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. in Chemistry

Sr.	Course No.	Subject	Teaching Schedule		Hours	Credits	
No			L	Т	Р	/week	
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	Indian Knowledge System	2	0	0	2	2
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
		18	0	10	28	23	

SEMESTER-I

SEMESTER-II

Sr.	Course No.	Subject	Teaching Schedule		Hours	Credits	
No				-		/week	
			L	Т	Р		
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
		20	0	10	30	25	

SEMESTER-III

Sr.	Course No.	Subject	Teach	Teaching Schedule		Hours	Credits
No			L	Т	Р	/week	
1	CY-631	Organometallics	4	0	0	4	4
2	CY-632	Interpretative Molecular	4	0	0	4	4
		Spectroscopy					
3	CY-633	Solid State & Materials Chemistry	4	0	0	4	4
4	CY-7MN	Programme Elective-II*	4	0	0	4	4
5	CY-796	Summer Internship/Industrial	0	0	0	0	1
		Training [#]					
6	CY-798	MSc Dissertation	-	-	-	-	8
	Total		16	0	0	16	25

[#]Summer Internship/Industrial Training will be undertaken by the students just after second semester during summer vacation and its evaluation will be done in third semester

Sr.	Course No.	Subject	Teaching Schedule		Hours	Credit	
No			L	Т	Р	/week	
1	CY-7MN	Programme Elective-III*	4	0	0	4	4
2	CY-7MN	Programme Elective-IV*	4	0	0	4	4
3	CY-70N	Institute Elective**	4	0	0	4	4
4	CY-797	Community Connect***	0	0	0	0	1
5	CY-800	MSc Dissertation	-	-	-	-	10
		12	0	0	12	23	

SEMESTER-IV

*Programme Elective-I-IV: Any course listed in Annexure I (List of Electives)

**Institute Elective: Any course listed in Annexure II (List of Open/Institute Electives)

Total Programme Core Credit = 56; Total Programme Elective Course Credit = 16; Total Institute Elective Course Credit = 04, Industrial Training,/Summer Internship =1, Community Connect =1, Dissertation Credit =18

Total Credit of the Programme = 23+25+25+23=96

Types of Courses and credits in each Semester

Types of Courses	1st	2nd	3rd	4th	Total Credits
PC	23	25	8	0	56
PE	0	0	8	8	16
OE/IE	0	0	0	4	04
SI/IT	0	0	1	1	02
Dissertation	0	0	8	10	18
	96				



ANNEXURE-I List of Programme Electives

Sr.	Course No.	Subject
No		
1	CY-711	Polymer Chemistry
2	CY-712	Natural Products and Medicinal Chemistry
3	CY-713	Bioinorganic Chemistry
4	CY-714	Advanced Physical Chemistry
5	CY-715	Supramolecular Chemistry
6	CY-716	Computational Chemistry
7	CY-717	Biochemistry
8	CY-718	Biomolecular Spectroscopy
9	CY-719	Green Chemistry
10	CY-720	Heterocyclic Chemistry
11	CY-721	Catalysis

ANNEXURE-II List of Open/Institute Electives

Sr. No	Course No.	Subject
1	CY- 701	Polymer and Composites
2	CY- 702	Nanomaterials

Course Name:	Inorganic Chemistry-
Course Code:	CY-611
Course Type:	Programme Core
Contact Hour	s/Week: 4 L

Course Credits: 04

Course Objectives

- To make the students conversant with bonding theories of coordination complexes.
- To impart knowledge on 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 Bonding VSEPR, 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 favor 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

- 1. Inorganic Chemistry: Principles of Structure and Reactivity by Huheey, James E., Harper Collins College Publishers.
- 2. Chemistry of the Elements by Greenwood, N.N. and Earnshaw, A., Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
- 3. Principles of Instrumental Analysis by Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A, Saunders GoldenSunburst Series.

- 1. Advanced Inorganic Chemistry by Cotton, F.A., Murillo, C.A.; Bochmann, M., Wilkinson, G., John Wiley & Sons.
- 2. Inorganic Electronic Spectroscopy by Lever, A.B.P, Elsevier Science Publishers B.V.
- 3. Inorganic Chemistry by Shriver, D.F.; Atkins, P.W., Oxford University Press.
- 4. Physical Methods for Chemists by Drago, Russell S, Saunders College Publishing.
- 5. Analytical Chemistry by Christian, G. D, John Wiley & Sons, Inc.
- 6. Instrumental Methods of Analysis by Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A., Wadsworth Publishing

Course Name:Organic Chemistry-ICourse Code:CY-612Course Type:Programme CoreContact Hours/Week:4L

Course Credits: 04

Course Objectives

- 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 applications in organic chemistry.

Course Content

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes. Arynes: Generation and reactivity of arynes, nucleophilic aromatic substitution reactions, SNAr mechanism; Ipso effect. Huckel's rule. Energy level of π M.O., Annulenes, anti-aromaticity, aromaticity, homoaromaticity.

Reaction Mechanism, Reaction coordinate diagram, Kinetic and thermodynamics control, Hammond's postulate, transition states and intermediates, Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship (LFER), substituent and reaction constants, Taft equation. Method of determining mechanisms, isotope effects.

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; Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

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

1. A Guide Book to Mechanism in Organic Chemistry by Sykes, Peter, Longman.

- 2. Organic Reactions and their Mechanisms by Kalsi, P.S., New Age International Publishers.
- 3. Stereochemistry of Organic Compounds by Kalsi, P.S., New Age International Publishers.
- 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. Stereochemistry of organic compounds: Principles and Applications bY D. Nasipuri.
- 4. Stereochemistry of organic compounds by Ernest L. Eliel.
- 5. Modern Physical Organic Chemistry by Eric. V. Anslyn and D. A Dougherty.

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

- 1. Quantum Chemistry by Levine, I. N., PHI Learning Pvt. Ltd., Delhi.
- 2. Chemical Applications of Group Theory by Cotton, F. A., Wiley Eastern.

- 1. Quantum Chemistry by McQuarrie, D. A, Reprint, Viva Books.
- 2. Molecular Quantum Mechanics by Atkins, P., Oxford University Press

Course Name:	Molecular Spectroscopy
Course Code:	CY-614
Course Type:	Core
Contact Hou	rs/Week· AI

- To enable students to learn molecular spectroscopy as an important tool to interpret molecular structures.
- 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 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. Electronic 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, de-excitaion by fluorescence, 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, ESR Spectroscopy: Principle of ESR and interpretation of ESR spectra of -CH₃ and -CH₂ radicals, Mössbauer Spectroscopy: Principle and applications

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 the structure of compounds.
- 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

- 1. Fundamentals of Molecular Spectroscopy by Banwell, C.N. and McCash, E.L.M., McGraw-Hill, N. Y.
- 2. Molecular Spectroscopy by Graybeal, J.D., McGraw-Hill.

- 1. Principles of Magnetic Resonance by Slichter, C.P., Springer Verlag.
- 2. Physical Chemistry by Atkins, P. and Paula, J.de, Oxford Univ. Press.

Course Name: Indian Knowledge System Course Code: CY-615 Course Type: Core

Contact Hours/Week: 2L

Course Credits: 02

Course Objectives

- To create awareness among the students about the history and culture of our land.
- Ushering new areas of research in the field of Indian knowledge system.
- To explore the scientific and rational facets of traditional Indian knowledge.

Course Content

Bhāratīya Civilization and Philosophy: Genesis of the land, Antiquity of civilization, Traditional Knowledge System, The Vedas, Main Schools of Indian Philosophy, Ancient Education System: Takṣaśilā University and Nālandā University, Knowledge Export from Bhārata. Science, Astronomy, and Mathematics: Concept of Matter, Life and Universe, Gravity, Velocity of Light, Aeronautics, Vedic Cosmology and Modern Concepts, Sun, Earth, Moon, and Eclipses, Concepts of Zero and Pi, Number System, Vedic Mathematics. Engineering, Technology, and Architecture: Pre-Harappan and Sindhu Valley Civilization, Juices, Dyes, Paints and Cements, Glass and Pottery, Metallurgy, Engineering and Technology in Vedic and Post-Vedic ages, Marine Technology. Life, Environment, and Health: Life Science in Plants, Anatomy, Physiology, Agriculture, Ecology and Environment, Äyurveda, Integrated Approach to Healthcare, Medicine, Microbiology, Surgery, and Yoga.

Course Outcomes

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

CO1: Promote the youths to explore the various fields of research associated with Indian knowledge system.

- CO2: Relate the ancient Indian education to the various aspects of the modern scientific approach.
- CO3: Add career, professional and business opportunities in this field.

Books

1. Histrory of Science in India Volume-1, Part-I, Part-II, Volume VIII, by Sibaji Raha, et al. National Academy of Sciences, India and The Ramkrishan Mission Institute of Culture, Kolkata (2014).

2. Pride of India- A Glimpse of India's Scientific Heritage edited by Pradeep Kohle et al. Samskrit Bharati (2006).

3. Textbook on The Knowledge System of Bhārata by Bhag Chand Chauhan

References

1. Vedic Physics by Keshav Dev Verma, Motilal Banarsidass Publishers (2012).

2. India's Glorious Scientific Tradition by Suresh Soni, Ocean Books Pvt. Ltd. (2010).

Course Name: Inorganic Lab-I Course Code: CY-616 Course Type: Programme Core (Lab) 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 impart knowledge of colorimetry and estimation of ions present in the mixture solution
- To provide hand on practice of various separation techniques.

List of Experiments

- 1. Analysis of calcium and magnesium ions using EDTA.
- 2. Gravimetric Estimation of silver and zinc in the given solution of complex.
- 3. Gravimetric Estimation of copper and zinc in the given solution of complex.
- 4. Gravimetric Estimation of copper and silver in the given solution of complex.
- 5. Colorimetric estimation of Fe(II) ions by thiocyanate.
- 6. Estimation of Cu(II) ions in a given solution colorimetrically
- 7. Simultaneous determination of Cr and Mn in a given mixture colorometrically.
- 8. To extract iodine by solvent extraction and also quantify the extracted iodine.

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

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: Colorimetric estimation of various ions.
- CO4: Develop understanding of solvent extraction technique.

Course Name: Organic Lab-I Course Code: CY-617 Course Type: Programme Core (Lab) Contact Hours/Week: 4P

Course Credits: 02

Course Objectives

- To provide skills for separation and purification of organic compounds from mixture.
- To provide skills for identification of organic compounds based on qualitative analysis and spectroscopic methods.
- To extend student's comprehension and skill development in synthetic organic chemistry.

List of Experiments

- 1. Qualitative analysis of mixtures of two solid organic compounds (3-4 such samples): Separation of the components and identification of compounds through various qualitative tests and spectroscopic tools.
- 2. Separation of mixture of organic compounds using TLC and column chromatography.
- 3. Synthesis of hydroxynaphthaldehyde from β -naphthol and characterization of the product using FTIR.
- 4. Two-step synthesis of benzilic acid from benzoin via benzil and characterization of the final product using FTIR.

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

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 spectroscopic tools
- CO3: Execute various organic reactions safely and effectively for synthetic applications.

Course Name: **Physical Lab-I** Course Code: **CY-618** Course Type: **Programme Core (Lab)** Contact Hours/Week: **2P**

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, titrations, 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 the critical micelle concentration of a soap by surface tension method.
- 3. Verification of lambert beer's law for KMnO₄ under different experimental conditions.
- 4. To find composition of Ferric ions-salicylic acid complex by Job's method.
- 5. To determine the dissociation constant of phenolphthalein colorimetrically.
- 6. To compare the strengths of two acids by studying acid-catalyzed hydrolysis of an ester.
- 7. To study the kinetics of hydrolysis of ethyl acetate by NaOH.
- 8. Determine the specific reaction rate of the potassium persulphate-iodide reaction by initial rate method.
- 9. To study the kinetics of iodination of acetone in the presence of acid by initial rate method
- 10. To study the iodination of acetone using a colorimeter.

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

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: Study the kinetics of the reactions and identify the liquids based on above-mentioned parameters.

- 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 crystalfield 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 (d1 to d10) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1st row transition metal ions. 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

- 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. Shriver and Atkins Inorganic Chemistry by Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., Oxforduniversity press.

- 1. Ligand Field Theory and Its Applications by Figgis, B.N., and Hitchman, M.A, Wiley Eastern Ltd.
- 2. Inorganic Chemistry Principle of Structure & Reactivity by Huheey, J.E., Keiter, E.A., Keiter, R.L., Pearson Education.

Course Name: Organic Chemistry-II Course Code: CY-622 Course Type: Programme Core Contact Hours/Week: 4L

Course Credits: 04

Course Objectives

- To make students familiar with the concepts and applications in concerted organic reactions 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

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 addition 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. Ene reaction. Photochemistry: Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1, 3-, 1, 4and 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 prismanesin isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loefller-Freytag reaction.

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 reactions.
- CO2: Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions.

CO3: Discuss important photochemical reactions with organic compounds.

CO4: Outline the main mechanistic aspects for the photochemical transformations.

Books

- 1. Pericyclic Reactions by Fleming, I., Oxford Science Publications.
- 2. Pericyclic Reactions by Marchand, A.P. & Lehr, R.E., Academic Press.
- 3. Organic Photochemistry by Coxon and Halton.

- 1. Advanced Organic Chemistry: Reactions, Mechanism and Structure by March Jerry, John Wiley.
- 2. Organic Chemistry by Morrison, R.T., Boyd, R.N, Prentice Hall.
- 3. Aspects of Organic Photochemistry by Horspool, W.M. Academic Press.

Course Name: Physical Chemistry-II Course Code: CY-623 Course Type: Programme Core Contact Hours/Week: 4L

Course Credits: 04

Course Objectives

- To highlight the concept of equilibrium in chemical reactions and their detailed qualitative along with 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 ΔG° , Le Chatelier's principle. Relationships between K_{p} , K_{c} and K_{x} for reactions involving ideal gases. Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, 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. 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

- 1. Physical Chemistry by Castellan, G.W., Narosa.
- 2. Physical Chemistr by Barrow, G.M., Tata McGraw Hill.

- 1. Electroanalytical Chemistry: Theory and Applications by Sane, R.T. and Joshi, A.P., Quest Publications.
- 2. Priniciples of Electrochemistry by Koryta, J., Dvorak, J., Kavan, L, John Wiley and Sons, New York.
- 3. Electrochemical Methods-Fundamentals and Applications by Bard, A.J. and Faulkner, L.R., John Wiley.

Course Name:Organic Synthetic MethodologyCourse Code:CY-624Course Type:Programme CoreContact 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 offunctional 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: Beckmann rearrangement, Arndt-Eistert reaction, Favorskii rearrangement, 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, important strategies of retrosynthesis, Linear and convergent synthesis, reversal of polarity (umpolung), enzymatic catalysts.

Course Outcomes

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

- CO1: Identify suitable reagents and methodologies for single 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 andbiologically important molecules.

Books

- 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, New Central Book Agency.
- 3. Fundamentals of Organic Synthesis The retrosynthetic analysis by R. K. Kar, New Central Book Agency.

- 1. Advanced Organic Chemistry, Part B: Reactions and Synthesis by Carey, F. A. and Sundberg, R. J., Springer.
- 2. Organic Synthesis by Smith, M.B., Academic Press

Course Name: Inorganic Lab-II Course Code: CY-625 Course Type: Programme Core (Lab)

Contact Hours/Week: 4P

Course Objectives

- To develop experimental skills of synthetic inorganic chemistry.
- To prepare different coordination complexes.
- To impart knowledge of substitution reactions in metal complexes
- Characterization of complexes by spectroscopic techniques

List of Experiments

1. To prepare pure and dry sample of Chloropentaammine cobalt(III) Chloride and its IR measurements.

Course Credits: 02

- 2. Preparation of cis- and trans-[Co(en)₂Cl₂]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 (CH₃COO)₄(H₂O)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.
- 7. Preparation of Tris(thiourea) cuprous(I) sulphate [Cu(tu)₃]₂SO₄.2H₂O (Where tu stands for thiourea) and its physicochemical characterization including IR Study.
- 8. Energy optimization, depiction of HOMO-LUMO, energy calculations of transition metal complexes and correlation with spectroscopic data using computational tools.

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

Course Outcomes

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

- CO1: Understand synthetic methods of inorganic chemistry.
- CO2: Prepare and characterize various complexes and analyze the samples thoroughly.
- CO3: Develop in-depth understanding of substitution reactions.
- CO4: Characterize the synthesized coordination compounds by spectroscopic techniques.

Course Name: **Physical Lab-II** Course Code: **CY-626** Course Type: **Programme Core (Lab)** Contact Hours/Week: **4P**

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.
- To demonstrate the use of different techniques to monitor reaction kinetics.

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. Conductometric measurement of degree of hydrolysis of a salt.
- 3. Conductometric titration of a weak acid with strong base.
- 4. Conductometric titration of mixture of strong and weak acid with strong base.
- 5. Potentiometric titration of polyprotic acids with strong base.
- 6. Potentiometric titration of mixture of strong and weak acid with strong base.
- 7. Determination of the specific and molecular rotation of fructose at different concentrations and toobtain the value of intrinsic rotation for fructose.
- 8. To study the kinetics of inversion of cane sugar by optical rotation measurement.
- 9. To study the kinetics of saponification of ethyl acetate by NaOH conductometrically.

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

Course Outcomes

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

CO1: Operate potentiometers, polarimeter, and conductivity meters.

CO2: Measure reaction rate constant for reactions.

Course Name: **Organic Lab-II** Course Code: **CY-627** <u>Course Type: **Programme Core (Lab)**</u> Contact Hours/Week: **2P**

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 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.

List of Experiments

- 1. Synthesis of Adipic acid from cyclohexanol (oxidation).
- 2. Synthesis of p- Iodonitrobenzene from p-nitroaniline (diazotization & substitution).
- 3. Synthesis of N- Bromo succinimide (Bromination).
- 4. Synthesis of Dibenzal acetone from benzaldehyde (Claisen-Schmidt reaction).
- 5. Synthesis of Cinnamic acid from benzaldehyde (Knoevenaegal reaction).
- 6. Synthesis of Benzanilide (Schotten-Baumann reaction).
- 7. Synthesis of o-Benzoylbenzoic acid (Friedel Craft's reaction).
- 8. Synthesis of Benzyl alcohol and benzoic acid from benzaldehyde (Cannizzaro's reaction).
- 9. Synthesis of Trinitrophenol (picric acid) from phenol (nitration).
- 10. Synthesis of Benzanilide from benzophenone through benzophenone oxime (Beckmann Rearrangement)
- 11. Synthesis of Norbornene-5,6-dicarboxylic anhydride from cyclo-pentadiene and maleic anhydride (Diels-Alder reaction).
- 12. Energy optimization of organic molecules and depiction of HOMO-LUMO structure and their energy calculations and correlation with spectroscopic data using computational tools

Note: The concerned course coordinator will prepare the actual list of experiments/problems at the start of semester based on above generic list

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

CO4: Separate and purify the products after the reaction to plan and implement the scheme for multi-step organic synthesis.

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. Transition metal complexes with carbones 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, σ -bonded organotransition metal transition metal complexes and their reactivity, bimetallic and cluster complexes. Mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands. Main group organometallics: Carboranes, metalloboranes and metallocarboranes; Synthetic applications of organoboranes, Applications of organosilicon compounds in organic synthesis. Applications of organometallics 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 organometallics.
- CO2: Demonstrate the applications of organometallic compounds in synthetic organic reactions.
- CO3: Apply organometallics and clusters as catalysts in various chemical reactions highly usefulin industry.

Books

- 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. Basic Organometallic Chemistry by Gupta, B.D. and Elias A.J., University Press (India) Pvt. Ltd.

- 1. Organotransition Chemistry by Hill, A.F., The Royal Society of Chemistry, Cambridge.
- 2. Oxford Premier Series on Organometallics by Bochmann, M. (Ed.), Vol. 1 and 2, Oxford Press.
- 3. Modern Methods of Organic Synthesis by Carruthers, W. Cambridge University Press.

Course Name:Interpretative Molecular SpectroscopyCourse Code:CY-632Course Type:Programme CoreContact Hours/Week:4L

Course Objectives

- To provide fundamental and practical aspects about applications of molecular spectroscopy.
- To solve and confirm the structure of small organic molecules using spectroscopic and spectrometric tools.
- Major emphases will be on optical spectroscopy (UV-Visible, FT-IR) associated with the electronic/molecular transition processes and their stereochemistry, mass spectral studies and nuclear magnetic resonance (NMR) associated with structure and dynamics.

Course Content

Electronic spectroscopy: Introduction to plane and circularly polarized light, Application of Electronic spectroscopy in organic molecules, Solvent effect, cotton effect and octant rule. Infrared spectroscopy: Introduction for organic molecules, factors influencing vibrational frequencies, analysis of spectra of compounds with various functional groups and identity by finger printing. Mass spectrometry: Basic principles, hard and soft ionization techniques (mass analyzer in ESI-MS and MALDI-MS, high resolution MS), isotope abundance, fragmentation processes of organic molecules, Fragmentation associated with functional groups. Nuclear magnetic resonance: Introduction, chemical shift δ , inductive and anisotropic effects on δ , chemical structure correlations of δ , Effect of magnetic field strength on sensitivity and resolution, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant *J*, first order and second order spectru (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, relaxation processes, NOE effects, DEPT, determination of number of attached hydrogens, ¹H and ¹³C chemical shifts to structure correlations, Multinuclear NMR (COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY). 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: Analyze 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: Solve the structure of unknown organic compounds using a combination of spectroscopic techniques (including UV-vis, mass spectrometry, infrared spectrometry, 1D and 2D proton and carbon NMR spectroscopy)

Books

- 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.

References

1. Spectroscopic Methods in Organic Chemistry by Williams, D. and Fleming, I., McGrawHill Education (India) Private Limited.

Course Name: Solid State and Materials Chemistry Course Code: CY-633 Course Type: Programme Core Contact Hours/Week: 04 L

Course Credits: 04

Course Objectives

- To introduce the fundamentals of solid state, nanomaterials 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

Materials Chemistry: Basics of nanomaterials, Top-down and bottom-up synthesis approaches, Spectroscopic and microscopic characterizations techniques, Size-shape dependent properties, Applications. Symmetry in the crystalline state, X-Ray diffraction: Crystal planes and directions, Crystal symmetry, Lattice planes and Miller Indices, 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. 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/chemical properties along with applications in various fields.
- CO3: Understand the role of colloids and surface chemistry in various physical and chemical processes along with their practical applications

Books

- 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.

- 1. Fundamentals of Interface and Colloid Science by Lyklema, J., Academic Press San Diego.
- 2. Physical Chemistry of Surfaces by Adamson, A.W., John Wiley and Sons, New York.
- 3. Nanotechnology by WM Breck CBS Publishers & Distributors Pvt. Ltd.

- To introduce about polymers and composites
- To enable the students to understand the structure- property relationship of polymers
- To enable the students to understand the methods of molecular weight determination
- To make the students aware with the properties and manufacturing of various polymer matrixcomposites

Course Content

Basic concepts (classification, nomenclature, glass transition temperature, 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, Polymerization Techniques - bulk, solution, emulsion, suspension, progress of polymerization, rate of polymerization, degree of polymerization, living radical polymerization technique, Polymer molding techniques: Extrusion, Compression molding, Injection molding, 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, Effect of fibrous reinforcement on composite strength, Types of reinforcement such as natural, glasses, carbon/graphite, aramid fibers, high strength and high modulus fibers, Processing and production techniques like, Hand-layup, Spray-layup, Compression molding, bag moulding, pultrusion, Prepegs, dough molding, sheet molding, resin transfer molding, their manufacture and characterization, 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 properties 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: Understand about structures of polymers and their effect on different properties of polymers.
- CO4: Identify the application of a specific polymer/composites in a particular field

Books

- 1. Introduction to Physical Polymer Science by L. H. Sperling, Wiley Interscience, New York.
- 2. Textbook of Polymer Science by F. W. Billmeyer, John Wiley, London.
- 3. Polymer Science by Gowariker et al, Wiley Eastern, New Delhi.

- 1. Principles of Polymerization by G. Odian, Wiley Interscience. New York.
- 2. Principles of Polymer Chemistry by P. J. Flory, Cornell University Press, Ithaca.
- 3. Hand Book of Fibre glass and Advanced Plastic Composites by G. Lubin.
- 4. Polymer Science and Technology by J. R. Fried, Pearson Prentice Hall
- 5. Nanocomposite Science and Technology by Pulickel M. Ajayan, Linda S. Schadler, Paul V. Braun, Wiley.

- 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–SO₂, CO₂, H₂S, CCl₄ and chemical warfare agents, destructive adsorption, detoxification by adsorption, air purification, desulphurization, biocidal applications, modification of nanocrystalline metal oxides and their applications. Characterization 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

- 1. Nanoscale Materials in Chemistry by Klabunde, K.J. (Ed.), Wiley Interscience, 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.

- 1. Nanotechnology by WM Breck CBS Publishers & Distributors Pvt. Ltd.
- 2. 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.

- To provide 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.
- To impart knowledge on molecular weight determination of polymers and an overview of mechanical and rheological properties of polymers.

Course Content

Introduction to Polymers: An introduction to the history, recent developments, applications and processing of polymers, Classification of polymers, Nomenclature, Types of polymerization, morphology, degree of polymerization, glass transition temperature, factors influencing glass transition temperature and melting, molecular weight and distribution, 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-growthpolymerization and their kinetics such as - polyesters, polycarbonates, polyamides, polyimides, epoxy, phenolic resins, 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. Polymerization techniques such as - bulk, solution, suspension and emulsion polymerization, Cationic and anionic polymerization, Copolymerization, reactivity ratios, composition of copolymers, blocks and graft copolymers, Complex catalyst polymerization & mechanism. ATRP and Ring opening metathesis polymerization, Conducting polymers, Smart polymers.

Course Outcomes

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

- CO1: Understand different aspects of polymer chemistry.
- CO2: Choose a contemporary method of polymer synthesis.
- CO3: Determine the molecular weight of the polymer
- CO4: Learn about the applications of conducting and smart polymers.

Books

- 1. Principles of polymerization by George Odian, Wiley.
- 2. Polymer Chemistry by Seymour/Carraher's, Marcel Dekker, Inc.

- 1. Polymer Chemistry by P. C. Heimenz, T. P. Lodge, CRC press.
- 2. The synthesis, characterization, reactions and applications of polymers by Comprehensive Polymer Science, Pergamonpress.

Course Name:Natural Products and Medicinal ChemistryCourse Code:CY-712Course Type:Programme ElectiveContact Hours/Week:4L

Course Credits: 04

Course Objectives

- To provide fundamental understanding of chemistry of natural products and their structures, classification, occurrence, biosynthetic pathways and secondary metabolites.
- To impart knowledge on the laboratory synthetic routes and pharmacological properties of selected natural products.
- To make the students conversant with the general structural features, physicochemical properties and mechanism of action of different classes of drugs.
- To make student understand structure-activity relationship of different drug molecules in order to design better one.

Course Content

Natural Products: Terpenes and Steroids: Introduction, Classification, Isoprene rule, determination of structure of terpenoids and steroids, biosynthesis of mono-, sesqui-, di- and tri-terpenoids and steroids. (Conversion of acetylCoA to Mevalonic acid, to squalene, to lanosterol, lanosterol to Cholesterol, Cholesterol to hormones), diosgenin and its utility in commercial hormone synthesis. General chemistry and total synthesis Cholesterol. Alkaloids: Introduction, nomenclature and classification, Isolation and structure elucidation of alkaloids, Total synthesis of morphine. Flavonoids and related polyphenols: Introduction, classification and uses & application. 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, 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, detail chemistry, biosynthesis and properties.
- CO2: Investigate plant material as natural products and their further applications as starting materials for medicines used for the treatment of cancer, cardiovascular diseases, bacterial and fungal infections etc.
- 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

- 1. Natural Products by O. P. Agrawal.
- 2. Organic Chemistry Vol. II by Finar, I.L. & Finar, A.L. Addison-Wesley.
- 3. Introduction to Medicinal Chemistry by Patrick, G.L., Oxford University Press.

- 1. Organic Chemistry Vol.1 by Finar, I.L. Longman.
- 2. Principles of Medicinal Chemistry by Lemke, T.L. & William, D.A., Foye's, USA.

Course Name:Bioinorganic ChemistryCourse Code:CY-713Course Type:Programme ElectiveContact 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 specificapplications 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 and role of copper, zinc and iron therein.

Course Outcomes

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

- CO1: Identify the typical role of different metal ions in biological processes.
- CO2: Understand the involvement of metal ions in structural, recognition, and redox/non-redox catalytic activities of various metalloenzymes.
- CO3: 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.
- CO4: Understand metal-ion mediated post-translational modifications on proteins, DNA cleavage and associated toxicity.

Books

- 1. Bioinorganic Chemistry by Bertini, I., Gray, H.B. Lippard, S.J. and Valentine, J.S, University Science Book.
- 2. Principles of Bioinorganic Chemistry by Lippard, S.J. and Berg, J., University Science Books, U.S.A.

- 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. Special Collection Articles on Bioinorganic Chemistry, Chemical Reviews, Vol. 96 (1996) 2237-3042.
- 4. Selected Articles on Bioinorganic Chemistry Chemical Reviews, Vol. 104 (2004) 3705-4242.

Course Name: Advanced Physical Chemistry Course Code: CY-714 Course Type: Programme Elective Contact Hours/Week: 4L

Course Objectives

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

Course Content

Advanced chemical kinetics: Kinetics of simple and complex reactions, theories of unimolecular reactions, Potential energy surfaces. Kinetic theory of collisions. Transition state theory. Reaction cross-sections, rate coefficients, reaction probabilities. Catalysis-Enzyme catalysis and homogeneous catalysis. Salt effect, 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. Photochemical reactions. Ultrafast reactions 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 theoryof 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.

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: Understand and define various parameters in chemical reactions.
- CO4: Solve problems in chemical kinetics and statistical thermodynamics.

Books and References

- 1. Chemical Kinetics by Laidler, K. J., Prentice Hall.
- 2. Chemical Kinetics and Reaction Dynamics by Houst McGraw, P. L., Hill Higher Education.
- 3. Physical Chemistry by Atkins, P. and Paula, J. De, Oxford University Press.

- 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. Chemical Kinetics and Dynamics by Steinfeld, J. I., Francisco, J. S. and Sase, W. L. J. S. Prentice Hall.

- 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 host-guest 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-complementaryspecies 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 iondipole 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

1. Supramolecular Chemistry by Steed, J.W. and Aswood, J.L., Wiley.

2. Introduction to Supramolecular Chemistry by Dodziuk, H., Springer.

References

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:Computational ChemistryCourse Code:CY-716Course Type:Programme ElectiveContact 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, Semiempirical and quantum chemical methods for calculation of different molecular properties.
- To make the students conversant with the simulation methods.

Course Content

Potential Energy Surfaces: Introduction, Potential Energy Surfaces and Geometry, Potential Energy Surfaces and Thermodynamics, Potential Energy Surfaces and Kinetics, Thermodynamic vs. Kinetic Control of Chemical Reactions, Potential Energy Surfaces and Mechanism etc. Molecular Mechanics, Quantum Chemical Models and Graphical Models: Introduction to MM, SYBYL and MMFF Force Fields, Limitations of Molecular Mechanics Models, Schrödinger Equation, Born-Oppenheimer Approximation, Hartree-Fock Approximation, LCAO Approximation. Gaussian Basis Sets, STO-3G Minimal Basis Set, 3-21G, 6-31G and 6-311G Split-Valence Basis Sets, 42 6-31G*, 6-31G**, 6-311G* and 6-311G** Polarization Basis Sets, 43 3-21G(*) Basis Set etc. Semi-Empirical Models, Molecules in Solution, Cramer/Truhlar Models for Aqueous Solvation. Application of MM and QM model. Introduction to graphical Model: Molecular Orbitals, Electron Density, Spin Density, Electrostatic Potential, Polarization Potential, Local Ionization Potential, Property Maps, Electrostatic Potential Map, LUMO Map, Local Ionization Potential Map, Spin Density Map, Animations, Choice of Quantum Chemical Model. Applications of Graphical Model. Case studies: i) Stabilizing "Unstable" Molecules: Introduction, Favoring Dewar Benzene, Making Stable Carbonyl Hydrates, Stabilizing a Carbene: Sterics vs. Aromaticity, Favoring a Singlet or a Triplet Carbene ii) Kinetically-Controlled Reactions: Introduction, Thermodynamic vs. Kinetic Control, Rationalizing Product Distributions, Anticipating Product Distributions, Altering Product Distributions, Improving Product Selectivity etc.

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

- 1. Introduction to Computational Chemistry by Jensen, F., John Wiley & Sons Ltd.
- 2. Molecular Modeling: Principles and Applications by Leach, A., PrenticeHall.
- 3. Essentials of computational chemistry: Theories and models by Cramer, C.J., John Wiley & Sons.

References

1. Quantum Chemistry by Levine, I.N., PHI Learning Pvt. Ltd., Delhi.

Course Name:BiochemistryCourse Code:CY-717Course Type:Programme ElectiveContact 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, types of naturally occurring sugars, carbohydrate metabolism (glycolysis, glycogen metabolism, electron transport and oxidative phosphorylation), Classification and biological importance of fatty acids and lipids, chemical synthesis of phospholipids and glycolipids, lipid metabolism; Secondary structure of DNA and RNA, stabilizing forces, polymorphic nature of DNA, 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.

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.
- CO3: Demonstrate knowledge and understanding in enzyme kinetic behaviour and mechanisms.

Books

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.

References

1. Introduction to Protein Structure by Carl Branden and John Tooze, Garland Publishing Company.

2. Biophysical Chemistry by Cantor and Schimmel, Publisher W. H. Freeman & Co.

^{1.} Lehninger Principles of Biochemistry by David L. Nelson, W H Freeman & Co.

Course Name: **Biomolecular Spectroscopy** Course Code: **CY-718** Course Type: **Programme Elective** Contact Hours/Week: **4**L

Course Credits: 04

Course Objectives

- To introduce the fundamental concepts of biophysical techniques
- To apply spectroscopic methods for the study of structures and functions of biological macromolecules
- To demonstrate the kinetics and thermodynamics parameter of biomacromolecular interactions

Course Content

Structures of biological macromolecules (proteins and polynucleic acids). Structural transitions in biomacromolecules. Absorption spectroscopy. Fluorescence Spectroscopy: Introduction, steady-state and time resolved spectroscopy, fluorescence quenching- static and dynamic, Förster resonance energy transfer (FRET), Photoinduced electron transfer (PET), fluorescence anisotropy, Single Molecule Fluorescence Spectroscopy- Fluorescence Correlation Spectroscopy, fluorescence Stop flow and kinetics, Protein Fluorescence, Fluorescence Sensing for biological system, Application of fluorescence techniques in biomolecules. Dynamic light scattering (DLS), Circular Dichroism (CD), and Isothermal titration Calorimetry (ITC) – techniques and applications in biomacromolecular structure and interaction. Macromolecule-small molecule binding studies by using spectroscopic tools.

Course Outcomes

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

- CO1: Understand spectroscopic techniques and their application in biomolecules
- CO2: Understand photophysical processes in biological macromolecules
- CO3: Solve problems on structure of biological macromolecules by spectroscopy

Books

- 1. Fluorescence Spectroscopy, by J. R. Lakowicz, Springer.
- 2. Biophysical Chemistry by C.R. Cantor and P.R. Schimmel.

- 1. Physical Biochemistry by K.E.van Holde, C. Johnson, P. S. Ho.
- 2. Molecular Fluorescence Principles and Applications by B. Valeur, Wiley-VCH, (2002).
- 3. Protein-Ligand Interactions by S. E.Harding and B. Z. Chowdhry.

Course Name: Green Chemistry Course Code: CY-719 Course Type: Programme Elective 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., 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. Future Trends in Green Chemistry.

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 green processes and methods in real world problems.
- CO3: Implement the concept of green chemistry for sustainable future.

Books

- 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.

- 1. Real-World cases in Green Chemistry by Cann, M.C. & Connely, M.E., American Chemical Society, Washington.
- 2. Hazardous Reagent Substitution, Royal Society of Chemistry, Green Chemistry Series by Sharma, R.K. & Bandichhor, R.
- 3. Introduction to Green Chemistry by Ryan, M.A. & Tinnes, M., American Chemical Society, Washington.
- 4. 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.
- 5. Green Chemistry: An Introductory Text by Lancaster, M., RSC publishing.
- 6. Collection of Articles on Green Chemistry, Green Chem., Vol. 24 (2022)

Course Name:Heterocyclic ChemistryCourse Code:CY-720Course Type:Programme ElectiveContact Hours/Week:4L

Course Credits: 04

Course Objectives

- To familiarize the students with chemistry of heterocyclic compounds
- To impart knowledge on synthetic methods of heterocyclic compounds
- To discuss reactivity of different heterocyclic compounds along with synthetic applications

Course Content

Introduction to heterocycles: Nomenclature and aromaticity of heterocyclic molecules. Five membered hetrocycles with one heteroatom: Synthesis and reactivity of furan, pyrrole and thiophene. Synthesis and reactivity of benzofused heterocycles: indole, carbazole, benzofurans, benzothiophenes. Six membered heterocyclic compounds with one hetero atom: Synthesis and reactivity of pyridine, quinoline and isoquinoline, Comparison of reactivity with benzene and naphthalene, Preparation of pyridine salts and pyridine *N*-oxides and their synthetic applications. Five and six membered rings with two or more heteroatoms: Synthesis and reactivity of pyrazole, imidazole, triazole, oxadiazole, oxadiazoles, thiadiazoles, triazole, pyrimidines, purines, pyrazines, qunioxalines and phenothiazines. Mesoionic compounds.

Course Outcomes

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

- CO1: Comprehend the molecular structure of heterocyclic compounds.
- CO2: Pick an appropriate method for synthesis of heterocyclic compounds.
- CO3: Predict the product in the reactions involving heterocycles

Books

- 1. Heterocyclic Chemistry by Gilchrist, T. L., Pearson Education, India.
- 2. Heterocyclic Chemistry by Joule, J. A. and Mills, K., Wiley-Blackwell.
- 3. Heterocyclic chemistry, Vol. II: Five-Membered Heterocycles by Gupta, R. R., Kumar, M. and Gupta, V., Springer.

- 1. Heterocyclic Chemistry by Sainsbury, M., Wiley.
- 2. Handbook of Heterocyclic Chemistry by Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin, V. V., Elsevier.

Course Name:	Catalysis
Course Code:	CY-721
Course Type:	Programme Elective
Contact Hours/	Week AI

Course Objectives

- To familiarize the students with different types of catalysis and their mechanisms
- To impart knowledge on kinetics of surface reactions
- To discuss industrial applications of catalysis

Course Content

Course Credits: 04

Basic principles of catalysis: Introduction, types of catalysis, adsorption isotherms (Freundlich Isotherm, Langmuir adsorption isotherm, BET isotherm), chemisorption isotherms. Kinetics of surface reactions: rate determining step, various types of reactions: unimolecular surface reactions, bimolecular surface reactions, Kinetics of complex reactions-reversible reactions, side or parallel reactions and consecutive reactions. Mechanism of catalytical reactions: General considerations, reasons for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), basic concepts of catalysis (molecular activation by coordination and addition), proximity interaction (insertion/inter-ligand migration and elimination, rearrangement), hydrogenation, dehydrogenation and dehydration. Applications: Petrochemical industry - reforming and refining, environmental protection, autoexhaust catalysts. Enzyme Catalysis: Transition states and enzyme catalysis; Enzymes in chemical bio-transformations; Pre-steady state and steady state kinetics; Kinetics in industrial processes, Toxicological considerations and safety in handling enzymes; Enzyme immobilization and concept of protein and enzyme engineering, Applications of enzymes in industry and medicine. Photocatalysis- semiconductors, modifications, photocatalytic applications

Course Outcomes

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

- CO1: Comprehend the type of catalysis and its mechanism
- CO2: Understand the process of adsorption and surface reactions
- CO3: Pick suitable catalyst for an industrial process

Books

- 1. Introduction to the Principles of Heterogeneous Catalysis by J. M. Thomas and W. J. Thomas, Academic Press, (1967).
- 2. Homogeneous Transition Metal Catalysis by Christopher Masters, Springer Netherlands, 1981
- 3. Enzyme catalysis in organic synthesis, third Edition Editor(s): Karlheinz Drauz, Harald Gröger, Oliver May, Wiley-VCH Verlag GmbH & Co, 2012

- 1. Catalysis by C. Kuriacose, Macmillan India Limited, 1991.
- 2. Adsorption and Catalysis by Solids by D. K. Chakrabarty, Wiley Eastern Ltd., 1990.
- 3. Physical chemistry of solid surfaces by A. W. Adamson, Academic Press, 1995.
- 4. Petrochemical Economics, by Duncan Seddon, Catalytic Science Series, Volume 8.
- 5. Environmental Catalysis, Edited by: F J J G Janssen and R A van Santen, Catalytic Science Series, Volume 1.