Programme Name: M.Sc. (Chemistry) **Duration: 2 Years**

Programme Educational Objectives (PEOs)

1. To produce and train students at post graduate level for thriving career in chemical industry academics and research institutions of repute.
2. To train students in multidisciplinary and interdisciplinary areas in chemical sciences.
3. To train students who can apply their specialized and modern approach for the environmentally benign synthesis.

Programme Outcomes (POs)

Students shall be able to

1. Work in chemical industry, academic and research institutions.
2. Work in the areas like pharmaceuticals, nanotechnology, material science, biophysical, bioinorganic sensors, catalysis, green chemistry for sustainable development etc.
3. Analyze data obtained from sophisticated equipments (FT-NMR, FT-IR, UV -Vis, GC, GC-MS, Spectrofluorimeter etc.) for structure elucidation and chemical analysis.
4. Apply green chemistry approach towards planning and execution of research in frontier areas of chemical sciences.

Scheme and Syllabus of M.Sc. (Chemistry)

First Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY101	Analytical Chemistry	3	1	0	3.5
2.	PCY102	Inorganic Chemistry	3	0	0	3.0
3.	PCY109	Stereochemistry and Photochemistry	3	0	0	3.0
4.	PCY104	Quantum Chemistry	3	0	0	3.0
5.	PCY201	Electrochemistry and Thermodynamics	3	0	0	3.0
6.	PCY206	Inorganic Chemistry Lab	0	0	6	3.0
7.	PCY108	Chemical Biology (For non-medical group)	3	1	0	3.5
	PIM101	Basic Mathematics (For medical group)				
8.	PHU 002	Professional Communication	2	1	0	2.5
		Total	**20**	**3**	**6**	**24.5**

Second Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY215	Molecular Spectroscopy	3	1	0	3.5
2.	PCY202	Coordination Chemistry	3	0	0	3.0
3.	PCY203	Organic Reaction Mechanisms	3	0	0	3.0
4.	PCY208	Industrial and Green Chemistry	3	0	0	3.0
5.	PCY209	Organic Chemistry Lab	0	0	3	1.5
6.	PCY207	Physical Chemistry Lab	0	0	6	3.0
7.	PCY	Elective – I	3	0	0	3.0
8.	PCS-XXX	Programming for Bioinformatics	2	0	2	3.0
		Total	**17**	**1**	**11**	**23.0**

Third Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY316	Chemical Kinetics and Surface Chemistry	3	1	0	3.5
2.	PCY302	Symmetry and Group Theory	3	0	0	3.0
3.	PCY307	Catalysis and Reagents	3	0	0	3.0
4.	PCY308	Organic Structure Analysis	3	1	0	3.5
5.	PCY309	Analytical Chemistry Lab	0	0	3	1.5
6.	PCY305	Inorganic Synthesis Lab	0	0	3	1.5
7.	PCY306	Organic Synthesis Lab	0	0	6	3.0
8.	PCYXXX	Elective – II	3	0	0	3.0
	PCY391	Seminar/minor projects*	-	-	-	2.0
		Total	**15**	**2**	**12**	**24.0**

*May be undertaken/completed in academic or industry.

Fourth Semester

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCY401	Heterocyclic Chemistry and Natural Products	3	0	0	3.0
2.	PCY402	Advanced Topics in Chemistry	3	1	0	3.5
3.	PCY 491	Dissertation	-	-	-	10.0
		Total	6	1	0	12.5

Elective – I

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCY211	Medicinal and Pharmaceutical Chemistry	3	0	0	3.0
2.	PCY212	Synthetic and Natural Polymers	3	0	0	3.0
3.		Supramolecular Chemistry	3	0	0	3.0
4.		Biofuels	3	0	0	3.0

Elective - II

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCY321	Rearrangements and Retrosynthesis	3	0	0	3.0
2.		Photophysical Chemistry	3	0	0	3.0
3.		Biopolymer and Protein Chemistry	3	0	0	3.0
4.		Environmental Chemistry	3	0	0	3.0

Total Number of Credits = 88.0

PCY101 ANALYTICAL CHEMISTRY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

Course objective: To introduce concepts and applications of various analytical techniques.

Optical Methods: Principle, applications and limitations of Spectrophotometery, Beer-Lambert Law, Analysis of mixtures, Atomic Absorption Spectrometery, Atomic Emission Spectroscopy, Plasma and Electric Discharge Spectroscopy, Spectrofluorimetry, Nepheleometry and Turbidimetry.

Electroanalytical Methods: Introduction to Electrochemical Cells, Potentiometry: Types of Electrodes, Reference and indicator electrodes, Glass electrode, Ion-selective electrodes, Liquid membrane electrodes, Clark's electrode, Biosensor. Coulometry: Different methods, Coulometric titrations. Conductometric titrations. Voltammetry: Principles, Voltammograms, Equation of voltamogram, Modified Voltametric Methods, DPV, Cyclic Voltammetry, Amperometry, Anodic stripping voltammetry.

Chromatography: Classification, Retention time and retardation factor, Resolution and separation factor; General idea about adsorption, partition and column chromatography, Paper and thin layer chromatography, Gas Chromatography (GC) and High Performance liquid Chromatography (HPLC) - Instrumentation, methodology and applications.

Thermogravimetry: TGA, DTA, DSC - Instrumentation, methodology, applications.

Course learning outcomes (CLOs): The students will be able to interpret

1. various optical methods like AES, AAS, plasma and electric discharge spectroscopy, spectrofluorimetry, nephelometry and turbidimetry.
2. potentiometric, coulometric, and voltametric methods of analysis.
3. chromatographic techniques and applications.

Recommended Books

1. *Skoog, D.A., Holler, F.J., and Crouch, S.R., Principles of Instrumental Analysis, Thomson Learning (2007).*
2. *Willard, H.H., Merritt Jr. L., Dean, J.A. and Settle, F.A., Instrumental Methods of Analysis, CBS Publishers (2007) 7thed.*
3. *Christian, G.D., Analytical Chemistry, Wiley (2007) 6thed.*
4. *Bassett, J., Denney, R.C., Jeffery, G.H., and Mendham, J., Vogel's Textbook of Quantitative Chemical Analysis, Pearson Education (2007).*
5. *Skoog, D.A., West, D.M., Holler, F.J., and Crouch, S.R., Fundamentals of Analytical Chemistry, Brooks/Cole (2003) 8thed.*

Evaluation Scheme:

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation))
30	45	25

PCY102 INORGANIC CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s) : None

Course objective: To impart knowledge of chemistry of main group elements, f-block elements, organometallic compounds, their stability and catalytic application, and introduction to nuclear chemistry.

Chemistry of some main group elements: Synthesis, Properties and Structure of halides and oxides, Polymorphism of Carbon, Phosphorus and Sulfur. Synthesis, Properties and Structure of Boranes, Carboranes, Borazines, Silicates Carbides, Silicones, Phosphazenes, Sulphur-Nitrogen, Phosphorous-Nitrogen compounds, Peroxo compounds of Boron, Carbon and Sulphur, Oxy-acids of Nitrogen, Phosphorus, Sulphur and Halogens, Interhalogens, Pseudohalides and Noble gas compounds.

Chemistry of f-block elements: General discussion on the properties of the f-block elements. Spectral and Magnetic properties, Use of Lanthanide compounds as shift reagents.

Nuclear Chemistry: Nuclear reactions, Nuclear decay laws, Radioanalytical Techniques.

Organometallics: Organic-transition metal chemistry, Complexes with π-acceptor and σ-donor ligands, 18-electron and 16-electron rules, Isolobal analogy, Structure and Bonding, Transition metal to Carbon bonds in synthesis. Metal cluster compounds, Metal-metal bond, Metal Carbenes, Carbonyl and non-carbonyl clusters, Fluxional molecules, Application of orgnaometallic compounds as Homogeneous and Heterogeneous Catalysts.

Course learning outcomes (CLOs): The students will be able to know

1. the chemistry of main group elements, synthesis and properties of few main group compounds.
2. general properties and separation of lanthanides and actinides.
3. basics of nuclear chemistry and radio analytical techniques.
4. stability of organometallic compounds and clusters, and their applications as industrial catalysts.

Recommended Books

1. *Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., Advanced Inorganic Chemistry, John Wiley, (2003) 6thed.*
2. *Huheey, J.E., Keiter, E.A. and Keiter, R.L., Inorganic Chemistry, Pearson Education, (2002) 4th ed.*
3. *Greenwood, N.N., and Earnshaw, A., Chemistry of the Elements, Butterworth-Heinemann, (1997) 2nd ed.*
4. *Lee, J.D., Concise Inorganic Chemistry, ELBS, (1996) 5th ed.*
5. *Sharpe, E., Inorganic Chemistry, Pearson Education (2003) 3rd ed.*
6. *Crabtree, R.H., Organometallic Chemistry of the Transition Metals, John Wiley & Sons (2005).*
7. *Collman, J.P., Hegedus, L.S., Norton, J.R. and Finke, R.G., Principles and Applications of Organo-transition Metal Chemistry, University Science Books (1989).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation))
30	50	20

PCY109 STEREOCHEMISTRY AND PHOTOCHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To impart advanced knowledge of aromaticity, stereochemistry of organic compounds, pericyclic and photochemical reactions.

Stereochemistry: Conformational analysis of Cycloalkanes and Decalins, Effect of conformation on reactivity, Conformation of sugars, Steric-strain due to unavoidable crowding. Chirality, R-S nomenclature, Diastereoisomerism in Acyclic and Cyclic systems, E-Z isomerisms, Interconversion of Fischer, Newman and Sawhorse projections, Molecules with more than one chiral center, Threo and erythro isomers, Methods of resolution, Optical purity, Enantiotopic and diastereotopic atoms, Groups and faces, Stereospecific and Stereoselective synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape. Stereochemistry of the compounds containing Nitrogen, Sulphur and Phosphorus.

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddditions - antarafacial and 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 rearrangements, Ene reaction.

Photochemistry: Introduction, Photochemistry of Alkenes, rearrangement of 1,4- and 1,5-dienes. Photochemistry of Carbonyl Compounds: Intramolecular reactions of carbonyl compounds – Saturated, Cyclic and Acyclic, β,γ-unsaturated and α,β-unsaturated compounds, Photo-Fries reactions of Anilides. Photo-Fries rearrangement. Barton reaction.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, Energy level of π-molecular orbitals, Annulenes, Antiaromaticity, Homo-aromaticity.

Course learning outcomes (CLOs): The students will be able to explain

1. conformational analysis of cycloalkanes, reactivity, chirality, interconversion, resolution and asymmetric synthesis.
2. aromaticity, nonaromaticity and antiaromaticity in carbocyclic and heterocyclic compounds.
3. molecular orbital symmetry and possibility of thermally and photochemically pericyclic reactions.
4. basics of photochemical reactions of alkenes, carbonyl and aromatic compounds.

Recommended Books

1. *Carey, F. A., and Sundberg, R. J., Advanced Organic Chemistry, (Part A): Structure and Mechanism, Springer (2007) 5th ed.*
2. *March, J., and Smith, M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms and structures, John Wiley (2007) 6th ed.*
3. *Depuy, C.H., and Chapman, O. L., Molecular Reactions and photochemistry Pearson Education, Limited, (1972).*

4. *Horsepool, W. H., Organic Photochemistry. A Comprehensive Treatment, Ellis Horwood, Chichester, U.K (1992).*
5. *Clayden, Greeves, Narren, and Wothers, Organic Chemistry, Oxford University Press (2001).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes /Assignments/Lab Evaluation))
30	50	20

PCY104 QUANTUM CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course objective: To acquire knowledge of the quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry.

Quantum Mechanics: Postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems *viz.*, Particle in a box, The Rigid Rotor, The hydrogen atom.

Approximate Methods: The variation theorem, linear variation principle, perturbational methods.

Angular Momentum: Ordinary angular momentum, eigen functions and eigen values for angular momentum, addition of angular momenta, spin, antisymmetry and pauli exclusion principle.

Electronic Structure of Atoms: Electronic configuration, Russell-Saunders terms and coupling schemes, magnetic Effects: Spin-orbit coupling and Zeeman splitting.

Born-Oppenheimer Approximation: Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule, hybridization and valence MOs of H_2O and NH_3. Huckel theory of conjugated systems, bond order and charge density calculations, applications to ethylene and butadiene.

Course learning outcomes (CLOs): The students will be able to explain

1. Schrodinger equation for a particle in a box and quantum chemical description.
2. electronic and Hamiltonian operators for molecules.
3. quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
4. Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle.

Recommended Books

1. *Levine, N.I., Quantum Chemistry, Prentice Hall (2008) 5th ed.*
2. *Chandra, A.K., Introduction to Quantum Chemistry, Tata McGraw Hill (2004) 4th ed.*
3. *Atkins, P., and Friedman, R., Molecular Quantum Mechanics, Oxford University Press (2005) 4th ed.*

4. *Prasad, R.K., Quantum Chemistry, Wiley Easter (1992).*
5. *McWeeny, R., Coulson's Valence, Oxford University Press (1980) 3rd ed.*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes /Assignments/Lab Evaluation))
30	50	20

PCY201 ELECTROCHEMISTRY AND THERMODYNAMICS

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course objective: To impart knowledge of advanced electrochemistry, classical and statistical thermodynamics.

Electrochemistry: Nernst equation, Electrochemical cells, Concentration cells with and without liquid junction, Application of electrochemical cell, Thermodynamics of reversible electrodes and reversible cells, Redox indicators, Debye-Huckel treatment of dilute electrolyte solutions, Derivation of Debye-Huckel limiting law.

Classical Thermodynamics: Concepts involved in first, second and third law of thermodynamic, Free energy and entropy of mixing, Partial molar quantities, Gibbs-Duhem equation. Equilibrium constant, Temperature-dependence of equilibrium constant, Thermodynamic description of phase transitions, Determination of activity and activity coefficient by Debye Huckel law.

Statistical Thermodynamics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Partition function, Molar partition function, Thermodynamic properties in term of molecular partition function for diatomic molecules, Monoatomic gases, Rotational, Translational, Vibrational and Electronic partition functions for diatomic molecules.

Course learning outcomes (CLOs): The students will be able to

1. explain different thermodynamic parameters for chemical reactions
2. comprehend the redox processes in electrochemical systems.
3. explain Debye-Huckel theory and determination of activity and activity coefficient.
4. correlate and differentiate Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, theories of specific heat for solids.

Recommended Books

1. *Atkins, P.W., Physical Chemistry, W.H. Freeman (1997) 6th ed.*
2. *Puri, B.R., Sharma, L.R., and Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co. (2011) 45th ed.*
3. *Kapoor, K.L., A Text Book of Physical Chemistry, Vol. 3, Macmillan India (2005) 2nd ed.*
4. *Laidler, K.J., Chemical Kinetics, Dorling Kingsley (2007).*
5. *Rajaraman, J., and Kuriacose, J., Kinetics and Mechanism of Chemical Transformations, McMillan (2008).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes /Assignments/Lab Evaluation)
30	50	20

PCY206 INORGANIC CHEMISTRY LAB

L	T	P	Cr
0	0	6	3.0

Prerequisite(s): None

Course Objective: To impart knowledge of various techniques for analysis of inorganic compounds.

Introduction to good laboratory practices in chemistry.

Volumetric analysis: Covering the examples of precipitation titration, Complexometric titration, Oxidation reduction titration, Acid-base titration, Use of external indicator, Estimation of purity of organic molecules (e.g. aspirin).

Gravimetric analysis: Gravimetric estimation of cations and anions in the mixture or from alloys.

Spectrophotometeric determination: NO_3^- in water sample, $K_2Cr_2O_7$ in the presence of $KMnO_4$ and Fe(III) using 8-hydroxyquinoline.

Flame photometric determination: Li, Na, K and Ca.

Atomic absorption Spectrometry: Estimation of certain transition metals.

Course learning outcomes (CLOs): The students will be able to

1. interpret volumetric and gravimetric analysis of different cations and anions.
2. operate spectrophotometer, AAS and flame photometer for chemical analysis

Recommended Books

1. Mendham, J., Denney, R.C., Barnes, J.D., and Thomas, M. J.K., Vogel's Textbook of Quantitative Analysis, Pearson Education, (2007) 3rd ed.

2. Skoog, D.A., Holler, F.J., and Nieman, T.A., Principles of Instrumental Analysis, Thomson, (2006) 5th ed.

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes /Assignments/Lab Evaluation)
00	70	30

PCY108 CHEMICAL BIOLOGY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

Course Objective: To introduce molecular structure and interactions present in various bio-molecules that help in functioning and organization of living cell.

Introduction: Cell structure and functions, Scales of biological systems, Dimensions of bio-molecules and assemblies, Times of biological processes and biologically important energies, ATP. Water – physical properties and structure of water molecules, Interactions in aqueous solutions, Role of water in life, Biological buffers, Henderson-Hasselbalch equation.

Amino Acids and Peptides: Classification of amino acids and their properties, Polypeptides, Primary Structures, N-terminal and C-terminal determinations. Structure of peptide bond, synthesis of peptides, Solid phase peptide synthesis.

Nucleic Acids: Purine and pyrimidine bases, Nucleotides, Nucleosides, Base pairing via H-bonding, Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), Double helix model of DNA, Chemical and enzymatic hydrolysis of nucleic acids, The chemical basis for heredity, An overview of replication of DNA, Transcription, Translation and genetic code.

Carbohydrates: Biologically important monosaccharides, disaccharides and polysaccharides, Glycoproteins, Role of sugars in biological recognition, Blood group substances, Carbohydrate metabolism - Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, Pentose Phosphate pathway.

Lipids: Lipid classification, Lipid Bilayers, Membrane Proteins - integral membrane proteins, Lipid linked proteins, peripheral proteins, Overview of membrane structure and assembly. Liposomes, their biological functions.

Course learning outcomes (CLOs): Students will be able to

1. assess molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids.
2. be familiar with organization and working principles of various components present in living cell.

Recommended Books

1. *Voet, D.J., Voet, J.G., Pratt, C.W., Principles of Biochemistry, John Wiley, (2008) 3rd ed.*
2. *Berg, J.M., and Tymoczko, J.L., Stryer, L., Biochemistry, W.H. Freeman (2007) 6th ed.*
3. *Garrett, R.H., Grisham, C.M., Biochemistry, Brooks/Cole, Cengage Learning,(2010)4th ed.*
4. *Conn, E.E., and Stump, F., Outlines of Biochemistry, John Wiley (2006) 5th ed.*

Evaluation Scheme:

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
30	45	25

PCY215 MOLECULAR SPECTROSCOPY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

Course Objective: To impart the knowledge of electronic, rotation, vibration. NMR, FTIR, ESR, spectroscopy and their applications.

Unifying Principles: Electromagnetic radiation, Interaction of electromagnetic radiation with matter, Line width, Selection rules, Intensity of spectral lines, Born-Oppenheimer approximation, Rotational, Vibrational and Electronic energy levels.

Microwave Spectroscopy: Classification of molecules, Rigid rotor model, Effect of isotopic substitution on the transition frequencies, Intensities, Non-rigid rotor, Stark effect, Applications.

Vibrational Spectroscopy: Infrared Spectroscopy– Simple harmonic oscillator, Vibrational energies of diatomic molecules, Anharmonicity, Vibration-rotation spectroscopy, P, Q, R branches, Vibrations of polyatomic molecules, Group frequencies, Overtones, Hot bands, Applications.

Raman Spectroscopy - Classical and quantum theories of Raman effect, Pure rotational, Vibrational and Vibrational-Rotational Raman spectra, Mutual exclusion principle, Coherent anti Stokes Raman spectroscopy.

Electronic Spectroscopy: Energies of atomic and molecular orbitals, UV-Visible spectra, Spectra of hydrogen atom and alkali metal atoms, Applications, Franck-Condon principle, Electronic spectra of polyatomic molecules.

Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance Spectroscopy – Proton NMR, Shielding and Deshielding, of magnetic nuclei, Chemical shift, Spin-spin interactions and coupling constant 'J', Spin decoupling, Instrumentals, NMR studies of ^{13}C, ^{19}F and ^{31}P nuclei, NMR in chemical analysis and medical diagnostics.

Electron Spin Resonance Spectroscopy - Basic principles, Zero field splitting and Kramer's degeneracy, Factors affecting the 'g' value, hyperfine coupling constants, Instrumentation and Applications.

Mossbauer Spectroscopy: Basic principles, Application of the technique to the studies of (1) bonding, structures and oxidation state of Fe^{+2} and Fe^{+3} compounds.

Course learning outcomes (CLOs): The students will be able to

1. interpret microwave, vibration-rotation Raman and infra-red spectra for chemical analysis
2. analyze electronic spectra of different elements and simple molecules.
3. comprehend Nuclear Magnetic and Electron Spin Resonance spectroscopic techniques for organic compounds analysis and medical diagnostics.

Recommended Books

1. *Hollas, J.M., Modern Spectroscopy, John Wiley (1996) 3rd ed.*
2. *Windawi, H., and Floyd, F.L.H., Applied Electron Spectroscopy for Chemical Analysis (Chemical Analysis Vol. 63), John Wiley (1982).*
3. *Parish, R.V., NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Harwood (1991).*
4. *Chang,R., Basic Principles of Spectroscopy, McGraw-Hill (1971).*

5. *Ghosh, P.K., Introduction to Photoelectron Spectroscopy, **John Wiley** & Sons, New York (1983).*
6. *Carrington, A., and MacLachalan, A.D., Introduction to Magnetic Resonance, **Harper** and Row, New York, USA (1967).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
30	45	25

PCY202 COORDINATION CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s) : None

Course Objective: To introduce theories, reaction mechanism and stability of the coordination complexes, magnetic and electronic properties.

Coordination chemistry: Bonding in coordination compounds, Crystal field and molecular orbital theory, Splitting of d-orbitals in low-symmetry environments. Molecular orbitals energy level diagrams for common symmetries. Bonding involving π-donor ligands, Jahn-Teller effect, Tanabe-Sugano and Orgel diagrams, Interpretation of electronic spectra Including charge transfer spectra, Spectrochemical and Nephelauxetic series, Spectroscopic method of assignment of configuration in optically active metal complexes and their resolution. IUPAC nomenclature of coordination compounds.

Magnetism in coordination compounds: Quenching of orbital angular moment and Spin-orbit Coupling, Spectroscopic states.

Metal-ligand equilibrium in solution: Stepwise and overall formation constants and their determination, Factors affecting the stability of metal complexes.

Reaction Mechanism: Energy profile of a reaction, Reactivity of metal complexes, Inert and labile complexes, Kinetic application of valence bond and crystal field theories, Kinetics of octahedral substitution, Acid and base mediated hydrolysis, Reactions without metal ligand bond cleavage.
Redox reactions, Electron transfer reactions, mechanism of one electron transfer reactions, Energy conversion (solar) and photodecomposition of water, Outer sphere type reactions, Cross reactions and Marcus-Hush theory, Inner sphere type reactions, Berry pseudorotation.

Substitution reactions in square planar complexes, Trans effect, Mechanism of the substitution reaction.

Course learning outcomes (CLOs): The students will be able to

1. explain the formation, reaction mechanism and stability of coordination complexes.
2. interpret the electronic and magnetic properties of inorganic compounds.

Recommended Books

1. *Cotton, F.A., Wilkinson, G., Murillo, C.A., and Bochmann, M., Advanced Inorganic Chemistry, John Wiley (2003) 6th ed.*
2. *Huheey, J.E., Keiter, E. A., and Keiter, R. L., Inorganic Chemistry, Pearson Education (2002) 4th ed.*

3. Greenwood, N.N., and Earnshaw, A., Chemistry of the Elements, Butterworth-Heinemann (1997) 2nd ed.
4. Lever, A.B.P., Inorganic Electronic Spectroscopy, Elsevier Science (1985) 2nd ed.
5. Banerjea, D., Coordination Chemistry, Asian Books Private Limited (2007) 2nd ed.
6. McCleverty, J.A., and Meyer, T.J., Comprehensive Coordination Chemistry II, Vol. 9, Elsevier (2004) 1st ed.

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY203 ORGANIC REACTION MECHANISMS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To impart knowledge of mechanisms of substitution, addition, elimination and some named reactions in organic chemistry.

Aliphatic Substitution: Nucleophilic – S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. Neighbouring group mechanism, Classical and nonclassical carbocations, Phenonium ions, Norbornyl system, Common carbocation rearrangements, The S_Ni mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon, Reactivity effects of substrate structure, Attacking nucleophile, Leaving group and reaction medium, Phase transfer catalysis. Ambient nucleophile, Regioselectivity.

Aromatic Substitution: Electrophilic – Mechanism, Orientation and reactivity, o/p Ratio, Orientation in benzene ring with more than one substituent, Nitration, Halogenation, Sulphonation, Friedal Crafts alkylation and acylation, Sandmayer, Vilsmeier, Gatterman Koch, Gatterman, Kolbe-Schmidt reactions, Houben, Hoesch. Nucleophilic – Aromatic nucleophilic substitution mechanism (SNAr, SN1 and Arynes).

Addition Reaction: Addition to carbon-carbon multiple bonds, Mechanism of additions involving Electrophiles, Nucleophiles and Free radicals, Addition to conjugated systems, Orientation and reactivity, Hydroboration, Epoxidation, Birch reduction.
Addition to carbon-hetero multiple bonds, Addition to carbon oxygen double bond, $LiAlH_4$, $NaBH_4$, Aldol, Perkin, Claisen, Benzoin, Benzil-benzilic acid, Mannich, Dieckmann, Michael and Wittig reactions.

Elimination Reactions: β-Elimination – E_2 and E_1, α-elimination

Course learning outcomes (CLOs): The students will be able to explain

1. mechanistic aspects in nucleophilic and electrophilic substitution.
2. reaction conditions, products formation and mechanisms of some named reactions.
3. mechanisms of addition reactions of C=C and C=O bonds and elimination reactions.

Recommended Books

1. *Carey, F.A., and Sundberg, R.J., Advanced Organic Chemistry, (Part A), Springer (2007) 5th ed.*
2. *Carey, F.A., and Sundberg, R.J., Advanced Organic Chemistry, (Part B), Springer (2007) 5th ed.*

3. *March, J., and Smith, M.B., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, John Wiley (2007) 6th ed.*
4. *Clayden, Greeves, Narren, and Wothers, Organic Chemistry, Oxford University Press (2001).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY208 INDUSTRIAL AND GREEN CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course objective: To introduce basic principles of chemical industry and importance of green chemistry for industrial applications.

Industrial Chemistry Basics: Economic factors, Industrial Vs Laboratory chemistry, the raw material and basic processes, Material balance, Chemical processes used in industrial organic synthesis, Production of industrially important alcohols.

Sugar: Introduction, Manufacture of cane sugar, Extraction and Purification of juice, Defection, Sulphitation and Carbonation, Concentration and Evaporation, Crystallization, Separation of crystals, Drying, Refining, Grades, Recovery of sugar from molasses, Bagasse, Preparation of celotex, Manufacture of sucrose from beet root, Testing and estimation of sugar, Double sulphitation process.

Detergents: Introduction, Principal groups of synthetic detergents, Classification of surface active agents, Anionic, Cationic, Amphoteric and non-ionic detergents, Soaps, Alkyl and alkyl aryl sulphonates, Amide sulphonates, Miscellaneous compounds, Ecofriendly detergents containing enzymes.

Green Chemistry: Toxicity of chemicals, Chlorine and phosgene controversy, Principles of Green Chemistry, Concept of atom economy, Tools of Green Chemistry: Alternative feedstock/starting materials, Reagents, Solvents, Product/target molecules, The role of catalysis, chirotechnology and asymmetric catalysis, Non-conventional reaction media, bio catalysis, Chemical separations, Inclusion compounds, Separations of ions, Membranes, Recent literature examples of conventional Vs green synthesis.

Course learning outcomes (CLOs): The students will be able to

1. be familiar with the principals of industrial chemistry and procedures for production of some industrially important products.
2. realize the concepts and applications of green chemistry for industrial production.

Recommended Books

1. *Howard, W.L., Introduction to Industrial Chemistry, Wiley-Interscience (1986).*
2. *Riegel, E. R.R., Industrial Chemistry,Reinhold Publishing Corporation (1960) 6th ed*
3. *Matlack, A. S., Introduction to Green Chemistry, CRC Press, (2010), 2nd ed.*
4. *Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).*
5. *Ahluwalia, V. K., and Kidwai, M., New Trends in Green Chemistry, Anamaya Publishers (2004).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes /Assignments/Lab Evaluation)
30	50	20

PCY209 ORGANIC CHEMISTRY LAB

L	T	P	Cr
0	0	3	1.5

Prerequisite(s): None

Course Objective: To develop experimental skills of various separation and purification techniques.

Chromatography: Separation and identification of organic compounds in a given mixture by Thin Layer Chromatography, R_f values, Column chromatography.

Purification Techniques: Crystallization, Distillation, Steam distillation and Fractional distillation.

Extraction: Liquid-liquid extraction, Solid-liquid extraction (Soxhlet extraction) of natural products.

Synthesis: Synthesis of organic compounds, their purification and characterization: Asprin, Schiff's base, Diels-Alder adduct.
Determination of melting point and mixed melting point.

Course learning outcomes (CLOs): The students will be able to

1. assess chromatographic separation and identification of organic compounds.
2. distinguish purification, crystallization, and different distillation processes.
3. recognize synthesis, purification and characterization of aspirin, Schiff's base, Diels-Alder adduct.

Recommended Books

1. *Leonard, J., Lygo, B., and Procter, G., Advanced Practical Organic Chemistry, Blackie Academic (1995) 2nd ed.*
2. *Furniss, B.S., Hannaford, A.J., Smith, P.W.G., and Tatchell, A.R., Vogel's Textbook of Practical Organic Chemistry, Pearson Education (2006).*
3. *Pasto, D., Johnson, C., and Miller, M., Experiments and Techniques in Organic Chemistry, Prentice Hall (1991).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
00	70	30

PCY207 PHYSICAL CHEMISTRY LAB

L	T	P	Cr
0	**0**	**6**	**3.0**

Prerequisite(s): None

Course Objective: To have hand-on experiences of techniques for verifying physical and chemical properties.

1. Determination of relative and absolute viscosity of a given liquid.
2. Determination of surface tension of alcohols.
3. Determination of refractive indices of given liquids.
4. To verify Freundlich and Langmuir Adsorption isotherms for adsorption of acetic acid on activated charcoal.
5. Determination of partition coefficient of benzoic acid between organic solvent and water.
6. Determination of rate constant of hydrolysis of an ester and to study the effect of temperature and ionic strength on reaction rate.
7. To study kinetics of inversion of cane sugar by optical rotation measurement.

Course learning outcomes (CLOs): The students will be able to

1. be familiar with experimental techniques for controlling chemical reactions.
2. measure various physical and chemical properties of materials.

Recommended Books

1. *Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, S. Chand (2007).*

2. *Yadav, J.B., Advanced Practical Physical Chemistry, Krishna Prakasan Media (2008).*

3. *Das, R.C., and Behra, B., Experimental Physical Chemistry, Tata McGraw (1983).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
00	70	30

PCSXXX: PROGRAMMING FOR BIOINFORMATICS

L	T	P	Cr
2	0	2	3.0

Course objective: The course will provide students with basic understanding of Python programming language and its application to computational biology.

Introduction to Python: Basics of Python, Installation, Operators and Expressions, Control flow (if-else, Loops), Functions, Modules, Data Structures in python (List, Dictionary, Sets, Tuple), Problem Solving using Python, Object Oriented Programming Concepts(Classes, Polymorphism, Encapsulation), Input and Output (File Handling), Exceptions Handling, Standard Library, Command Line Argument, GUI Development in Python.

Introduction to Computational Biology Concepts (Using Biopython): Structure Analysis (Learn how to compare and align structures, identify ligand contacts, and extract ligands from PDB files), Trajectory Analysis (Learn how to analyze simulation trajectories, in particular handling large trajectory files that don't fit in memory), Conformational Sampling (Learn how to generate alternate protein conformations along ANM modes and to refine them using NAMD), Ensemble Analysis (Learn how to analyze large and heterogeneous ensembles of protein structures to infer dynamical properties), Elastic Network Models (Learn how to perform normal mode analysis and developing customized force constant functions), Druggability Suite (Learn how to setup and analyze druggability simulations containing small organic molecules using DruGUI) and Collective Molecular Dynamics (Learn how to sample transition pathways between known conformers using a multi scale hybrid methodology).

Bioinformatics (Advance): Parsing Bioinformatics file formats (BLAST, Clustalw, FASTA, Genbank), access to online services (NCBI, Expasy), interfaces to common and not-so-common programs (Clustalw, DSSP, MSMS), Applications and Prospects, Genome and protein information resources, sequence analysis, multiple sequence alignment, homology and analogy, pattern recognition, analysis package, NCBI basic alignment tools, DNA binding motif finding by sequence alignment, Gibbs sampling approaches, Regulatory module (a combination of DNA binding motifs) detection, Bayesian network approach to study the gene expression network based on expression quantitative trait loci (eQTL) data, Statistical methods for pre-mRNA alternative splicing

Introduction to Machine Learning: Supervised Learning, Unsupervised Learning, Clustering, Neural Network, Decision Tree, Support Vector Machine.

Laboratory Work: Basics of Python, Multiple Sequence Alignment, BLAST, Motif Finding, finding novel gene, Hands on ChemDraw and Marvin.

Assignment: Compulsory 4 weeks project on bioinformatics.

Course Learning Outcomes (CLOs): Students will be able to
1) write python program to understand biological processes.
2) generate *in silico* models for biological macromolecules
3) analyze interactions biological molecules using *in silico* modeling.

Recommended books:

1. *Guttag John, V, Introduction to Computation And Programming Using Python (2014).*
2. Karumanchi, N, Data Structure and Algorithmic Thinking with Python (2015).
3. Mckinney, W, Python For Data Analysis (2013).
4. Hetland, M, L, Beginning Python: From Novice To Professional (2008).
5. Downey, A, Elkner, J, Meyers, C, Learning with Python: How to Think Like a Computer Scientist (2015).

***Web Resource**:*

1. ***Byte of Python** http://python.swaroopch.com/*
2. ***BioPython** http://biopython.org/DIST/docs/tutorial/Tutorial.html*
3. ***Protein Dynamics and Sequence Analysis** http://prody.csb.pitt.edu/tutorials*
4. ***Command Line Tools for Genomic Data Science** https://www.coursera.org/learn/genomic-tools*

Evaluation Scheme:

S.No.	Evaluation	Marks
1.	MST	25
2.	EST	35
3.	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)	40

PCY 316 CHEMICAL KINETICS AND SURFACE CHEMISTRY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

Course objective: To impart knowledge of applications of reaction kinetics, surface reaction, adsorption and catalysis.

Reaction Kinetics: Introduction, Rates of chemical reactions, Methods of determining rate laws, Mechanisms of chemical reactions and steady state approximation, Kinetics of photochemical and composite reactions, Chain and oscillatory reactions, Collision and transition state theories, Stearic factor, Treatment of unimolecular reactions, Ionic reactions: salt effect. Homogeneous catalysis and heterogeneous catalysis, free radical polymerization, enzyme catalysis, and reaction dynamics. Effect of pressure on reaction rate, Kinetics of catalytic reactions, Kinetics of surface reaction, autocatalysis, unimolecular and bimolecular surface reaction.

Fast Reaction: Luminescence and Energy transfer processes, Study of kinetics by stopped-flow technique, Relaxation method.

Adsorption: Surface tension, Capillary action, Gibbs adsorption isotherm, Estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon), Catalytic activity at surfaces.

Properties and stability of colloids, Surface active agents, Reverse micelles, Critical micellar concentration (CMC), Factors affecting the CMC of surfactants, Thermodynamics of micellization, Micro emulsion.

Course learning outcomes (CLOs): The students will be able to

1. interpret mechanism for chemical reactions for optimizing the experimental conditions.
2. familiar with application of homogeneous and heterogeneous catalysis in chemical synthesis
3. explain the importance of adsorption process and catalytic activity at the solid surfaces
4. classify the colloidal material and their stability for many practical uses.

Recommended Books

1. *Atkins, P.W., Physical Chemistry, W.H. Freeman (1990).*
2. *Laidler, K.J., Chemical Kinetics, Dorling Kingsley (1998).*
3. *Rajaraman, J., and Kuriacose, J., Kinetics and Mechanism of Chemical Transformations, McMillan (2008).*
4. *Moroi, V., Micelles Theoretical and Applied Aspects, Springer (1986).*
5. *Gowarikar, V.A., Vishwanathan, N.V., and Sreedhar, J., Polymer Science, New Age International (1986).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	45	25

PCY302 SYMMETRY AND GROUP THEORY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To introduce the concepts and importance of symmetry and group theory in solving chemical problems.

Introduction: Symmetry elements and symmetry operation, Definitions of group, Subgroup, Relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, Representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh}). Character of a representation.

Character Table and their Uses: The great orthogonality theorem and its importance. Construction of character tables, Reducible and irreducible representations, Group theory and quantum mechanics, Projection operator, Using projection operator to construct symmetry adopted linear combinations (SALCs).

Chemical Applications: Molecular orbital theory and its application in organic and inorganic chemistry, Molecular vibrations, Normal coordinates.

Course learning outcomes (CLOs): The students will be able to explain

1. the concepts of symmetry and group theory in solving chemical structural problems.
2. molecular structure by the use of character tables and projection operator techniques.
3. the importance of symmetry and group theory in spectroscopic applications.

Recommended Books

1. *Cotton, F.A., Chemical Applications of Group Theory, John Wiley (1990) 3rd ed.*
2. *Rakshit, S.C., Molecular Symmetry Groups and Chemistry, The New Book Stall (1988).*
3. *Dass, N.N., Symmetry and Group Theory for Chemists, Asian Books Pvt. Ltd (2004).*
4. *Gopinathan, M.S., and Ramakrishnan, V., Group Theory in Chemistry, Vishal Publishers (2006).*

Evaluation Scheme:

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY307 CATALYSIS AND REAGENTS

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course objective: To impart knowledge of metal catalysis, reagents and their current applications.

Metal-Catalyzed Transformations in Organic Syntheses: Review of basic concepts in catalysis, Reactions of transition metal complexes, The Suzuki coupling, Cross-coupling reaction, Heck reaction and other Pd-catalyzed reactions, Copper catalysis, Buchwald-Hartwigamination, Metathesis reactions, Gold catalysis, Emerging topics (C-H functionalization, borrowing hydrogen).

Reagents in Organic Syntheses: Use of the following reagents in organic syntheses and functional group transformations, Complex metal hydrides, Gilman's reagent, Lithium dimethylcuprate, Lithium disopropylamide, Dicyclohexylcarbodimide, 1,3-Dithiane, Trimethylsilyl iodide, Tri-n-butyltin hydride, Woodward and Prevost hydroxylation, Osmium tetroxide, DDQ, Selenium dioxide, Phase transfer catalysts, Crown ethers, Peterson's synthesis, Wilkinson's catalyst.

Course learning outcomes (CLOs): The students will be able to

1. comprehend experimental techniques for different catalytic reactions.
2. interpret physical and chemical characterization of catalysts and catalytic reaction.
3. be familiar with various reagents and their applications in industry.

Recommended Books

1. *Hegedus, L.S., Transition Metals in the Synthesis of Complex Organic Molecules, University Science Book (2010) 3^{rd} ed.*
2. *Carruthers, W., Some Modern Methods of Organic Synthesis, Cambridge University Press (1987).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY308 ORGANIC STRUCTURE ANALYSIS

L	T	P	Cr
3	**1**	**0**	**3.5**

Prerequisite(s): None

Course Objective: To impart knowledge of spectroscopic techniques for structural analysis of organic compounds.

Ultraviolet and Visible Spectroscopy: Introduction, Ultraviolet bands for carbonyl compounds, Unsaturated carbonyl compounds, Dienes, Conjugated polyenes, Fieser – Woodward rules for conjugated dienes and carbonyl compounds, Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls.

Infrared Spectroscopy: Introduction, Characteristic vibrational frequencies of alkanes, Alkenes, Alkynes, Aromatic compounds, Alcohols, Phenols, Ethers, and amines. Detailed study of vibrational frequencies of carbonyl compounds (Ketones, Aldehydes, Esters, Amides, Acids, Anhydrides, Lactones, Lactams and Conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies.

Optical Rotatory Dispersion and Circular Dichroism: Definition, Deduction of absolute configuration, Octant rule for ketones.

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, Chemical shift, Spin-spin interaction, Shielding mechanism, Chemical shift values and correlation for protons bonded to carbon (Aliphatic, Olefinic, Aldehydic and Aromatic) and other nuclei (Alcohols, Phenols, Enols, Carboxylic acids, Amines, Amides & Mercapto), Chemical exchange, Effect of deuteration, Complex spin-spin interaction between two, three, four and five nuclei (first order spectra), Simplification of complex spectra. Continuous wave and FT-NMR.
^{13}C NMR Spectroscopy: General considerations, Nuclear Overhauser effect (NOE), Chemical shift (Aliphatic, olefinic, Alkyne, Aromatic, Heteroaromatic and carbonyl carbon), Coupling constants. Introduction to two dimension NMR spectroscopy.

Mass Spectrometry: Introduction, Ion production - EI, CI, FD and FAB, Factors affecting fragmentation, Ion analysis, Ion abundance. Mass spectral fragmentation of organic compounds, Common functional groups, Molecular ion peak, McLafferty rearrangement. Nitrogen rule, High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Structure elucidation of some model organic molecules by UV-Vis, IR, ^{1}H NMR, ^{13}C NMR and MS.

Course learning outcomes (CLOs): The students will be able to

1. identify functional groups using IR, λ_{max} for polyenes and α, β-unsaturated carbonyl compounds.
2. interpret Cotton effect curves for obtaining absolute configuration of chiral molecules with chromophores.
3. determine chemical structure by UV-Vis, IR, ^{1}HNMR, ^{13}CNMR and mass spectral data.

Recommended Books

1. *Crews, P., and Rodrigue, J., Organic Structure Analysis, Oxford University Press (1998).*
2. *Simpson, J.H., Organic Structure Determination using 2D NMR Spectroscopy, Academic Press, Elsevier (2008).*
3. *Pavia, D.L., Lampman, G.M., and Kriz, G.S., Introduction to Spectroscopy, Brooks/Cole Cengage Learning (2008) 4th ed.*
4. *Silverstein, R.M., and Webster, F.X., Spectrometric Identification of Organic Compounds, John Wiley & Sons, Inc. (2005) 7th ed.*
5. *Martin, M.L., Delpeuch, J.J., and Mirtin, G.J., Practical NMR Spectroscopy, Heyden (1980).*
6. *Kalsi, P.S., Spectroscopy of Organic Compounds, New Age International (P) Ltd (2008).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	45	25

PCY309 ANALYTICAL CHEMISTRY LAB

L	T	P	Cr
0	**0**	**3**	**1.5**

Prerequisite(s): None

Course Objective: To provide training on different analytical techniques for chemical analysis.

Conductometry: Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.

Potentiometry: To fabricate saturated calomel electrode and salt bridge, Determination of strengths of halides in a mixture by potentiometric titrations, Determination standard electrode potential of Fe^{2+}/Fe^{3+} system using potassium permanganate solution.

pHmetry: Titration of strong and weak acids against a base using a pH meter, Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.

Voltammetry: To determine half wave potentials of Zn and Cd ions, To study the electrochemistry of $Co(NH_3)_6^{3+}$ by cyclic voltammetry.

Course learning outcomes (CLOs): The students will be able to develop experimental skills on conductivity meter, potentiometer, pH meter and voltammeter for different applications.

Recommended Books

1. *James, A.M., and Prichard, F.E., Practical Physical Chemistry, Longman, Harlow (1974) 3rd ed.*
2. *Das, R.C., and Behra, B., Experimental Physical Chemistry, Tata McGraw-Hill (1983).*
3. *Ghosh, J.C., Experiments in Physical Chemistry, BharatiBhavan (1990).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
00	70	30

PCY305 INORGANIC SYNTHESIS LAB

L	T	P	Cr
0	**0**	**3**	**1.5**

Prerequisite(s) :None

Course Objective: To teach the synthesis of inorganic complexes and their characterization with instrumental techniques.

Inorganic synthesis: Synthesis, separation and purification of following inorganic compounds, and their characterization by various techniques viz., UV-Vis, FT-IR, Magnetic moment measurement, Conductivity measurements, NMR and Thermogravimetric analysis.
Werner's complex and their conductivity, cis and trans-$[Co(en)_2Cl_2]^+$, 1-Acetyl ferrocene and separation by TLC, $Hg[Co(SCN)_4]$ as standard for the magnetic moment measurement, Preparation and separation of isomers of $K_3[Fe(C_2O_4)_3]$, Cu(II) and Ni(II) complexes of Schiff base, $VO(acac)_2$, Conventional and green method for the preparation of isomers of tris(8-hydroxyquilinato)aluminum(III) complex.

Course learning outcomes (CLOs): The students will be able to

1. know the preparation and purification processes of different inorganic complexes.
2. be familiar with UV-Vis, FT-IR, magnetic moment measurement, conductivity measurements, NMR and thermogravimetric analysis for characterization of coordination complexes.

Recommended Books

1. *Jolly, W.L., Synthesis and Characterization of Inorganic Compounds, Prentice Hall, (1970)1st ed.*
2. *Angelici, R.J., Synthesis and Techniques in Inorganic Chemistry, W B Saunderers Co. (1969).*
3. *Sharma, R.K., Tucker, S., and Chaudhuri, M.K., Green Chemistry Experiments- A monograph, Tucker Prakashan (2007).*

Evaluation Scheme

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
00	70	30

PCY306 ORGANIC SYNTHESIS LAB

L	T	P	Cr
0	**0**	**6**	**3.0**

Prerequisite(s): None

Course Objective: To acquire knowledge of laboratory techniques for organic synthesis and characterization.

Handling of hazardous chemicals: Drying of Toluene using sodium metal.Safe quenching of the residual sodium using methanol/ethanol.Drying dichloromethane using P_2O_5.Safely disposing off P_2O_5 using methanol.

Preparation, Separation and purification of organic compounds, and their characterization by spectral techniques (UV, IR, ^{1}H NMR, ^{13}C NMR and MS).

Electrophilic Aromatic Substitution Reaction: Nitration of phenol.Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.Three Component Coupling: Synthesis of dihydropyrimidinone.

Multistep synthesis: Preparation of methylbenzoate from benzoic acid. Synthesis of m-nitromethylbenzoate from methylbenzoate.Demethylation of m-nitromethylbenzoate to get m-nitrobenzoic acid.

Applications: Resolution of α-phenyl ethylamine using tartaric acid and find its optical rotation.Introduction to Chemical Literature.Solving problems of structure elucidation of organic compounds based on UV, IR, ^{1}H-NMR, ^{13}C-NMR and MS.

Course learning outcomes (CLOs): The students will be able to

1. use to safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. develop synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
3. propose starting materials, functional groups, mechanism, and typical reaction conditions.
4. evaluate the characterization by physical and spectroscopic techniques.

Recommended Books

1. *Fessenden, R.J., and Fessenden, J.S., Techniques for Organic Chemistry, Willard Grant Press (1984).*
2. *Furniss, B.S., Hannaford, A.J., Smith, P.W.G. and Tatchell, A.R.,Vogel's Textbook of Practical Organic Chemistry, Dorling Kingsley (2008).*
3. *Ranu, B.C., Monograph on Green Chemistry Laboratory Experiments, DST (2000).*

Evaluation Scheme

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
00	70	30

PCY391 SEMINAR/ MINOR PROJECT

	L	T	P	Cr
	-	-	-	2.0

Prerequisite(s): None

Course Objective: To provide training for research work and handling of various instrument used in academic and industries

The students have to visit various reputed research institutes or industries according to their interest for six weeks (June-July). The training of these students is then evaluated by the faculty of school of chemistry and biochemistry. The evaluation is on the basis of 30 min presentation given by each student in the month of August. Grads are then decided on the basis of research work and presentation.

Course learning outcomes (CLOs): The students will be able to

1. comprehend safe laboratory practices for handling laboratory equipments and chemical reagents.
2. develop experimental skills for handling of various sophisticated instruments.

Recommended Books/literature

Literature from the websites of Royal Society of Chemistry, American Chemical Society, Elsevier, Wiley Sciences, Bantham, Springer etc.

Evaluation Scheme

REPORT	PRESENTATION
50	50

PCY401 HETROCYCLIC CHEMISTRY AND NATURAL PRODUCTS

	L	T	P	Cr
	3	0	0	3.0

Prerequisite(s): None

Course Objective: To introduce synthesis and reactivity of aliphatic and aromatic heterocyclic compounds, and importance of some natural products.

Nomenclature of Heterocycles: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, Fused and bridged heterocycles.

Aromatic Heterocycles: Classification (structural type), Criteria of aromaticity (bond lengths, Ring current and chemical shifts in ^1H NMR-spectra, Empirical resonance energy, Delocalization energy and

Dewar resonance energy, Diamagnetic susceptibility exaltations). Heteroaromatic reactivity and Tautomerism in aromatic heterocycles.

Heterocyclic Synthesis: Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

Small Ring Heterocycles: Three-membered and four-membered heterocycles - Synthesis and reactions of Aziridines, Oxiranes, Azetidines and Oxetanes.

Benzo-Fused Five-Membered Heterocycles: Synthesis and reactions of Benzopyrroles, Benzofurans, Benzothiophenes, Benzodiazoles and Benzotriazoles.

Five-Membered Heterocycles: Synthesis and reactions of Pyrrole, Thiophene, Furan, Pyrazoles, Oxazoles and Imidazoles.

Six-Membered Heterocycles: Synthesis and reactions of Quinoline, Isoquinoline, Coumarins, Chromones, Diazines, Triazines, Tetrazines and Thiazines.

Natural Products: Introduction, Structure, Chemistry of Terpenoids, Steroids, Alkaloids and Natural pigments.

Course learning outcomes (CLOs): The students will be able to

1. comprehend nomenclature of different heterocyclic compounds.
2. interpret synthesis and reactivity of fused, six membered and smaller heterocyclic compounds.
3. categorize and the importance of various natural products.

Recommended Books

1. *Gilchrist, T.L., Heterocyclic Chemistry, Prentice Hall (1997) 3rd ed.*
2. *Katritzky A.R., and Rees C.W., Comprehensive Heterocyclic Chemistry, Pergamon Press (1996).*
3. *Gupta, R.R., Kumar M., and Gupta, V., Heterocyclic Chemistry Vo1.1-3, Springer Verlag (2008).*
4. *Torsell, K.B.G., Natural Product Chemistry, Apotekasocieteten (1997).*
5. *Koskinen, A., Asymmetric Synthesis of Natural Products, Wiley (1993).*
6. *Apsimon J., Total synthesis of Natural Products (1-7) Wiley Interscience (1973-1988).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY402 ADVANCED TOPICS IN CHEMISTRY

L	T	P	Cr
3	**1**	**0**	**3.5**

Prerequisite(s): None

Course objective: To impart knowledge of certain advanced topics in chemistry such as biophysical, bioinorganic, and solid state chemistry.

Biophysical Chemistry: Primary, Secondary and Tertiary structures of proteins, Covalent and noncovalent interactions, Hofmeister series, Chaotropic and kosmotropic ions/cosolvents. Spectroscopic

(CD, FTIR, Fluorescence) and calorimetric methods to study folding, stability, and dynamics of proteins, Thermal, Chemical, and pH-denaturations of proteins, Ultrafast biological reactions, Folding intermediates and their detection test, Protein misfolding and its consequences.

Bioinorganic Chemistry: Heme and non-heme proteins, Haemoglobin and myoglobin as oxygen carriers, Bohr effect, Relaxed and tense (R & T) configurations of haemoglobin. Structure and functions of cytochromes, Hemerythrins and Hemocyanins. Biochemistry of iron, Iron storage and Transport, and ferritin, Transferrin., Blue copper proteins, Zinc protein (carbonic anhydrase), and Iron-sulfur proteins, Metal deficiency and disease, Toxic effects of metals.

Solids State Chemistry: Diffraction methods **(**X-ray, electron and neutron), Dislocations in solids, Schottky and Frenkel defects, Band theory of solids, significance of band gap, Conductors, Semi-conductors and insulators. Electrical conduction in metals, Superconductivity, Ferroelectric and piezo-electric materials. Classification of magnetic materials and their examples.

Course learning outcomes (CLOs): The students will be able to

1. evaluate kinetics, thermodynamics, and mechanism of protein folding.
2. assess the structure and biological functions of proteins and the role of metals in biology.
3. correlate the physicochemical properties, defects in solid, diffraction techniques, electrical and magnetic properties of materials.

Recommended Books

1. *Huheey, J.E., Keiter, E. A., and Keiter, R.L., Inorganic Chemistry, Pearson Education (2008) 4th ed.*
2. *Lesk, A.M., Introduction to Protein Science, Oxford University Press, (2010) 2nd ed.*
3. *Cowan, J.A., Inorganic Biochemistry-An Introduction, Wiley-VCH (1997) 2nd ed.*
4. *Cantor, C.R., and Schimmel, P.R., Biophysical Chemistry, Freeman (1980).*
5. *Van Holde, K.E., Johnson, W.C., and Ho, P.S., Principles of Physical Biochemistry, Pearson Education (1998).*
6. *Harding, S.E., and Chowdhry, B. Z., Protein-Ligand Interactions, Oxford University Press (2001).*
7. *Keer, H.V., Principles of the Solid State, New Age International (2004).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	45	25

PCY491 DISSERTATIONS

L	T	P	Cr
-	-	-	6.0

Prerequisite(s): None

Course Objective: To provide training for literature survey, experimental research work, instrumental techniques and their operational procedure useful for their future profession.

The students are doing six months project work in any of the research laboratory in school of chemistry and biochemistry according to their interest and availability of the position (January-June). This dissertation is submitted in the form of thesis. The training of these students is then evaluated by committee members of the faculty of school of chemistry and biochemistry as well as one member from outside of Thapar Institute of Engineering and Technology. The evaluation is on the basis of 30 min presentation given by each student in the month of August. Grades are then decided on the basis of their research work and presentation.

Course learning outcomes (CLOs): The students will be able to

1. analyze current literature research for research topic of his/her area of expertise.
2. rationalize the research gap for new innovation.
3. comprehend expertise for writing the research reports.
4. exposure for safe laboratory practices by handling high end equipments and chemical reagents.

Recommended Books/literature

Literature from the websites of Royal Society of Chemistry, American Chemical Society, Elsevier, Wiley Sciences, Bantham, Springer etc.

Evaluation Scheme

DISSERTATION	PRESENTATION
60	40

PCY211 MEDICINAL AND PHARMACEUTICAL CHEMISTRY

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course Objective: To acquire knowledge of drug design and development, pharmacokinetics, and pharmacodynamics.

Drug Design: Development of new drugs, Procedures followed in drug design, Concepts of lead compound and lead modification, Concepts of pro-drugs and soft- drugs, Structure-activity relationship (SAR), Factors affecting bioactivity, Resonance, Inductive effect, Isosterism, Bio-isosterism, Spatial considerations. Theories of drug activity: Occupancy theory, Rate theory, Induced fit theory. Concepts of drug receptors. Physico-chemical parameters: Lipophilicity, Partition coefficient, electronic ionization constants, Steric. Free-Wilson analysis, Hansch analysis, Relationships between Free-Wilson and Hansch analysis. LD-50, ED-50.

Pharmacokinetics: Introduction to drug absorption, Disposition, Elimination using pharmacokinetics, Important pharmacokinetic parameters in defining drug disposition and in therapeutics.

Pharmacodynamics: Introduction, Elementary treatment of enzyme stimulation, Enzyme inhibition, Sulphonamides, Membrane active drugs, Drug metabolism, Xenobiotics, Biotransformation.

Antineoplastic Agents: Introduction, Cancer chemotherapy, Role of alkylating agents and antimetabolites in treatment of cancer, Antibiotics and mitotic inhibitors.

Cardiovascular Drugs: Introduction, Cardiovascular diseases, Drug inhibitors of peripheral sympathetic function, Central intervention of cardiovascular output.

Psychoactive Drugs: Introduction, CNS depressants, General anaesthetics, Mode of action of hypnotics, Sedatives, Anti-anxiety drugs, Benzodiazipines, Buspirone. Antipsychotic drugs - the neuroleptics, Antidepressants, Butyrophenones, Serendipity and drug development, Stereochemical aspects of psychotropic drugs.

Antibiotics: Cell wall biosynthesis, Inhibitors, β-lactam rings, Antibiotics inhibiting protein synthesis.

Course learning outcomes (CLOs): The students will be able to
1. comprehend drug designing and development, their SAR and QSAR.
2. explain the mode of action of different drugs.
3. describe the role of drugs to inhibit the particular enzymes and treatment of disease.

Recommended Books

1. *Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Beale Jr., J.M., Block, J.H. (2012) 12th ed.*
2. *Pandeya, S.N., and Dimmock, J.R., An Introduction to Drug Design, New Age International (2008).*
3. *Abraham, D.J., and Rotella, D.P., Burger's Medicinal Chemistry and Drug Discovery, Vol-1, Ed. John Wiley & Sons (2010) 7th ed.*
4. *Brunton, L.L., Chabmer, B.A., and Knollmann, B.C., Goodman and Gilman's Pharmacological Basis of Therapeutics, Ed. McGraw-Hill (2011) 12th ed.*
5. *Silverman, R.B., The Organic Chemistry of Drug Design and Drug Action, Elsevier(2004) 2nd ed.*
6. *Lednicer, D., Strategies for Organic Drug Synthesis and Design, John Wiley & Sons. (2008) 2nd ed.*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY212 SYNTHETIC AND NATURAL POLYMERS

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course Objectives: To acquire knowledge of different techniques of polymerization, their molecular weight determination and processing of polymers.

Classification of Polymers: Homopolymers, Co-polymers, Linear polymers, Branched polymers, Cross linked or three dimensional polymers, Block co-polymers, Organic and inorganic polymers, Natural and synthetic polymers, Chain and step growth polymers, Thermoplastic and thermosetting, Fibers, Foams, Adhesives and elastomers.

Mechanisms of Polymerization: Step growth-, Radical-, Chain-, Ring opening-,Cationic-, and anionic polymerization.

Copolymerization: Importance of copolymerization, Types of co-polymers, Co-polymer composition, Methods of determination of reactivity ratio, and co-polymerization behavior.

Techniques of Polymerization: Bulk, Solution, Emulsion, Suspension and interfacial polymerization.

Polymer Molecular Weights: Molecular weight determination using viscometry, Osmometry, Light-scattering, Ultracentrifuge, Gel permeation chromatography and end group analysis.

Application and Processing of polymers: Phenol-formaldehyde, Urea-formaldehyde, Melamine-formaldehyde, Epoxy Resins and curing Agents, Polyamides: Nylon-6, Nylon-6,6, Processing of thermoplastics and thermosetting resins for films, Fibers, Foams, Sheets and tubing.

Structure and Properties of polymers: Morphology and order in crystalline polymers, polymer structure and physical properties.

Conducting Polymers: Synthesis of conducting polymers, Preparation of conducting polymers for various devices like electronic devices, Chemical sensors, Solar cells, Light emitting devices, Biomedical devices

Natural Polymers: Structures, Properties and applications of shellac, Lignin, Rubber, Starch and proteins.
Chemical modification of cellulose and polystyrene, Polyelectrolyte's, Polymer liquid crystals.

Course learning outcomes (CLOs): The student will be able to

1. interpret different mechanisms of polymerization.
2. determine number, weight and viscosity average molecular weights by various techniques
3. correlate thermoplastic and thermosetting polymer processing
4. recognize conducting polymers and their applications.

Recommended Books

1. Gowarikar, V. R., Polymer Science, New Age International Pvt. Ltd., New Delhi (1997).
2. Odian, G., Principles of Polymerization, John Wiley & Sons (2001).
3. Peacock, A., and Calhoun, A., Polymer Chemistry-properties and applications, Hanser Publishers, Munich, (2006).
4. Chandra, R., and Adab, A., Rubber and Plastic Waste, CBS Publishers & Distributors, New Delhi, (1994).
5. Bahadur, P., and Sastry, N. V., Principles of Polymerisation, Narosa Publishing House, New Delhi (2002).

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY --- SUPRAMOLECULAR CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To impart knowledge of types of supramolecules, structures their applications as organic materials, sensors, and devices.

Introduction: Concepts and development, Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-π, anion-π, π-π and van der Waal interactions, Ionophores, Porphyrin and other tetrapyrrollic macrocycles, Coenzymes, DNA and biochemical self-assembly.

Host–guest Chemistry: Synthesis and structures of crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarene, Cyclodextrins, Cyclophanes, Cryptophanes, Carcerands and hemicarcerands, , Preorganisation and complimentarity, Lock and key analogy.

Supramolecular Polymers: Self-assembly molecules: Design, Synthesis and Properties of the molecules, Self assembly by H-bonding, Catenanes, Rotaxanes, Relevance of supramolecular chemistry to mimic biological system.

Molecular Devices: Molecular Electronic devices, Molecular switches and Molecular logic gates. Examples of recent developments in supramolecular chemistry from current literature.

Course learning outcomes (CLOs): The students will be able to

1. know molecular recognition and nature of bindings involved in biological systems
2. interpret the structure of supramolecules of various types in solution and solid state
3. recognize applications of supramolecules in miniaturization of molecular devices

Recommended Books

1. *Lehn, J. M., Supramolecular Chemistry-Concepts and Perspectives, Wiley –VCH (1995).*
2. *Beer, P.D., Gale, P. A., and Smith, D. K., Supramolecular Chemistry, Oxford University Press (1999).*
3. *Steed, J. W., and Atwood, J. L., Supramolecular Chemistry, Wiley (2000).*

Evaluation Scheme

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY---BIOFUELS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To acquire knowledge of different methods of biofuel production, application, and their advantages.

Introduction: Drivers for alternative fuels, security, cost and environmental considerations, carbon sequestration and the impact of biofuels, review of current processes for biofuel production from biomass.

Economic Models: Costing of current and future processes for biofuel production from biomass, biomass availability, models of biomass concentration and utilization.

Feedstock Chemistry: Chemistry of triglycerides and carbohydrates, Improving biomass yield and properties for easier processing and conversion, Pretreatment of biomass, Enzymatic hydrolysis, Processes and alternatives, Enzymes immobilization techniques.

Fermentation: Processes and alternatives, Aqueous processing of sugars.

Bio-Diesel and other alternative liquid fuels, Policy of biofuels, Biofuels around the world: Brazil, India and China.

Course learning outcomes (CLOs): The students will be able to discuss biofuel production technologies, and their applications.

Recommended Books:

1. *Bhojvaid, P.K., Biofuels: Towards a greener and secure energy future, TERI Press (2006).*
2. *Adholeya, A., and Kumar P., Dadhich Production and Technology of Bio-diesel: Seeding a change, TERI press (2008).*
3. *Scragg, A. H., Biofuels: Production, Application and Development, CABI (2009).*
4. *Olsson, L., Biofuels, Springer, (2007).*
5. *Furfari, A., Biofuels: Illusion Or Reality? : the European Experience, Editions TECHNIP (2008).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY321--- REARRANGEMENTS AND RETROSYNTHESIS

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course Objective: To teach the concepts and critical bond forming reactions in organic synthesis and molecular rearrangements.

Molecular rearrangements: Rearrangements involving migration to electron-deficient carbon, Nitrogen and oxygen: Wagner-Meerein, Pinacol-pinacolone, Wolff, Benzil-benzilic acid rearrangements; Migration to heteroatoms; Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements; Baeyer-Villiger, Hydroperoxide rearrangements and Dakin reaction.
Rearrangements involving migration to electron-rich carbon: Favorski, Stevens, Sommelet-Hauser, Wittig rearrangements; Aromatic rearrangements: Migration around the aromatic nucleus, Migration of groups

from side chain to the nucleus, Rearrangement of aniline derivatives, Rearrangements involving migration from oxygen to the ring: Phenolic ethers, Fries, Claisen rearrangements.

Retrosynthesis: Synthons and synthetic equivalents, Definitions, Guidelines, Functional group interconversions, Use of acetylenes and aliphatic nitrocompounds in organic synthesis; Two-group C-C disconnections – Diels-Alder reaction, 1,3- and 1,5-difunctional compounds (Michael addition and Robinson annulation), Order of events in organic synthesis, Reversal of polarity (umpolung), Cyclisation reactions.

Course learning outcomes (CLOs): The students will be able to interpret

1. mechanistic pathway of organic reactions.
2. retrosynthetic approach to planning organic syntheses.
3. conversion of different functional group *via* rearrangement reaction.

Recommended Books

1. *Carruthers, W., Some Modern Methods of Organic Synthesis, Cambridge University Press (1987).*
2. *Warren, S., Organic Synthesis: The Disconnection Approach, Wiley (2007).*
3. *Sanyal, S. N., Reactions, Rearrangements & Reagents, BharatiBhavan (2004).*
4. *Chemistry Education: Research and Practice in Europe, 2002, Vol. 3, No. 1, pp. 33-64.*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY--- PHOTOPHYSICAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To acquire knowledge of photochemistry and photophysical principles, their applications on simple and macromolecules.

Principles and Concepts: Laws of photochemistry, Atomic and molecular term symbols, Electronic transitions, Jablonski diagram and photophysical processes, Radiative transitions, Absorption and emission, Absorption coefficient, Phosphorescence, Intersystem crossing, Mechanisms of singlet-triplet conversion (spin-orbit coupling), Spin rephasing, Spin flip, Examples of ISC between states of different configurations, Radiative rates, Radiationless transitions, Internal conversion, Energy gap law, Deuterium effect.

Electronically Excited States: Electronic, Vibrational and spin configurations, Excited state lifetime, Steady state and time resolved emission, Factors affecting excited state energy, Solvent effect, TICT, Origin of energy difference between singlet and triplet states, Excited state kinetics, Quantum yield expressions, Excimer and exciplex, Kinetics of luminescence quenching, Static and dynamic, Stern-Volmer analysis, Deviation from Stern-Volmer kinetics, Photoinduced electron transfer rates, Free energy dependence of electron transfer on rate, Photoinduced energy transfer, FRET, ESPIT, TBET, Rate and efficiency calculation of FRET.

Applications of Photochemistry and Photophyscial Principles: Measurement of fluorescence and phosphorescence and lifetimes, Introduction to time-resolved techniques for absorption and emission measurements, Detection and kinetics of reactive intermediates, Photochromic reactions and memory devices, Sensors, Switches and molecular machines, TiO_2 photocatalysis, , Flash photolysis.

Course learning outcomes (CLOs): The student will be able to
1. assess photochemistry and photophysical principles.
2. identify and characterize of transient intermediates by ultrafast modern techniques.
3. know the theory and application of photochemistry and photophysical principles of macromolecules.

References:

1. *Lakowicz, J. R., Principles of Fluorescence Spectroscopy, Springer, New York (2006), 3rd ed.*
2. *Kavarnos, G. J., Fundamentals of Photoinduced Electron Transfer, VCH publishers Inc., New York (1993).*
3. *Valeur, B., Molecular Fluorescence: Principles and Applications, Wiley-VCH Verlag GmbH, Weinheim (2002).*
4. *Turro, N. J., Ramamurthy, V., and Scaiano, J. C., Modern Molecular Photochemistry of Organic Molecules, University Science, Books, CA (2010).*
5. *Ninomiya, I., and Naito, T., Photochemical Synthesis, Academic Press, New York (1989).*

Evaluation Scheme

MST	EST	Sessional (May include Project/ Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY--- BIOPOLYMER AND PROTEIN CHEMISTRY

L	T	P	Cr
3	**0**	**0**	**3.0**

Prerequisite(s): None

Course objective: To provide knowledge of structure, function, and physicochemical properties of biopolymers and proteins.

Biopolymers: The structure, Function, and Properties of synthetic (Dextran, Ficoll) and natural biopolymers (DNA, nucleic acids, nucleotides, proteins), Conformation of nucleic acids (DNA, t-RNA, micro-RNA), Molecular architecture for some biological structures such as collagen, Tissue, Silk, Wool, and shell. Introduction to biomedical materials and “drug delivery” formulations.

Proteins: Principles of biophysical chemistry (pH, buffer, reaction kinetics, Thermodynamics, **C**olligative properties), Structure and physical properties of amino acids, Physical principle of structure, Function, and Folding of proteins, Conformations of proteins (Ramachandran plot, Secondary, Tertiary and Quaternary structure; Domains; Motif and Folds), Determination of protein structures by spectroscopic methods (CD, FTIR, NMR), Mechanisms of protein folding, Thermodynamics of protein folding by spectroscopic and calorimetric methods, Ultrafast folding dynamics study by laser flash photolysis, Protein conformational study by NMR and fluorescence spectroscopy, Measurement of hydrodynamic radii by dynamic light scatter.

Course learning outcomes (CLOs): The students will be able to evaluate

1. physico-chemical properties, and molecular architecture of biopolymers.
2. folding, stability, and dynamics of protein.
3. the dynamics and fast kinetics by Stopped flow and laser flash photolysis methods.

Recommended Books

1. *Cantor, C.R., and Schimmel, P.R., Biophysical Chemistry, Freeman (1980).*
2. *Holde, V., Johnson, K. E., and Ho, P.S., Principles of Physical Biochemistry, Prentice Hall (1998).*
3. *Lakowicz, J.R., Principles of Fluorescence spectroscopy, Springer (1999).*
4. *Creighton, T.E., Protein Folding, W.H. Freeman (1992).*
5. *Jirgensons, B., Optical Rotatory Dispersion of Proteins and other Macromolecules, Springer-Verlag (1969).*
6. *Lesk, A.M., Introduction to Protein Science, Oxford University Press, (2010) 2nd ed.*

Evaluation Scheme

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
30	50	20

PCY--- ENVIRONMENTAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Course Objective: To study chemical processes taking place in earth's atmosphere and hydrosphere, and to learn air pollution control methods.

Introduction: Environmental chemistry, Environmental composition, Chemical processes.

Earth's atmosphere: Chemical composition, Reactions in atmosphere, Stratospheric chemistry, Catalytic decomposition of ozone, CFCs and related compounds, Ozone hole. Tropospheric chemistry – Chemistry of photochemical smog, Precipitation, Acid rain, Production and removal of nitric acid, Sulphuric acid. Atmospheric aerosols – Sources, Concentrations, Control. Chemistry of global climate.

The hydrosphere: Physical and chemical properties of water, Distribution of species in aquatic systems: Single variable diagrams, Two variable diagrams, Method of calculating pE°.

Gases in water: Henry's law, Concentration of oxygen in natural waters, Carbon dioxide in water. Alkalinity – Water as acid neutralising agent, Environmental relevance.

Organic matter in water – Origin, Environmental issues, Reactions, Consumption of oxygen.

Metals in aqueous environment - Classification, Complexes, Metal speciation of calcium, Copper and mercury, their behaviour in hydrosphere.

Environmental Chemistry of Colloids and Surfaces: Colloid size and surface area, Surface area Properties of colloidal materials: Surface charge, Electrical double layer, Ion exchange, Adsorption, Quantitative descriptions of adsorption: The Langmuir relation, Partitioning of small organic solutes. Colloidal material in natural environment.

Air Pollution: Introduction and control methods

Course learning outcomes (CLOs): Students will be able to explain

1. different concepts of atmosphere, stratospheric and tropospheric chemistry, photochemical smog, acid rain, atmospheric aerosols, global climate.
2. gases in hydrosphere, organic matter in water, humic material, metals in aqueous environment.
3. chemistry of colloids with reference to environment.
4. air pollution and its control.

Recommended Books:

1. *Van-Loon G.W., and Duffy S.J., Environmental Chemistry, Oxford University Press (2005) 3rded.*
2. *Rao C.S., Environmental Pollution Control Engineering, New Age International Publishers, New Delhi, 2nd Edition (2006).*
3. *Sindhu P.S., Environmental Chemistry, New Age International Publishers (2002) 2nded.*
4. *De A.K., Environmental Chemistry, New Age International Publishers (2008)6thed.*

Evaluation Scheme

MST	EST	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)
30	50	20