Write mechanism of organic reactions involving reactive intermediates. Apply these reactions in organic synthesis.

CO3: Discuss the importance of the configuration of chiral organic compounds, including those with no chiral centre, in relation to chemical and physical properties.

CO4: Critically assess the key stereochemical features of substitution, addition, elimination mechanisms.

Books and References

1. Advanced Organic Chemistry: Reactions, Mechanism and Structure by March, Jerry, John Wiley.
2. Advanced Organic Chemistry by Carry, F. A., Sundberg, R.J., Plenum.
3. A Guide Book to Mechanism in Organic Chemistry by Sykes, Peter, Longman.
4. Organic Chemistry by Morrison, R. T.; Boyd, R. N, Prentice Hall.
5. Organic Reactions and their Mechanisms by Kalsi, P. S., New Age International Publishers.
6. Stereochemistry of Organic Compounds by Kalsi, P.S., New Age International.

Course Name: **Physical Chemistry-I**
Course Code: **CY-613**
Course Type: **Core**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To educate the students about history of quantum chemistry and its detailed correlation to spectroscopic observations.
- To demonstrate the applicability of quantum parameters in solving important scientific problems such as rotation, vibration and electronic structure of atoms.
- To impart knowledge of symmetry elements and group theory to the students.

Course Content

Fundamentals of quantum chemistry: Basic postulates, eigenvalues and eigenvectors, Hermitian operators, applications including translational, vibrational and rotational degrees of freedom - particle in 1D/2D/3D box, particle in a ring, rigid rotor, harmonic oscillator. Electronic, vibrational and rotational transitions.Solution of SchrÖdinger equation for the hydrogen atom; radial and angular functions, atomic orbitals and electron spin. Multi-electron systems, term symbols.

Applications of Quantum chemistry: Understanding of chemical bonding and Approximate techniques: Born-Oppenheimer approximation, variation and perturbation methods with examples. Valence bond theory including mathematical treatment of sp, sp^2 and sp^3 hybridized orbitals, molecular orbital theory with suitable examples, Huckel molecular orbital approach.

Group theory: Concept of molecular symmetry and groups, symmetry operations and symmetry elements in molecules, matrix representations of symmetry operations, point groups, representation of a group, reducible and irreducible representations, great orthogonality theorem and its consequences.

Applications of group theory: Applications of group theory to atomic orbitals in ligand fields, molecular orbitals, symmetry of normal modes of vibrations, prediction of infrared, Raman active vibrational modes, and electronic transitions.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Understand the importance of mathematical functions & operators in Quantum Chemistry.
CO2: Interpret the atomic structure & spectroscopic data more clearly.
CO3: Explore the symmetry elements present in molecules and their significance in chemical properties.

Books and References:

1. Quantum Chemistry by Levine, I. N., PHI Learning Pvt. Ltd., Delhi.
2. Quantum Chemistry by McQuarrie, D. A, Reprint, Viva Books.
3. Molecular Quantum Mechanics by Atkins, P., Oxford University Press.
4. Chemical Applications of Group Theory by Cotton, F. A., Wiley Eastern.

Course Name: **Molecular Spectroscopy**
Course Code: **CY-614**
Course Type: **Core**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- To enable students to learn molecular spectroscopy as an important tool to interpret molecular structure of compounds.
- To acquire theoretical knowledge of different spectroscopic techniques.
- To demonstrate an understanding of the rotational, vibrational and electronic spectroscopy of diatomic and polyatomic molecules.
- To enable the students to acquire the skill to determine the functional groups present in unknown molecules using vibrational (IR) spectra.
- To impart knowledge of magnetic properties of electrons and nucleus of atoms with the help of Magnetic resonance and ESR spectroscopy.

Course Content

Overview of molecular spectroscopy: Different aspects of molecular spectroscopy, the Born-oppenheimer approximation, transition probability, oscillator strength, the integrated absorption coefficient. Microwave spectroscopy: Classification of the rotors, intensity of the rotational lines, population of energy levels, non-rigid rotation, anharmonicity and centrifugal distortion, effect of isotopic substitution. Rotation spectra of the linear, spherical top and asymmetric top polyatomic molecules.Infrared and Raman spectroscopy: Types of vibration bands- overtones, combination bands, Fermi resonance phenomenon, finger print region, FTIR spectroscopy and application. Rayleigh and Raman scattering, polarizabilities, rotational and vibrational Raman spectra, selection rules, polarization of light and Raman effect, resonance Raman and coherent anti-Raman spectroscopy. UV-visible spectroscopy: Electronic spectra, Frank-Condon Principle, predissociation spectra, Fortrat diagram, conjugated polyene and enone systems, different types of charge transfer transitions and their basis. Charge transfer spectra in organic and inorganic systems. Photoelectron spectroscopy: The photoionization processes, Auger and autoionization processes, de-excitaion by fluorescence, outlines of UPS, XPS and Auger techniques and their applications in interpretation of valence and core shell spectra of atoms and molecules. Magnetic resonance spectroscopy: Nuclear moments, nuclear spin states in a magnetic field and the resonance phenomenon, relaxation processes and their importance. Bloch equation, Larmor frequency, shielding constant and chemical shifts. Spin-spin coupling ,Dynamic NMR and line shapes. General introduction to double resonance experiments and nuclear overhauser effect, chemical shift reagents, multinuclear NMR. ESR Spectroscopy: Principle of ESR and interpretation of its applications for ESR spectra of $-CH_3$ and $–CH_2$ radicals.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Demonstrate different spectroscopic techniques by using theoretical knowledge.
CO2: Become familiar with different spectroscopic techniques to explain structure of compound.
CO3: Interpret rotational, vibrational and electronic spectra of given material.
CO4: Demonstrate an understanding of electronic and magnetic properties with the help Magnetic resonance and ESR spectroscopy.

Books and References

1. Fundamentals of Molecular Spectroscopy by Banwell, C.N. and McCash, E.L.M., McGraw-Hill, N. Y.
2. Principles of Magnetic Resonance by Slichter, C.P., Springer Verlag.
3. Molecular Spectroscopy by Graybeal, J.D., McGraw-Hill.
4. Physical Chemistry by Atkins, P. and Paula, J.de, Oxford Univ. Press.

Course Name: **Solid State & Colloidal Chemistry**
Course Code: **CY-615**
Course Type: **Core**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To introduce the fundamentals of solid state and colloidal chemistry.
- To provide better understanding of the related concepts through various laws and theories
- To impart knowledge of about the various materials, classification, their structure, bonding, and related problems.

Course Content

Symmetry in the crystalline state: Crystal symmetry, elements of translation - screw axis and glide planes, symmetry in a cube, types and stereographic projections of crystal systems, space symmetry and space groups, Hermann Mauguin and Schoenflies notations, Lattice planes and Miller Indices.

X-Ray diffraction: Crystal planes and directions, Bragg's law of Diffraction, structure factor, integrated intensity and systematic absences/presences of reflections, indexing and simulation of powder X-ray diffraction pattern for simple systems such as CaF_2. Bonding in solids: Bonding in molecular solids – polymorphism, bonding in extended solids - ionic, covalent and metallic. Band theory of solids - classification of semiconductors, metals and insulators, free electron theory.Colloids & Surfaces: Classification and preparation of colloids, Electrical double layer phenomena, DLVO theory, Surfactants & CMC determination, Gibbs Isotherm. Adsorption, Different types of Adsorption, Langmuir & BET adsorption isotherms, Measurement of surface area of adsorbents.

Course Outcomes:

Upon successful completion of the course, students will be able to

CO1: Understand the importance of crystal symmetry, structure, molecular bonding in solid materials.

CO2 : Interpret the materials physical and chemical properties.

CO3: Understand the role of colloids and surface chemistry in various physical and chemical processes along with their practical applications

Books and References

1. New Directions in Solid State Chemistry by Rao, C.N.R. and Gopalakrishnan, J., Cambridge University Press.
2. Foundation of Colloid Science by Hunter, R. J., Oxford Univ. Press.
3. Solid State Chemistry and its Applications by West, A. R., Reprint, Wiley India.
4. Fundamentals of Interface and Colloid Science by Lyklema, J., Academic Press San Diego.
5. Physical Chemistry of Surfaces by Adamson, A.W., John Wiley and Sons, New York.

Course Name: **Inorganic Lab-I**
Course Code: **CY-616**

Contact Hours/Week: **4P** Course Credits: **02**

Course Objectives

- To identify individual ions present in the mixture solution and the chemistry behind it.
- To estimate various ions by titrimetry and spectral techniques.
- To synthesize coordination compound.

List of Experiments

1. Gravimetric Estimation of silver and zinc in the given solution of complex.
2. Gravimetric Estimation of copper and zinc in the given solution of complex.
3. Gravimetric Estimation of copper and silver in the given solution of complex.
4. Analysis of calcium and magnesium ions using EDTA.
5. Preparation of Tris(thiourea) cuprous(I) sulphate $[Cu(tu)_3]_2SO_4.2H_2O$ (Where tu stands for thiourea) and its physicochemical characterization including IR Study.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Estimate the ions present in the sample by different techniques.
CO2: Develop in depth understanding of titrimetry and gravimetry.
CO3: Prepare coordination compounds.

Course Name: **Organic Lab-I** Course Code: **CY-617**	
Contact Hours/Week: **4P**	Course Credits: **02**

Course Objectives

- To provide skills for separation and purification of organic compounds from mixtures.
- To provide skills for identification of organic compounds based on qualitative analysis method.
- To enable the students to synthesize the derivatives of organic compounds.

List of Experiments

Qualitative Analysis of mixtures of two solid organic compounds (Five such samples). For each sample:

1. Separation of the components.
2. Identification of the individual compounds through various tests.
3. Checking the purity of components by melting point.
4. Preparation of derivatives for each component, their recrystallization and recording of their melting point.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Separate and purify organic compounds from mixtures

CO2: Identify organic compounds based on qualitative tests and melting point determination

CO3: Design and develop route for the synthesis of different derivatives

Course Name: **Physical Lab-I**
Course Code: **CY-618**

Contact Hours/Week**: 02 P** Course Credits: **01**

Course Objectives

- To enable the students to measure the surface tension, viscosity and absorbance of liquids.
- To give hands-on experience of viscometers, stalagmometers and spectrophotometers to students.
- To demonstrate the effective quantitative analysis of liquid mixtures.

List of Experiments

1. Determination of percentage composition of a liquid mixture by viscosity measurement.
2. Determination of molecular weight of a polymer (say polystyrene) by viscosity measurement.
3. Determination of Parachor value for >CH2 group in a molecule.
4. Measurement of interfacial tension and to test the validity of Antonoff's rule.
5. Determination of the critical micelle concentration of a soap by surface tension method.
6. Verification of lambert beer's law for $KMnO_4$ solution.
7. Verification of lambert beer's law for $K_2Cr_2O_7$ under different experimental conditions.
8. To find composition of Ferric ions-salicylic acid complex by Job's method.
9. To determine the dissociation constant of phenolphthalein colorimetrically.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Measure the viscosity, surface tension and absorbance of unknown liquid samples and mixtures.
CO2: Get hands-on exposure to glassware such as viscometers and stalagmometers.
CO3: Identify the liquids based on above-mentioned parameters.

urse Name: **Inorganic Chemistry -II** Course Code: **CY-621** Course Type: **Core**	
Contact Hours/Week: **4L**	Course Credits: **04**

Course Objectives

- To make the students familiar with stereochemistry of coordination compounds.
- To enable students to understand stability constant of metal complexes and their determination methods.
- To impart knowledge of MOT diagram of metal complexes.
- To enable the students to understand electronic and magnetic properties of transition metal complexes.

Course Content

Structure, bonding and properties of transition metal complexes: Different types of ligands and coordination geometry (symmetry considerations), coordination number, isomerism (recapitulation), Stereoisomerism in inorganic complexes, HSAB concept, thermodynamic stability, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate and macrocyclic effect , successive and overall stability constants, determination of stoichiometry (Job's method) and stability constants by spectrophotometric, potentiometric and polarographic methods, Irving-William series,. Metal-ligand bonding: Overview of crystal field and ligand field theories of 4-, 5- and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal-bipyramidal and cubic complexes, measurement of CFSE (d_1 to d_{10}) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1^{st} row transition metal ions. Molecular orbital theory (MOT) of coordination compounds: Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ and π bonding, angular overlap model.Electronic spectra of coordination compounds: Energy states from spectral terms of dn configurations, selection rules for ligand-field and charge transfer transitions in metal complexes, band intensities, factors influencing band widths, splitting of various terms, Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral dn complexes, calculation of ligand field parameters, luminescence, phosphorescent complexes. Magnetic properties of coordination compounds: Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon, spin admixed states, metal-metal direct spin interaction and super exchange spin-spin interaction through bridging ligands, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties, single molecule magnets.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Demonstrate an understanding of isomerism and stereochemistry of coordination compounds.
CO2: Interpret the stability of complexes.
CO3: Demonstrate an understanding of electronic spectra of coordination compounds.
CO4: Able to analyze Tanabe – Sugano diagrams.

Books and References

1. Advanced Inorganic Chemistry by Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., John Wiley & Sons.
2. Concepts and Models in Inorganic Chemistry by Douglas, B.E., McDaniel, D.H. and Alexander, J.J., John Wiley & Sons.
3. Ligand Field Theory and Its Applications by Figgis, B.N., and Hitchman, M.A, Wiley Eastern Ltd.
4. Inorganic Chemistry Principle of Structure & Reactivity by Huheey,J.E., Keiter, E.A., Keiter, R.L., Pearson Education.
5. Shriver and Atkins Inorganic Chemistry by Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., Oxford university press.

Course Name: **Organic Chemistry-II**
Course Code: **CY-622**
Course Type: **Core**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- The aim is to make students familiar with the concepts and applications in concerted organic and organic photochemistry.
- The foundation for photochemistry is outlined and discussed based on the nature of relevant chemical bonds and the properties of light.

Course Content

Nature of Bonding in Organic Molecule: Delocalized chemical bonding, conjugation, Cross conjugation, resonance hyper conjugation, Bonding in fullerenes, Tautomerism, Aromaticity in benzenoid and non benzenoid Compounds. Alternant and non alternant hydrocarbons, Huckel's rule. Energy level of π M.O., Annulenes, anti aromaticity, aromaticity, Homo aromaticity, Bonds weaker than covalent, addition compound, crown ether complexes and cryptands, Inclusion compound, cyclo dextrins, Catenanes & rotaxanes. Effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment. Reaction Mechanism, Structure and Reactivity types of mechanism, types of reactions, methods of determining mechanism and isotope effects, thermodynamics and kinetic requirement. Kinetic and thermodynamics control, Hammond's postulate, Curtin-Hammett Principle, Potential energy diagrams, transition states and intermediates, The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.Method of determining mechanisms, isotope effects. Pericyclic Reactions Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO, PMO and Hückel–Mobius approach. Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene and allyl system Electrocyclic reactions conrotatory and disrotatory motions 4n, 4n +2 and allyl system. Cycloadditions-antarafacial suprafacial additions, 4n and 4n+2 systems, 2+2 additiion of ketenes, 1, 3-dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements-Suprafacial and antarafacial shifts of H. Sigmatropic shifts involving carbon moieties, [3, 3]-and [5, 5]-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangement. Fluxional tautomerism. Ene reaction. Photochemistry :Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes; dimerizations. Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α,β- unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno–Buchi reactions; photoreductions. Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loeflller-Freytag reaction. Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence, etc.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Understand the theoretical basis of pericyclic reaction and help them to find a way to carry out these types of reaction.
CO2: Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions.
CO3: Discuss the most important photochemical reactions for organic compounds.
CO4: Outline the main mechanistic aspects for the photochemical transformations.

Books and References

1. Advanced Organic Chemistry: Reactions, Mechanism and Structure by March Jerry, John Wiley.
2. Advanced Organic Chemistry by Carry, F. A.; Sundberg, R.J. Plenum.
3. Organic Chemistry by Morrison, R. T., Boyd, R. N, Prentice Hall.
4. Pericyclic Reactions by Fleming, I., Oxford Science Publications.
5. Pericyclic Reactions by Marchand, A. P. & Lehr, R. E., Academic Press.
6. Aspects of Organic Photochemistry by Horspool, W. M. Academic Press.

Course Name: **Physical Chemistry-II**
Course Code: **CY-623**
Course Type: **Core**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To highlight the concept of equilibrium in chemical reactions and their detailed qualitative and quantitative analysis.
- To impart mechanistic understanding of basic electrochemical cells and their applications.
- To discuss more recent advances in electrochemistry based imaging and sensing technology.

Course Content

Chemical and Ionic Equilibrium:Free energy change in a chemical reaction and its relation to reaction quotient. Thermodynamic derivation of the law of chemical equilibrium.Distinction between ΔG and ΔGo, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases.
Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree ofionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect.Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salt solutions.Buffer solutions.Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Introduction to electrochemistry: Types of electrochemical cells, Arrhenius and Debye-Huckel-Onsager theory for electrolytes, Nernst Equation, Application of EMF and conductometric measurements in determining (i) free energy, enthalpy, entropy and kinetic parameters of reactions, (ii) equilibrium constants, and (iii) solubility limits of different salts. Commonly used electrode types and their functioning.Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Detailed qualitative discussion of potentiometric/conductometric titrations (acid-base, redox, precipitation),Advanced Electrochemistry: Principle and applications of Voltammetry, Polarography and Amperometric titrations.Working and usage of Scanning Tunneling Microscope.Electrochemical sensors for biomolecules and pathogens. Fuel cells: Different types and their advantages.

Course Outcomes

Upon successful completion of the course, students will be able to
CO1: Understand the mechanism of working of Electrolytic and Galvanic Cells.
CO2: Utilization of Conductance and EMF values in calculation of Thermodynamic parameters.
CO3: Use Electrochemical approaches for Imaging, Sensing and Storage Applications.

Books and References

1. Physical Chemistry by Castellan, G.W., Narosa.
2. Physical Chemistr by Barrow, G.M., Tata McGraw Hill.
3. Electroanalytical Chemistry: Theory and Applications by Sane, R.T. and Joshi, A.P., Quest Publications.
4. Priniciples of Electrochemistry by Koryta, J., Dvorak, J., Kavan, L, John Wiley and Sons, New York.
5. Electrochemical Methods-Fundamentals and Applications by Bard, A.J. and Faulkner, L.R., John Wiley.

Course Name: **Organic Synthetic Methodology** Course Code: **CY-624** Course Type: **Core**	
Contact Hours/Week: **4L**	Course Credits: **04**

Course Objectives

- To make the students conversant with the common steps of organic synthesis (i.e. oxidation and reduction of functional groups)
- To impart knowledge about the synthetically useful reactions in organic chemistry
- To introduce the fundamental concepts related to retrosynthetic analysis for organic compounds

Course Content

Oxidations: Oxidations of hydrocarbon, alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based reagents, ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation), ketones to α-hydroxy ketones, α,β-unsaturated ketones, ester/lactones (Baeyer-Villiger), alcohols to carbonyls (chromium, manganese, DMSO, hypervalent iodine and TEMPO based reagents), alcohols to acids or esters. Reductions: Catalytic hydrogenation, reduction by dissolving metals, reduction with hydride transfer reagents, reduction with borane and dialkyl borane, other methods-Wolff-Kishner reduction, desulphuration of thio-acetals, di-imide, low valent titanium species, trialkyl silane. Name reactions: Baylis-Hillman reaction, Beckmann rearrangement, Arndt-Eistert reaction, Favorskii rearrangement, Nef reaction, Sakurai reaction, Tishchenko reaction, Brook rearrangement, Tebbe olefination, Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling. Protection and deprotection of functional groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection, illustration of protection and deprotection in multi-step synthesis. Retrosynthetic analysis: Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, reversal of polarity (umpolung).

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Identify suitable reagents and methodologies for one-step and multi-step organic synthesis

CO2: Demonstrate the capability of predicting the products from different reactions with their stereochemistry, if applicable

CO3: Apply the principles of retrosynthetic analysis to formulate proper synthetic route for the industrially and biologically important molecules.

Books and References

1. Modern Methods of Organic Synthesis by Carruthers, W. and Coldham, I., Oxford University Press.
2. Application of Redox and Reagents in Organic Synthesis by R. K. Kar, National Central Book Agency.
3. Advanced Organic Chemistry, Part B: Reactions and Synthesis by Carey, F. A. and Sundberg, R. J., Springer.
4. Organic Synthesis by Smith, M.B., Academic Press.

Course Name: **Inorganic Lab -II** Course Code: **CY-625**	
Contact Hours/Week: **4P**	Course Credits: **02**

Course Objectives

- To prepare different coordination complexes.
- Characterization of complexes by using IR technique.

List of Experiments

1. To prepare pure and dry sample of Chloropentaammine cobalt(III) Chloride and its IR measurements.
2. Preparation of cis- and trans-$[Co(en)_2Cl_2]Cl$. And its IR study.
3. Preparation of $Na_2[Fe(CN)_5NH_3]$. H_2O and its characterization by IR.
4. Preparation of $Cu_2(CH_3COO)_4(H_2O)_2$ and its IR study
5. Preparation of $Hg[Co(CNS)_4]$ and to study its properties.
6. Preparation of cis-and trans-K $[Cr(C_2O_4)_2(H_2O)_2$ and its IR study.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Prepare and characterize various complexes and analyze the samples thoroughly.

CO2: Develop in-depth understanding of substitution reactions.

Course Name: **Physical Lab-II**
Course Code: **CY-626**

Contact Hours/Week**: 04 P** Course Credits: **02**

Course Objectives

- To teach the working of electrochemical cells.
- To show the diverse applications of conductance and EMF measurements.
- To demonstrate the usage of different types of electrodes in such instruments.

List of Experiments

1. Determination of cell constant of a cell and study the effect of dilution on equivalent conductance of strong/weak electrolytes.
2. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid like acetic acid.
3. Conducometric measurement of degree of hydrolysis of a salt.
4. Conductometric titration of a weak acid with strong base.
5. Conductometric titration of mixture of strong and weak acid with strong base.
6. Conductometric titration of a weak acid with weak base.
7. Potentiometric titration of polyprotic acids with strong base.
8. Potentiometric titration of mixture of strong and weak acid with strong base.
9. Determination of pKa of weak acid/base.
10. Determination of concentration of halides in a solution.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Operate potentiometers and conductivity meters.

CO2: Measure concentration, K_d of different electrolytes.

CO3: Identify the liquids based on above-mentioned parameters.

Course Name: **Organic Lab-II**
Course Code: **CY-627**

Contact Hours/Week**: 02 L** Course Credits: **01**

Course Objectives

- To demonstrate organic synthesis process of various compounds.
- To demonstrate the name reactions experimentally and their importance in Chemistry.
- To impart knowledge about the organic synthesis of materials.

List of Experiments

1. Adipic acid from cyclohexanol (oxidation).
2. p- Iodonitrobenzene from p-nitroaniline.
3. N- Bromo succinimide (Bromination).
4. Dibenzal acetone from benzaldehyde (Claisen-Schmidt reaction).
5. Cinnamic acid from benzaldehyde (Knoevenaegal reaction).
6. Benzanilide (Schotten-Baumann reaction).
7. o-Benzoylbenzoic acid (Friedel Craft's reaction).

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Understand the chemical synthesis processes.
CO2: Understand the various chemical reactions and their mechanism more clearly.
CO3: Explore the various chemical processes of oxidation/reduction and their applications.

Course Name: **Organometallics** Course Code: **CY-631** Course Type: **Core**	
Contact Hours/Week: **4L**	Course Credits: **04**

Course Objectives

- To make students familiar with the organometallic compounds.
- To make the students enable for proper understanding of the structure and bonding in the main group and transition metal-organometallic complexes.
- To impart knowledge on the application of organometallic compounds in organic synthesis and industrially relevant chemical reactions.

Course Content

Structure, bonding and reactivity of organometallics: 18 electron rule and its applications, limitations of 18 electron rule, description of bonding models for π-acceptor ligands including CO, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, physical evidences and consequences of bonding. Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.Organotransition metal chemistry: σ-Bonded transition metal-alkyls, -aryls, -alkenyls(vinyls), -alkynyls(acetylides), reactions in σ–organyls: homolytic cleavage, reductive elimination, β-metal hydrogen elimination.Transition metal complexes with carbenes and carbynes, reactions of carbine and carbyne complexes such as ligand substitution, nucleophilic, electrophilic attack, dismutation, and ligand coupling reactions.Concept of hapticity, transition metal complexes of alkenes (Ziese salt), alkynes, allyls, butadienes; π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes, reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxionalty, bimetallic and cluster complexes.Main group organometallics: Carboranes, metalloboranes and metallocarboranes; Synthetic applications of organoboranes, Organosilicon compounds: Preparation and their applications in organic synthesis.Applications of organometallics and clusters in catalysis: Alkene metathesis, Cativa and Monsanto processes for production of acetic acid, carbonylation and decarbonylation reactions, Wacker process, cyclooligomerisation of acetylene using Ni/Cr catalysts, Mobil and Fischer-Tropsch processes, polymer-bound catalysts, metal carbonyl clusters in catalysis.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Understand the electron count, structure, bonding and reactivity of different organometallic compounds.

CO2: Demonsrste the applications of organometallic compounds in synthetic organic reactions.

CO3: Apply the organometallics and clusters as catalysts in various chemical reactions, which are highly useful in industry.

Books and References

1. Inorganic Chemistry Principle of Structure and Reactivity by Huheey, J.E., Keiter, E.A. and Keiter, R.L., Pearson Education Inc.
2. Advanced Inorganic Chemistry by Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., John Wiley & Sons.
3. Organotransition Chemistry by Hill, A.F., The Royal Society of Chemistry, Cambridge.
4. Oxford Premier Series on Organometallics by Bochmann, M. (Ed.), Vol. 1 and 2, Oxford Press.
5. Basic Organometallic Chemistry by Gupta, B.D. and Elias A.J., University Press (India) Pvt. Ltd.
6. Modern Methods of Organic Synthesis by Carruthers, W. Cambridge University Press.

Course Name: **Interpretative Molecular Spectroscopy**
Course Code: **CY-632**
Course Type: **Core**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- The objective of the course is to provide fundamental and practical aspects about molecular spectroscopy.
- This course focuses on using spectroscopy to solve experimental problems and provide interpretation of observed phenomena.
- Major emphases will address subject matter in optical spectroscopy (UVVisible, FT-IR, Raman,) associated with the electronic/molecular processes, and nuclear magnetic resonance (NMR) associated with structures and dynamics.

Course Content

Electronic spectroscopy: Electronic transitions in organic molecules, Woodward-Fieser rules for alkenes, Woodward rules for enones, aromatic compounds**. Infrared and Raman spectroscopy:** For simple organic molecules, predicting number of active modes of vibrations, analysis of representative spectra of compounds with various functional groups, application of isotopic substitution. **Mass spectrometry:** Basic principles, hard and soft ionization techniques, mass analyzer in ESI-MS and MALDI-MS, high resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecules, deduction of structure through mass spectral fragmentation. **Nuclear magnetic resonance:** Effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order and second order spectra, examples of AB, AX, ABX, AMX and AA′BB′ systems, simplification of second order spectrum, selective decoupling, double resonance, use of chemical shift reagents for stereochemical assignments, 13C NMR, T1 relaxation, NOE effects, DEPT, determination of number of attached hydrogens,1H and 13C chemical shifts to structure correlations, study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (fullvalene and related systems). Multinuclear NMR, COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY, VGSE. **Combined Spectroscopic applications**: Structure elucidation of organic/inorganic compounds using spectroscopic methods.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Analyse and interpret spectroscopic data collected by the methods discussed in the course.

CO2: Explain spectra and relate the observations to electronic, molecular and dynamic processes occurring in the samples.

CO3: Identify unknown organic compounds using a combination of spectroscopic techniques (including UV-vis, mass spectrometry, infrared spectrometry, raman, 1D and 2D proton and carbon NMR spectroscopy)

Books and References

1. Spectrometric Identification of Organic Compounds by Silverstein, R. M., Webseter, F. X. and Kiemle, D., John Wiley & Sons.
2. Organic Spectroscopy by Kemp, W. L., Palgrave.
3. Spectroscopy by Pavia, D. L., Cengage.
4. Spectroscopic Methods in Organic Chemistry by Williams, D. and Fleming, I., McGraw Hill Education (India) Private Limited.

Course Name: **Physical Lab-III**
Course Code: **CY-633**

Contact Hours/Week**: 04 P** Course Credits: **02**

Course Objectives

- To impart experimental skills to measure kinetic parameters of chemical reactions.
- To teach the detailed working principle and applications of polarimeter.
- To demonstrate the use of different techniques to monitor reaction kinetics.

List of Experiments

1. Determination of the specific and molecular rotation of fructose at different concentrations and to obtain the value of intrinsic rotation for fructose.
2. To study the kinetics of inversion of cane sugar by optical rotation measurement.
3. To compare the strengths of two acids by studying acid-catalyzed hydrolysis of an ester.
4. To study the kinetics of hydrolysis of ethyl acetate by NaOH.
5. Determine the specific reaction rate of the potassium persulphate-iodide reaction by initial rate method.
6. To study the kinetics of iodination of acetone in the presence of acid by initial rate method.
7. To study the kinetics of saponification of ethyl acetate by NaOH conductometrically.
8. To study the iodination of acetone using a colorimeter.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Operate polarimeter and colorimeter for studying different chemical reactions.
CO2: Measure reaction rate constant and order for reactions.

Course Name: **Organic Lab-III**
Course Code: **CY-634**

Contact Hours/Week: **4P** Course Credits: **02**

Course Objectives

- To extend student's comprehension and skill development in synthetic organic chemistry.
- To impart knowledge on the advances at the forefront of synthetic organic chemistry.
- To enable the students for planning and carry out the synthesis of different organic molecules having applications in healthcare, materials science, food processing etc.
- To develop the ability of the students to adapt and apply methodologies for solving problems in synthetic organic chemistry.

List of Experiments

1. Synthesis of Hydroxynaphthaldehyde (Reimer tiemann Reaction).
2. Two-step synthesis of Benzilic acid from Benzoin via Benzil.
3. Two-step synthesis of Benzanilide from Benzophenone (Beckmann Rearrangement) through Benzophenone oxime.
4. Synthesis of Trinitrophenol (picric acid) and picrate derivative.
5. Preparation of benzyl alcohol and benzoic acid (Cannizzaro's reaction).
6. Studies of TLC, column chromatography and paper chromatography for organic mixtures.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Execute various organic reactions safely and effectively for synthetic applications.

CO2: Use proper glassware set-up, handling of hazardous chemicals, and following appropriate techniques and procedures for any synthetic reaction.

CO3: Separate and purify the products after the reaction.

CO4: Plan a scheme for multi-step organic synthesis and will be able to implement that.

Course Name: **Inorganic Lab -III**
Course Code: **CY-635**

Contact Hours/Week: **2P** Course Credits: **01**

Course Objectives

- To impart knowledge of colorimetry and estimation of ions present in the mixture solution
- To provide hand on practice of various separation techniques.
- Separation of various ions using chromatography.

List of Experiments

1. Colorimetric estimation of Fe(II) ions by thiocyanate.
2. Estimation of Cu(II) ions in a given solution colorimetrically
3. Simultaneous determination of Cr and Mn in a given mixture colorometrically.
4. To extract iodine by solvent extraction and also quantify the extracted iodine.
5. To extract iodine by solvent extraction using DCM as solvent. Also quantify the extracted iodine
6. Separation of cations using paper chromatography
7. To study the effect of solvent o Rf value and the resolution for the mixture of dyes.
8. To separate ions by using ion-exchange resins.
9. To separate mixture of ions using column chromatography.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Colorimetric estimation of various ions.

CO2: Separation of mixture by chromatographic techniques.

Course Name: **Natural Products and Medicinal Chemistry** Course Code: **CY-701** Course Type: **Programme Elective-I**	
Contact Hours/Week: **4L**	Course Credits: **04**

Course Objectives

- To familiarise students with different natural products and to provide fundamental understanding on the concept of natural products as secondary metabolites, their structures, classification, occurrence, and biosynthetic pathways.
- To impart knowledge on the typical synthetic routes and pharmacological properties of various natural products.
- To make the students conversant with the general structural features, physicochemical properties and mechanism of action of different classes of drugs.
- To understand structure-activity relationship of different drug molecules.

Course Content

Terpenes and Steroids: Classification and biosynthesis of mono- sesqui-, di- and triterpenoids and steroids. Acetyl CoA, Mevalonic acid, acetoacetyl CoA, squalene to lanosterol, lanosterol to Cholesterol, Cholesterol to estradiol and progesterone, diosgenin and its utility in hormone synthesis. General chemistry of the following compounds- Cholesterol, Artemisinin, Gibbereline A3, Azadirachtin. Alkaloids and Polyphenols: Isolation and structure elucidation of alkaloids, Biosynthesis of alkaloids using thiokinase, mixed function oxygenases, methyl transferases, amino acid decarboxylases. Total synthesis of morphine, reserpine and ergotamine. Biosynthesis of flavonoids and related polyphenols. Synthesis of apigenin, luteolin, quercetin, Diadzen, myrtucommulone A, prenylflavone, binaringenin and biflavanoids. Medicinal Chemistry: Introduction to the history of medicinal chemistry, General mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids, Drug metabolism and inactivation. Receptor structure and sites. Drug discovery, development, design and delivery systems. General introduction to antibiotics, Mechanism of action of lactam antibiotics, non-lactam antibiotics and quinilones; antiviral and anti-AIDS drugs. Neurotransmitters, classes of neurotransmitters, Drugs affecting collingeric and adrenergic mechanisms. Anti-histamines, anti-inflammatory, anti-analgesics, anticancer and anti-hypertensive drugs, New developments, e.g. gene therapy, anti-sense & anti-gene strategies and drug resistance.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Provide an overview on natural product chemistry through identification of different types of natural products, their occurrence, structure, biosynthesis and properties.

CO2: Investigate plant materials and natural products and their further applications as starting materials for medicines used for the treatment of cancer, cardiovascular diseases, bacterial and fungal infections.

CO3: Recognize the drug structure and predict its pharmacological action.

CO4: Identify the pharmacophore and its physico-chemical features.

CO5: Describe the mechanism of action, use and mode of application of the selected drugs on the basis of their structure.

Books and References

1. Organic Chemistry Vol. 2by Finar, I. L. & Finar, A. L. Addison-Wesley.
2. Organic Chemistry Vol. 1by Finar, I. L. Longman.
3. Secondary Metabolites by Mann, J. Oxford University Press, Oxford, UK.
4. Advanced Organic Chemistry,Parts A&B by Carey,F.A. & Sundberg,R. J. Plenum: U.S.
5. Introduction to Medicinal Chemistry: How Drugs Act and Why? by Gringauz, A., John Wiley & Sons.
6. Introduction to Medicinal Chemistry by Patrick, G. L., Oxford University Press.
7. Principles of Medicinal Chemistry by Lemke, T. L. & William, D. A., Foye's, USA.

Course Name: **Biochemistry**
Course Code: **CY-702**
Course Type: **Programme Elective-I**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- To understand the fundamental principles of Biochemistry based on the structure and function of biomolecules.
- To enable students in acquiring knowledge and to understand the regulation of biological/biochemical processes.
- To understand the role of nucleic acids in the controlling process of life system.
- To impart knowledge on enzyme action, metabolism of glucose, fats, amino acids as source of energy.

Course Content

Introduction to Chemical Biology: Chemical principles of biological systems, structure of amino acids, Primary, secondary, tertiary structures of proteins, Motifs of protein structure, Folding and flexibility of protein structures, protein folding thermodynamics, carbohydrate structure and its metabolism (glycolysis, glycogen metabolism, electron transport and oxidative phosphorylation), lipid metabolism; amino acid metabolism, basic knowledge on nucleic acid structure, DNA replication and gene expression for recombinant DNA technology, DNA transcription; RNA processing and translation. Techniques for Bioseparation: Method of solubilization, Chromatographic separation techniques: gel-filtration, ion exchange, affinity techniques, Electrophoresis, Nucleic acid fractionation Enzymes: Enzyme kinetics, enzyme catalysis, enzyme activators, enzyme inhibitors and inhibition mechanisms. Spectroscopic Tools in Biology: Different spectroscopic methods like absorption, fluorescence, surface plasmon resonance; circular dichroism, infrared, NMR and different mass spectrometric techniques.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Understand the structure of Protein and DNA, DNA replication, RNA and protein synthesis.

CO2: Gain proficiency in basic biochemical techniques for isolation, purification and characterization of biomolecules.

CO3: Demonstrate knowledge and understanding in enzyme kinetic behaviour and mechanisms, Biochemical and biophysical tools for characterization of biomolecules and their interactions.

Books and References

1. Lehninger Principles of Biochemistry by David L. Nelson, W H Freeman & Co.
2. Biochemistry by Donald Voet and Judith G. Voet, Wiley.
3. Biochemistry by Jeremy M. Berg, Lubert Stryer, John L. Tymoczko, W H Freeman & Co.
4. Introduction to Protein Structure by Carl Branden and John Tooze, Garland Publishing Company.
5. Biophysical Chemistry by Cantor and Schimmel, Publisher W. H. Freeman & Co.

Course Name: **Computational Chemistry** Course Code: **CY-703** Course Type: **Programme Elective-I**	
Contact Hours/Week: **4L**	Course Credits: **04**

Course Objectives

- To introduce the students about the computational methods in chemistry for determination of atomic and molecular properties.
- To impart knowledge on energy minimization techniques, Semi empirical and Abintio methods for calculation of different molecular properties.
- To make the students conversant with the simulation methods.

Course Content

Fundamentals of electronic structure: Basis function–hydrogen-like, Slatertype and Gaussian type orbitals, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets, correlation consistent basis sets, basis set super position error, energy minimization methods–derivative and non-derivative methods-simplex method, steepest descents method, Newton-Raphson method, minima, maxima and saddle points. Semi empirical and Abintio methods: Approximation methods, self-consistent field treatment of polyatomic molecules, closed shell systems–restricted HartreeFock calculations, open shell systems–ROHF and UHF calculations, The Roothan–Hall equations, Koopman's theorem, HF limit and electron correlation, introduction to post Hartree-Fock and density functional methods. Electronic properties: Dipole moment, electrostatic potential, frequencies, population analysis, Mulliken and Lowdin analysis, solvent effects, polarizable and nonpolarizable models. Introduction to simulation methods: Molecular mechanics, Monte carlo and molecular dynamics simulations, periodic boundary conditions, radial distribution function, calculation of thermodynamic properties.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Choose an appropriate computational tool (in terms of applicability, accuracy, and economy) for the calculation of a given chemical problem.

CO2: Perform, understand, and interpret the results of computational calculations.

CO3: Use computational methods to interpret typical chemical phenomenon, reactivity, electronic properties and thermodynamic properties.

Books and References

1. Introduction to Computational Chemistry by Jensen, F., John Wiley & Sons Ltd.
2. Molecular Modeling: Principles and Applications by Leach, A., Prentice Hall.
3. Essentials of computational chemistry: Theories and models by Cramer, C. J., John Wiley & Sons.
4. Quantum Chemistry by Levine, I. N., PHI Learning Pvt. Ltd., Delhi.

Course Name: **Polymer Chemistry**
Course Code: **CY-704**
Course Type: **Perogramme Elective-II**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- The objective of this course is provides an introduction to polymer science with respect to synthesis, polymerization kinetics and network formation/gelation of macomolecules formed by step-growth and chain-growth polymerization.
- To understand the Polymer structure/conformation and transitions from liquid (melt and solutions) to solid (polymer crystals and glass) states using equilibrium thermodynamics, kinetics and free volume considerations.
- Molecular weight determination of polymers using osmotic pressure, viscometry and size exclusion chromatography (SEC) and an overview of mechanical and rheological properties of polymers is also given.

Course Content

Introduction to Polymers: An introduction to the history, recent developments, applications and processing of polymers, Classification of polymers, addition and condensation polymerization, chain growth and step polymerization, Nomenclature, molecular weight and distribution, glass transition temperature, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships. Organic Polymer Chemistry I: Systematic study of polymers with emphasis centered on those synthesized by step-growth polymerization and their kinetics such as - polyesters, polycarbonates, polyamides, polyimides, epoxy, phenolic resins, amino plastics, polyurethanes etc. Organic Polymer Chemistry II: Systematic study of polymers with emphasis centered on those synthesized by addition polymerization and their kinetics such as ethers, acetals, lactones, lactams . Polymerisation techniques such as - bulk, solution, suspension and emulsion polymerization
Cationic and anionic polymerisation mechanism of ionic polymerisation, effect of gegen ions, temperature and solvent on polymerization. Copolymerisation, reactivity ratios,composition of copolymers, block and graft copolymers Complex catalyst polymerisation, mechanism of reaction. ATRP and Ring opening metathesis polymerization and their kinetics. Physical state and transitions, factors affecting glass transition and melting temperature.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Comprehend the molecular structure of heterocyclic compounds.
CO2: Pick the appropriate methods for the preparation of heterocyclic compounds.
CO3: Acquire skills to predict the outcomes of interactions of heterocyclic compounds.
CO4: Learn about the applications of the most important as well as less common heterocycles.

Books and References

1. Principles of polymerization by George Odian, Wiley.
2. Polymer Chemistry by P. C. Heimenz, T. P. Lodge, CRC press.
3. Polymer Chemistry by Seymour/Carraher's, Marcel Dekker, Inc.
4. The synthesis, characterization, reactions and applications of polymers by Comprehensive Polymer Science, Pergamon press.

Course Name: **Advanced Physical Chemistry**
Course Code: **CY-705**
Course Type: **Programme Elective-II**

Contact Hours/Week**: 04 L**
Course Credits: **04**

Course Objectives

- To introduce the theory and detailed analysis of ultrafast chemical reactions.
- To impart knowledge about irreversible chemical reactions and calculation of thermodynamic parameters of such systems.
- To utilize the basic quantum principles for understanding molecular behaviour.

Course Content

Advanced chemical kinetics: Kinetics of simple and complex reactions, theories of unimolecular reactions, kinetics-proton transfer and electron transfer reactions, fast reactions–rapid flow, stopped-flow and relaxation techniques, molecular beam method, diffusion controlled reactions, oscillatory reactions, linear free energy relationship, elucidation of mechanism from kinetic data. Irreversible Thermodynamics: Meaning and scope of Irreversible Thermodynamics, thermodynamic criteria for non-equilibrium states, phenomenological laws – linear laws, Gibbs equation, Onsager's reciprocal relations, entropy production, Prigogine's principle of maximum entropy production, non-equilibrium stationary states. Advanced quantum chemistry***:*** Dirac Bra-ket notation, addition of angular momentum, use of ladder operators– rigid rotor and harmonic oscillator, variation method– treatment of He atom, perturbation method–examples of anharmonic oscillator, He atom, Stark and Zeeman splitting, Hartree-Fock method.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Solve vibrational, rotational and electronic structure problems of molecules.
CO2: Obtain kinetic parameters of very fast and complex chemical reactions.
CO3: Measure the thermodynamic parameters of non-equilibrium reactions.

Books and References

1. Reaction Kinetics by Laidler, K.J., Anand Sons, New Delhi.
2. Non-Equilibrium Thermodynamics in Biophysics by Katchalsky, A &Curren, P. F., Harvard University press.
3. Quantum Chemistry by McQuarrie, D. A., Viva Books.
4. Molecular Quantum Mechanics by Atkins, P., Oxford University Press.

Course Name: **Supramolecular Chemistry**
Course Code: **CY-706**
Course Type: **Programme Elective-II**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To introduce the fundamentals of supramolecular chemistry and its importance.
- To demonstrate the role of supramolecular chemistry in understanding of molecular bonding and structure.
- To impart knowledge of synthesis of supramolecules and their applications.

Course Content

Fundamentals of supramolecular chemistry: Definitions, brief overview and examples; types of non-covalent interactions (H-bonding, electrostatic (ion-ion, ion-dipole, dipole-dipole), hydrophobic and steric, π-π, van der Waals), concepts of hostguest complexation with examples from ionophore chemistry, complexation of ions, molecular baskets, chalices and cages– podands, crown ethers, cryptands, calixarenes, macrocyclic effect, complexation of neutral molecules, self-assembly, molecular boxes and capsules, self-complementary species and self-replication. Supramolecular chemistry and biological processes: Cation binding (biological relevance, affinity and selectivity, artificial ionophores, natural and artificial cation channels). Anion and neutral molecule binding –relevance factors affecting affinity and selectivity, anion and neutral molecule binding in biology, artificial hosts for anions, katapinands, guanidinium receptors, receptors based upon Lewis acid-base concepts, enantio-selective anion recognition, cyclodextrins, anion binding based upon ion-dipole interactions, simultaneous anion-cation binding, neutral molecule recognition and binding. Synthesis of supramolecules: Synthesis of macrocycles, synthesis of receptors for cations anions, and neutral molecules, non-covalent synthesis, metal directed self-assembly of complex supramolecular architecture– rotaxanes, catenanes. Physical methods in supramolecular chemistry: Spectroscopy in supramolecular chemistry, determination of stoichiometry, stability constants, and geometry of complexes, binding constant determination, dynamics of supramolecular systems (solid state vs solution behavior).Application of supramolecular chemistry: Supramolecules in catalysis, as membrane transport, sensors, phase-transfer catalysts, supramolecular devices and switches, memories, logic gates and related systems, molecular scale machines (mechanical rotors, gears and brakes), conversion of light into fuels and light into electricity.

Course Outcomes:

Upon successful completion of the course, students will be able to -

CO1: Understand the chemical systems composed of a discrete number of molecules.
CO2: Interpret the molecular structure and various processes of their formation.
CO3: Explore the applications of supramolecules and their significance.

Books and References

1. Supramolecular Chemistry by Steed, J.W. and Aswood, J.L., Wiley.
2. Introduction to Supramolecular Chemistry by Dodziuk, H., Springer,.
3. Supramolecular Chemistry by Beer, P.D., Gale, P.A. and Smith, D.K., Oxford Chemistry Printers.
4. A Practical Guide to Supramolecular Chemistry by Cragg, P., Wiley-VCH.

Course Name: **Molecular Energetics and Dynamics**
Course Code: **CY-707**
Course Type: **Programme Elective-III**

Contact Hours/Week**: 4 L** Course Credits: **04**

Course Objectives

- To introduce the fundamental concepts and ideas of statistical thermodynamics and chemical kinetics
- To impart knowledge about the thermodynamics quantities, and state variables in understanding the behaviour of systems.
- To demonstrate the applicability of related kinetics laws and theories in solving problems in reaction kinetics, catalysis

Course Content

Statistical Thermodynamics: Statistical view of entropy. Laws of thermodynamics from statistical considerations. Molecular view of temperature and heat capacity. Boltzmann distribution. Thermodynamic quantities in terms of partition functions. Statistical mechanics of simple gases and solids. Kinetic theory of gases. Equilibrium constant, mean energies and heat capacities in terms of partition functions. Bose-Einstein and Fermi-Dirac statistics. Use of Statistical Thermodynamics in understanding molecular interaction in liquids.

Chemical Kinetics: Differential and integrated rate laws for zero, first and second order reactions. Complex Reactions. Catalysis. Temperature dependence and Arrhenius law. Potential energy surfaces. Kinetic theory of collisions. Transition state theory. RRK and RRKM theories. Reaction cross-sections, rate coefficients, reaction probabilities. Enzyme catalysis and homogeneous catalysis. Salt effects. Photochemical reactions. Ultrafast reactions.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Understand the meaning and the role of thermodynamic description of systems

CO2: Understand and define various parameters in chemical reactions.

CO3: Solve problems in chemical kinetics and statistical thermodynamics.

Books and References

1. Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology by Dill, K. A. and Bromberg, S., Garland Science.
2. Molecular Thermodynamics by McQuarrie, D. A. and Simon, J. D., Viva Books.
3. Atkins Physical Chemistry by Atkins, P. and Paula, J. De, Oxford University Press.
4. Chemical Kinetics by Laidler, K. J., Prentice Hall.
5. Chemical Kinetics and Dynamics by Steinfeld, J. I.,Francisco, J. S. and Sase, W. L. J. S. Prentice Hall.
6. Chemical Kinetics and Reaction Dynamics by Houst McGraw, P. L., Hill Higher Education.

Course Name**: Green Chemistry**
Course Code: **CY-708**
Course Type: **Programme Elective-III**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To educate the students about green chemistry, its importance and detailed correlation to industries and environment.
- To demonstrate the applications and significance of green chemistry in real world problems.

Course Content

Introduction to Green Chemistry: History of emergence of Green Chemistry through some industrial disasters, environmental movements for public awareness and some important environmental laws, Definition of Green Chemistry, Need for Green Chemistry, goals of Green Chemistry, Green Chemistry advances towards a sustainable future, Green Chemistry v/s Environmental Chemistry, Green Chemistry and its interdisciplinary nature, Twelve Principles of Green Chemistry and their illustrations with examples. Catalysis for Green Chemistry with examples. Catalytic oxidation using H_2O_2, Bio-catalysis, Photo-catalysis, Green reagents, Green solvents including solvent free synthesis of some organic compounds and inorganic complexes, alternative sources of energy, Green energy and sustainability. Application of Green Chemistry in real world cases: Wealth from waste Industrial Case Studies Green Nanotechnology Greener approaches for nanoparticle synthesis Pharmaceutical Industries: The largest waste producer Problems and solutions through Green Chemistry Benefits of Greening Industries, Need for Academia-Industry Collaborations, Innovations Stemming from Academia-Industry Collaborations Emerging Green Technologies. Green Solvents, Next generation Catalyst Design, Microwave assisted synthesis etc.

Course Outcomes

Upon successful completion of the course, students will be able to

CO1: Understand the need and importance of green chemistry.

CO2: Explore various processes and methods for implementing in real world problems.

Books and References

1. Green Chemistry- Theory and Practical by Anastas, P.T. & Warner, J.C., Oxford University Press.
2. Introduction to Green Chemistry by Matlack, A.S., Marcel Dekker.
3. Real-World cases in Green Chemistry by Cann, M.C. & Connely, M.E., American Chemical Society, Washington.
4. Hazardous Reagent Substitution, Royal Society of Chemistry, Green Chemistry Series by Sharma, R.K. & Bandichhor, R.
5. Introduction to Green Chemistry by Ryan, M.A. & Tinnes, M., American Chemical Society, Washington.
6. Green Chemistry Experiments: A Monograph by Sharma, R.K., Sidhwani, I.T. & Chaudhari, M.K., I.K. International Publishing House Pvt. Ltd. New Delhi, Bangalore.
7. Green Chemistry: An Introductory Text by Lancaster, M., RSC publishing.

Course Name: **Bioinorganic Chemistry**
Course Code: **CY-709**
Course Type: **Programme Elective-IV**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- To understand how metal ions interact with biological environments and how these interactions can influence the properties of metal centers.
- To explain how nature tailors the properties of metal centers in different metalloenzymes for their specific applications based on the principles of coordination chemistry.
- To introduce the concept of metallotherapy (medical applications of metal ions) and metal derived toxicity.

Course Content

Inorganic biochemistry: Metalloproteins and enzymes– Role of metal ions in the active sites, structure and functions of metalloproteins and enzymes containing Mg, Ca, V, Mn, Fe, Co, Ni, Cu and Zn ions. Detailed structure and mechanistic studies of the following–Mn-photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, Ni-urease, hydrogenase, nitrogen fixation, Cu-blue copper protein, tyrosinase, galactose oxidase, superoxide dismutases, Zn-carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, Mo and W containing enzymes, xanthine oxidase. Biological importance of Vitamin B12 and coenzymes, and their biomimetic studies.Chemical toxicity and metallotherapy: Toxic chemicals in the environment, toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens, metal containing drugs in therapy, interaction of heavy metal ions with DNA, DNA cleavage, structure-activity relationship and mode of action. Organometallic compounds as therapeutic drugs and enzyme inhibitors.
Metal ions and diseases: Role in Alzheimer's disease– Aggregation of proteins, role of copper, zinc and iron.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO2: Identify the typical role of different metal ions in biological processes.

CO3: Understand the involvement of metal ions in structural, recognition, and redox/non-redox catalytic activities of various metalloenzymes.

CO4: Interpret the information obtained from optical, vibrational, ESR, Mössbauer spectroscopy, X-ray diffraction, electrochemical and other selected methods for the characterization of biomolecular compounds containing metal atoms.

CO5: Understand metal-ion mediated post-translational modifications on proteins, DNA cleavage and associated toxicity.

Books and References

1. Elements of Bioinorganic Chemistry by Mukherjee, G.N. and Das, A., U.N. Dhur & Sons Pvt. Ltd., Calcutta.
2. Bioinorganic Chemistry by Hussian Reddy K., New Age International (P) Ltd.
3. Bioinorganic Chemistry by Bertini, I., Gray, H.B. Lippard, S.J. and Valentine, J.S, University Science Book.
4. Principles of Bioinorganic Chemistry by Lippard, S.J. and Berg, J., University Science Books, U.S.A.

Course Name: **Heterocyclic Chemistry**
Course Code: **CY-710**
Course Type: **Programme Elective-IV**

Contact Hours/Week: **4L** Course Credits: **04**

Course Objectives

- The objective of this course is to familiarize the students with chemistry of heterocyclic compounds, different methods of their synthesis and studying their various reactions.
- Emphasis is given on the most important heterocyclic systems, such as pyridines, quinolines, isoquinolines, pyrroles, furanes, tiophenes, indoles, pyrimidines, purines, imidazoles, aziridines and oxiranes.
- To discuss some of the key applications of various heterocyclic compounds in diverse fields such as in biology, dyes, photosensitizers, coordination compounds and polymeric materials.

Course Content

Heterocycles: Systematic nomenclature of heterocyclic compounds (Hantzsch-Widman, replacement and fusion methods), biological importance of heterocyclic compounds. Five-membered heterocycles with one heteroatom**:** Chemical structures of furan, pyrrole and thiophene, and degree of aromaticity. General syntheses methods for 5-member rings. Paal-Knorr, Feist-Benary, Hantzsch and Knorr syntheses. Electrophilic substitution, reactants employed and orientation of the substituent on the ring. Benzo derivatives of five-membered heterocycles with one heteroatom: Preparation of indole and carbazole derivatives. Fisher, Bischler, Madelung and Reissert syntheses. Preparation and reactivity of benzofurans (coumarins), benzothiophenes, dibenzofurans and dibenzothiophenes. Pyridines, quinolines and isoquinoles**:** Influence of the imine group on the reactivity of the pyridine ring. Nucleophilic and electrophilic substitutions on pyridine, quinolines and isoquinolines. Comparison of reactivity with benzene and naphthalene. Preparation of pyridine salts and pyridine *N*-oxides and synthetic applications. Skraup, Friedlander, Pfintzinger Bischler-Napieralski and Pictet syntheses. Heterocycles with 5 or 6 members and two or three heteroatoms: Syntheses and reactivity of **o**xazoles, thiazoles, oxadiazoles, thiadiazoles, benzothiazoles, benzothiadiazoles, triazole, benzotriazole, pyrimidines, pyrazines, quinoxalines and triazines.

Course Outcomes

Upon successful completion of the course, the students will be able to

CO1: Comprehend the molecular structure of heterocyclic compounds.

CO2: Pick the appropriate methods for the preparation of heterocyclic compounds.

CO3: Acquire skills to predict the outcomes of interactions of heterocyclic compounds.

CO4: Learn about the applications of the most important as well as less common heterocycles.

Books and References

1. Heterocyclic Chemistry by Gilchrist, T. L., Pearson Education, India.
2. Heterocyclic Chemistry by Joule, J. A. and Mills, K., Wiley-Blackwell.
3. Handbook of Heterocyclic Chemistry by Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin, V. V., Elsevier.
4. Principles, Three- and Four-Membered Heterocycles by Gupta, R. R., Kumar, M. and Gupta, V., Springer.
5. Heterocyclic chemistry, Vol. II: Five-Membered Heterocycles by Gupta, R. R., Kumar, M. and Gupta, V., Springer.
6. Heterocyclic Chemistry by Sainsbury, M., Wiley.

Course Name: **Polymer and Polymer Composites**
Course Code: **CY-881**
Course Type: **Open Elective**

Contact Hours/Week**: 04 L** Course Credits: **04**

Course Objectives

- To introduce the basics of polymer and composites
- To enable the students to understand the structure- property relationship of polymers
- To discuss the characterization of polymers by molecular weight
- To make the students aware with the properties and manufacturing of various polymer matrix composites

Course Content

Basic concepts (classification, nomenclature, molecular weight and distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationship), Methods of determination of molecular weight, distribution, size and shape of macromolecules, Mark-Houwink relationship, Thermodynamics of polymer solutions, Rubber elasticity concepts, thermodynamic equation of state, theories, Polymerization Techniques - bulk, solution, emulsion- description of the process, progress of polymerization, rate of polymerization, degree of polymerization, suspension, living radical polymerization technique. Mechanical properties of polymers and methods of determination, selected commercial polymers and applications Introduction to composite materials, comparison of different materials with composites - advantages and disadvantages, Principles of composite reinforcement, Effect of fibrous reinforcement on composite strength, Types of reinforcement such as natural, glasses, carbon/graphite, aramid fibers, high strength and high modulus fibers, Surface treatment and various forms of fibers. Processing and production techniques like hand-layup, bag moulding, filament winding, pultrusion, Prepegs, their manufacture and characterization, Sheet moulding and dough moulding compounds and their processing, resin transfer mouldings. Role of polymers/composites for high-tech areas such as light emitting diode, OSR in satellite communication, photovoltaic etc, High temperature polymers such as polyimides, polyetherimides, PEEK, silicone etc, their preparations, properties & applications, Liquid Crystalline, polymers - their synthesis and properties of such polymers and applications, self reinforced composites, Concept of nanofillers and polymer nanocomposites. High energy absorbing polymer, Super absorbent polymers - their synthesis, properties and applications' Polymers, for biomedical applications.

Course Outcomes

Upon successful completion of the course, students will be able to -

CO1: Develop knowledge in polymerization techniques
CO2: Determine the molecular weight of the polymer
CO3: Understanding about various structure of polymers and their effect on different properties of polymers.
CO4: Identify the application of a specific polymer/composites in a particular field

Books and References

1. Introduction to Physical Polymer Science by L. H. Sperling, Wiley Interscience, New York.
2. Principles of Polymerization by G. Odian, Wiley Interscience. New York.
3. Principles of Polymer Chemistry by P. J. Flory, Cornell University Press, Ithaca.
4. Textbook of Polymer Science by F. W. Billmeyer, John Wiley, London.
5. Polymer Science by Gowariker et al, Wiley Eastern, New Delhi.
6. Hand Book of Fibre glass and Advanced Plastic Composites by G. Lubin.
7. Polymer Science and Technology by J. R. Fried, Pearson Prentice Hall
8. Nanocomposite Science and Technology by Pulickel M. Ajayan, Linda S. Schadler, Paul V. Braun, Wiley.

Course Name: **Nanomaterials** Course Code: **CY-882** Course Type: **Open Elective**
Contact Hours/Week**: 04 L** Course Credits: **04**
Course Objectives • To introduce the students about the nanomaterials and their importance in technology. • To demonstrate the top down and bottom up synthesis approaches and their applications. • To impart knowledge about the various spectroscopic and miscroscopic techniques for characterizing nanomaterials.
Course Content
Introduction to nanoscale materials: The nano-length scale, quantum confinement effect, consequences of quantum confinement of electrons, conceptual development of band theory – from molecules to clusters/quantum dots to macroscopic crystals, material dependence of nanoscale and quantum size-effect, consequences of carrier confinement in semiconductors and metals. Structure of nanomaterials: Crystalline and amorphous nanomaterials, nanocrystals, surface energy and crystal facets, equilibrium shape of nanocrystals, surface energy as a function of surface curvature, chemical potential and solubility as a function of surface curvature and particle size, Ostwald ripening, nucleation and growth of nanoparticles. Synthesis and applications of nanomaterials: Concepts of top-down and bottom-up approaches, chemical, aerogel, aerosol, spray-pyrolysis, microemulsion, solvothermal, sonochemical, and microwave methods of synthesis. Reactivity studies by adsorption–SO_2, CO_2, H_2S, CCl_4 and chemical warfare agents, destructive adsorption, detoxification by adsorption, air purification, desulphurization, biocidal applications, modification of nanocrystalline metal oxides and their applications. Characterisation of nanomaterials: Surface area measurement, determination of size and texture, composition and elemental analysis.Electron probe methods (Scanning Electron Microscopy, Transmission Electron Microscopy); Scanning probe microscopy methods (Atomic Force Microscopy and Scanning Tunneling Microscopy.
Course Outcomes Upon successful completion of the course, students will be able to CO1: Understand the concept of nanoscience/nanomaterials and its role in nanotechnology. CO2: Explore the various nanostructures, methods of preparation and their applications in various fields. CO3: Understand various chemical and physical properties of materials at nanoscle.
Books and References 1. Nanoscale Materials in Chemistry by Klabunde, K.J. (Ed.), WileyInterscience, New York. 2. Nanoparticles: From Theory to Application by Schmid,G. (Ed.), WileyVCH,Weinheim. 3. Nanostructures and Nanomaterials: Synthesis, Properties and Applications by Cao, G. and Wang, Y., World Scientific. 4. The Chemistry of Nanomaterials: Synthesis, Properties and Applications by Rao, C.N.R., Müller, A. and Cheetham, A.K., Vol. 1 and 2, Wiley-VCH Verlag, Weinheim.