



# **COURSES SCHEME**

**&**

# **SYLLABUS**

**FOR**

**M.SC.**

**CHEMISTRY**

**2015**

**COURSE SCHEME & SYLLABUS FOR M.SC. (CHEMISTRY)****SEMESTER – I**

<b>SR. NO.</b>	<b>COURSE NO.</b>	<b>TITLE</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>CR</b>
1	PCY108	CHEMICAL BIOLOGY (FOR NON-MEDICAL GROUP)	3	1	0	3.5
	PIM101	BASIC MATHEMATICS (FOR MEDICAL GROUP)				
2	PCY101	ANALYTICAL CHEMISTRY	3	1	0	3.5
3	PCY102	INORGANIC CHEMISTRY	3	0	0	3.0
4	PCY109	STEREOCHEMISTRY AND PHOTOCHEMISTRY	3	0	0	3.0
5	PCY104	QUANTUM CHEMISTRY	3	0	0	3.0
6	PCY201	ELECTROCHEMISTRY AND THERMODYNAMICS	3	0	0	3.0
7	PCY206	INORGANIC CHEMISTRY LAB	0	0	6	3.0
8	PHU002	PROFESSIONAL COMMUNICATION	3	1	0	3.5
<b>TOTAL</b>			<b>21</b>	<b>3</b>	<b>6</b>	<b>25.5</b>

**SEMESTER – II**

<b>SR. NO.</b>	<b>COURSE NO.</b>	<b>TITLE</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>CR</b>
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		ELECTIVE – I	3	0	0	3.0
8	PCY205	COMPUTER PROGRAMMING AND APPLICATION	2	0	2	3.0
<b>TOTAL</b>			<b>17</b>	<b>1</b>	<b>11</b>	<b>23.0</b>

### SEMESTER – III

SR. NO.	COURSE NO.	TITLE	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		ELECTIVE – II	3	0	0	3.0
	PCY391/PCY392	SEMINAR/MINOR PROJECTS*	-	-	-	2.0
<b>TOTAL</b>			<b>15</b>	<b>2</b>	<b>12</b>	<b>24.0</b>

\* MAY BE UNDERTAKEN/COMPLETED WITHIN SCHOOL OR WITHIN THAPAR UNIVERSITY.

### SEMESTER – IV

SR. NO.	COURSE NO.	TITLE	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	PCY491	DISSERTATION	-	-	-	6.0
<b>TOTAL</b>			<b>6</b>	<b>1</b>	<b>0</b>	<b>12.5</b>

### ELECTIVE – I

SR. NO.	COURSE NO.	TITLE	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	PCY213	SUPRAMOLECULAR CHEMISTRY	3	0	0	3.0
4	PCY214	BIOFUELS	3	0	0	3.0

**ELECTIVE – II**

<b>SR. NO.</b>	<b>COURSE NO.</b>	<b>TITLE</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>CR</b>
1	PCY321	REARRANGEMENTS AND RETROSYNTHESIS	3	0	0	3.0
2	PCY322	PHOTOPHYSICAL CHEMISTRY	3	0	0	3.0
3	PCY323	BIOPOLYMER AND PROTEIN CHEMISTRY	3	0	0	3.0
4	PCY432	ENVIRONMENTAL CHEMISTRY	3	0	0	3.0

**TOTAL NUMBER OF CREDITS = 85.0**

## PCY108 CHEMICAL BIOLOGY

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>1</b>	<b>0</b>	<b>3.5</b>

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

**Introduction:** Cell structure and functions, Scales of biological systems, Dimensions of biomolecules 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 (CLO):

Students will acquire knowledge of:

1. Molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids.
2. 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).
2. Berg, J.M., and Tymoczko, J.L., Stryer, L., *Biochemistry*, W.H. Freeman (2007).
3. Garrett, R.H., Grisham, C.M., *Biochemistry*, Brooks/Cole, Cengage Learning, (2010).
4. Conn, E.E., and Stump, F., *Outlines of Biochemistry*, John Wiley (2006).

### Evaluation Scheme:

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

## PIM101: BASIC MATHEMATICS

L T P Cr  
3 1 0 3.5

**Course Objective:** The objective is to develop basic computing skills and application of quantitative and statistical operations required for biological studies and rationalization of experimental designs.

**Algebra:** Linear and quadratic equations; Complex numbers, Argand plane and polar representation of a complex number, square root of a complex number; Permutations and Combinations; Binomial theorem for positive/negative index and its simple applications; Arithmetic and Geometric progression.

**Trigonometry:** Review of trigonometric functions, sum and product formulae for trigonometric functions, Trigonometric Equations and C-D formulas for trigonometric functions; Identities related to  $\sin(2x)$ ,  $\cos(2x)$  and  $\tan(2x)$ .

**Determinants and Matrices:** Matrices, Operations on Matrices, Determinants and its properties, singular and non-singular matrices, Adjoint and inverse of a matrix and its properties, Solution of system of linear equations using Cramer's rule and inverse of a matrix.

**Differentiation:** Review of sets, relations and functions, Limit, Continuity and Differentiability, Differentiation of standard functions (polynomials, trigonometric, inverse trigonometric exponentials and logarithmic); Product rule, Quotient rule, applications of derivatives in Graphing

**Integration:** Integral as anti-derivative. Integration by substitution, by partial Fractions and by parts. Definite integral and its properties. Areas of bounded regions

**Coordinate geometry:** Rectangular Coordinate system, Straight lines, Circles. (in standard form).

### **Course Learning Outcomes (CLO):**

Students will acquire mathematical concepts in continuous learning and connecting ideas like numerical analysis, calculus, coordinate geometry to other subjects and support learning through applications of mathematics.

### **Recommended Books:**

1. *Mathematics, A Text book (Parts I & II), 2011, NCERT, New Delhi.*
2. *Thomas, G.B. and Finney, R.L. Calculus and Analytical Geometry, Pearson Education. (2007).*
3. *Shanti Narayan, Differential and Integral Calculus, S. Chand (2005).*
4. *Krishnamurthy V.K., Mainra V.P. and Arora J.L. An introduction to Linear Algebra. Associated East West Press (2007).*

## PCY101: ANALYTICAL CHEMISTRY

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>1</b>	<b>0</b>	<b>3.5</b>

**Course Objective:** To introduce concepts of various analytical techniques.

**Optical Methods:** Principle, applications and limitations of Spectrophotometry, Beer-Lambert Law, Analysis of mixtures, Atomic Absorption Spectrometry, Atomic Emission Spectroscopy, Plasma and Electric Discharge Spectroscopy, Spectrofluorimetry, Nephelometry 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 (CLO):

The students will acquire knowledge of:

1. Principles of 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).*
3. *Christian, G.D., Analytical Chemistry, Wiley (2007).*
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).*

### Evaluation Scheme:

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

## PCY102: INORGANIC CHEMISTRY

L T P Cr  
3 0 0 3.0

**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  $\pi$ -acceptor and  $\sigma$ -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 organometallic compounds as Homogeneous and Heterogeneous Catalysts.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. Chemistry of main group elements, and 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).
2. Huheey, J.E., Keiter, E.A. and Keiter, R.L., *Inorganic Chemistry*, Pearson Education, (2002).
3. Greenwood, N.N., and Earnshaw, A., *Chemistry of the Elements*, Butterworth-Heinemann, (1997).
4. Lee, J.D., *Concise Inorganic Chemistry*, ELBS, (1996).
5. Sharpe, E., *Inorganic Chemistry*, Pearson Education (2003).
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

**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. Cycloadditions - antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic 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,  $\beta$ ,  $\gamma$ -unsaturated and  $\alpha$ ,  $\beta$ -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  $\pi$ -molecular orbitals, Annulenes, Antiaromaticity, Homo-aromaticity.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

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).
2. March, J., and Smith, M. B., *March's Advanced Organic Chemistry: Reactions, Mechanisms and structures*, John Wiley (2007).
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/Quizes/Assignments/Lab Evaluation))
30	50	20

PCY104: QUANTUM CHEMISTRY				
	L	T	P	Cr
	3	0	0	3.0

**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<sub>2</sub>O and NH<sub>3</sub>. Huckel Theory of Conjugated Systems, Bond Order and Charge Density Calculations, Applications to Ethylene and Butadiene.

**Course Learning Outcomes (CLO):**

The students will acquire knowledge of:

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).
2. Chandra, A.K., *Introduction to Quantum Chemistry*, Tata McGraw Hill (2004).
3. Atkins, P., and Friedman, R., *Molecular Quantum Mechanics*, Oxford University Press (2005).
4. Prasad, R.K., *Quantum Chemistry*, Wiley Easter (1992).
5. McWeeny, R., *Coulson's Valence*, Oxford University Press (1980).

**Evaluation Scheme:**

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

## PCY201: ELECTROCHEMISTRY AND THERMODYNAMICS

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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 Outcome (CLO):

The students will acquire knowledge of

1. Redox processes in electrochemical systems.
2. Debye-Huckel theory and determination of activity and activity coefficient.
3. 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).*
2. *Puri, B.R., Sharma, L.R., and Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co. (2011).*
3. *Kapoor, K.L., A Text Book of Physical Chemistry, Vol. 3, Macmillan India (2005).*
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

**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.

**Spectrophotometric Determination:**  $\text{NO}_3^-$  in water sample,  $\text{K}_2\text{Cr}_2\text{O}_7$  in the presence of  $\text{KMnO}_4$  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 (CLO):

The students will acquire knowledge of

1. Volumetric and gravimetric analysis of cations and anions.
2. Operation and application of spectrophotometer, AAS and flame photometer.

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

### Evaluation Scheme:

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

## PHU002: PROFESSIONAL COMMUNICATION

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>1</b>	<b>0</b>	<b>4</b>

**Course Objective:** To provide the students with essential skills required for effective communication, and, to apprise them of business communication and its role in corporate environment.

**Essentials of Communication:** Meaning, Definition, process and barriers. Emergence of communication as a key concept in the corporate and global world.

**Methods and Modes of Communication:** Verbal and nonverbal, Verbal Communication: Characteristics of verbal communication: Non-verbal Communication: Characteristics and types.

**Listening:** Importance of listening skills, cultivating good listening skills.

**Written Communication:** Paragraph and Essay writing, Book reviews, Movie Reviews, Editorials and articles.

Effective Business writing: Letters, Reports. Paper writing: Styles of paper writing: Short Communication, Review papers and Research papers, Referencing styles: MLA, Chicago Style and APA.

**Presentations:** Principles of effective presentation, power-point presentation, video and satellite conferencing.

**Interviews and Group Activities:** Personal interviews, group discussion and panel discussion (tutorial classes)

### **Course Learning Outcomes (CLO):**

Students will have understanding of:

1. The use of proper writing techniques relevant to the present day technological demands, including anticipating audience reaction,
2. How to write effective and concise letters
3. How to prepare informal and formal reports,
4. How to proofread and edit copies of business correspondence
5. How to develop interpersonal skills that contribute to effective personal, social and professional relationships

### **Recommended Books:**

1. *Lehman, C.M., DuFrene, D.D., and Walker, R, B-BCOM - An Innovative Approach to Learning and Teaching Business Communication. Cengage Learning New Delhi, 2011.*
2. *McMurrey, A.M and Buckley, J., Handbook for Technical Writing, Cengage Learning, New Delhi, 2008.*
3. *Lesikar, R.V and Flatley, M.E., Basic Business Communication-Skills for Empowering the Internet Generation, Tata McGraw-Hill Publishing Company Limited. New Delhi, 2005.*

## PCY215: MOLECULAR SPECTROSCOPY

L	T	P	Cr
3	1	0	3.5

**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  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  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  $\text{Fe}^{+2}$  and  $\text{Fe}^{+3}$  compounds.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis
2. Electronic spectroscopy of different elements and simple molecules.
3. Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

**Recommended Books:**

1. *Hollas, J.M., Modern Spectroscopy, John Wiley (1996).*
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 MacLachlan, 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

**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  $\pi$ -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 (CLO):

The students will acquire knowledge of:

1. Formation, Reaction mechanism and stability of the coordination complexes.
2. Interpretation of the electronic and magnetic properties.

### Recommended Books:

1. Cotton, F.A., Wilkinson, G., Murillo, C.A., and Bochmann, M., *Advanced Inorganic Chemistry*, John Wiley (2003).
2. Huheey, J.E., Keiter, E. A., and Keiter, R. L., *Inorganic Chemistry*, Pearson Education (2002).
3. Greenwood, N.N., and Earnshaw, A., *Chemistry of the Elements*, Butterworth-Heinemann (1997).
4. Lever, A.B.P., *Inorganic Electronic Spectroscopy*, Elsevier Science (1985).
5. Banerjea, D., *Coordination Chemistry*, Asian Books Private Limited (2007).
6. McCleverty, J.A., and Meyer, T.J., *Comprehensive Coordination Chemistry II*, Vol. 9, Elsevier (2004).

**Evaluation Scheme:**

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

## PCY203: ORGANIC REACTION MECHANISMS

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

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

**Aliphatic Substitution:** Nucleophilic –  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1$  and  $S_N^2$  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, Sandmeyer, Vilsmeier, Gatterman Koch, Gatterman, Kolbe-Schmidt reactions, Houben, Hoesch.

Nucleophilic – Aromatic nucleophilic substitution mechanism ( $S_{NAr}$ ,  $S_{N1}$  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:**  $\beta$ -Elimination –  $E_2$  and  $E_1$ ,  $\alpha$ -elimination.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

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).
2. Carey, F.A., and Sundberg, R.J., *Advanced Organic Chemistry, (Part B)*, Springer (2007).
3. March, J., and Smith, M.B., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, John Wiley (2007).
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

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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 (CLO):

The students will acquire knowledge of:

1. Principals of industrial chemistry and procedures for production of some industrially important products.
2. Concepts and applications of green chemistry in light of industrial chemistry.

### Recommended Books:

1. Howard, W.L., *Introduction to Industrial Chemistry*, Wiley-Interscience (1986).
2. Riegel, E. R.R., *Industrial Chemistry*, Reinhold Publishing Corporation (1960).
3. Matlack, A. S., *Introduction to Green Chemistry*, CRC Press, (2010).
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/Quizes/Assignments/Lab Evaluation)
30	50	20

## PCY209: ORGANIC CHEMISTRY LAB

L T P Cr  
0 0 3 1.5

**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: Aspirin, Schiff's base, Diels-Alder adduct.  
Determination of melting point and mixed melting point.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. Chromatographic separation and identification of organic compounds.
2. Purification, Crystallization, and different Distillation processes.
3. 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).
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

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>0</b>	<b>0</b>	<b>6</b>	<b>3.0</b>

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

### List of Experiments:

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 (CLO):

The students will acquire knowledge of:

1. Experimental techniques for controlling the chemical reactions.
2. Measurement of various physical and chemical properties.
3. Applying related experiments for their research work.

### 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/Quizes/Assignments/Lab Evaluation)
00	70	30

## PCY205: COMPUTER PROGRAMMING AND APPLICATION

L T P Cr.  
2 0 2 3.0

**Introduction to Computer's general concept:** Definition, Categories of Computer with description, Applications of Computers in various fields, CPU, Primary memory, secondary storage devices, Input/output devices, Computer as a system.

**Programming Languages:** Evolution of Programming Language, Tools used to convert computer program - compiler, interpreter, overview of machine language, assembly language, high level languages, Binary arithmetic for integer and fractional numbers.

**C Programming:** Introduction to algorithm, Flow charts, Problem solving methods, Need of programming languages. C character set, Identifiers and keywords, Data types, Declarations, Statement and symbolic constants, Input-output statements, Preprocessor commands, Operators, expressions and library functions, decision making and loop control statements, Functions, Storage Classes, Arrays, Strings, Pointers, Structure and union, File handling.

**Laboratory Work:** Laboratory experiments will be set in consonance with the materials covered in theory.

### ***Recommended Books:***

1. Peter Norton, Introduction to COMPUTERS, Tata McGraw Hill.
2. Kernighan, B. W. and Ritchie D.M., The C Programming Language, PHI (1989)
3. Kanetkar, Y., Let Us C, BPB (2007).
4. Forouzan, A., Structured Programming Approach Using C, Cengage India Pvt Ltd (2008).
5. GaryB Shelly, Thomas J Cashman and Misty E Vermaat, Introductions to COMPUTERS, Cengage Learning (2008).

## PCY316: CHEMICAL KINETICS AND SURFACE CHEMISTRY

L T P Cr

3 1 0 3.5

**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 Outcome:

The students will acquire knowledge of:

1. Mechanism for chemical reactions for optimizing the experimental conditions.
2. Application of homogeneous and heterogeneous catalysis in chemical synthesis
3. Importance of adsorption process and catalytic activity at the solid surfaces
4. Concept of 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

**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 (CLO):

The students will acquire knowledge of:

1. Concepts of symmetry and group theory in solving chemical structural problems.
2. Use of character tables and projection operator techniques.
3. Application of symmetry and group theory in spectroscopy.

### Recommended Books:

1. Cotton, F.A., *Chemical Applications of Group Theory*, John Wiley (1990).
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

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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-Hartwig amination, 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 diisopropylamide, Dicyclohexylcarbodiimide, 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 (CLO):

The students will acquire knowledge of:

1. Experimental techniques for different catalytic reactions.
2. Physical and chemical characterization of catalysts and catalytic reaction.
3. 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).*
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

**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.

**<sup>13</sup>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 spectrometry. 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, <sup>1</sup>H NMR, <sup>13</sup>C NMR and MS.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. IR range for functional groups,  $\lambda_{\max}$  for polyenes and  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds.
2. Cotton effect curves for obtaining absolute configuration of chiral molecules with chromophores.
3. Solve structural problems based on UV-Vis, IR, <sup>1</sup>HNMR, <sup>13</sup>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).*
4. *Silverstein, R.M., and Webster, F.X., Spectrometric Identification of Organic Compounds, John Wiley & Sons, Inc. (2005).*
5. *Martin, M.L., Delpuech, 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/Quizes/Assignments/Lab Evaluation)
30	45	25

## PCY309: ANALYTICAL CHEMISTRY LAB

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>0</b>	<b>0</b>	<b>3</b>	<b>1.5</b>

**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.,  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) 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  $\text{Fe}^{2+}/\text{Fe}^{3+}$  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  $\text{Co}(\text{NH}_3)_6^{3+}$  by cyclic voltammetry.

**Course Learning Outcomes (CLO):** The students will acquire knowledge of development of 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).
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/Quizes/Assignments/Lab Evaluation)
00	70	30

## PCY305: INORGANIC SYNTHESIS LAB

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>0</b>	<b>0</b>	<b>3</b>	<b>1.5</b>

**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)<sub>2</sub>Cl<sub>2</sub>]<sup>+</sup>, 1-Acetyl ferrocene and separation by TLC, Hg[Co(SCN)<sub>4</sub>] as standard for the magnetic moment measurement, Preparation and separation of isomers of K<sub>3</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>], Cu(II) and Ni(II) complexes of Schiff base, VO(acac)<sub>2</sub>, Conventional and green method for the preparation of isomers of tris(8-hydroxyquinolato)aluminum(III) complex.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. Preparation and purification of different inorganic complexes.
2. Application of 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).
2. Angelici, R.J., *Synthesis and Techniques in Inorganic Chemistry*, W B Saunders 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

**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<sub>2</sub>O<sub>5</sub>. Safely disposing off P<sub>2</sub>O<sub>5</sub> using methanol.

**Preparation, Separation and purification of organic compounds, and their characterization by spectral techniques (UV, IR, <sup>1</sup>H NMR, <sup>13</sup>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  $\alpha$ -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, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and MS.

### Course Learning Outcomes (CLO):

The students will acquire knowledge of:

1. Safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents.
2. Synthetic procedures: aqueous workup, distillation, reflux, separation, isolation, and crystallization.
3. Starting materials, functional groups, mechanism, and typical reaction conditions.
4. 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

## PCY401: HETEROCYCLIC CHEMISTRY AND NATURAL PRODUCTS

L	T	P	Cr
3	0	0	3.0

**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  $^1\text{H}$  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 (CLO):

The students will acquire knowledge of:

1. Nomenclature of different heterocyclic compounds.
2. Synthesis and reactivity of fused, six membered and smaller heterocyclic compounds.
3. Classification and importance of various natural products.

### Recommended Books:

1. Gilchrist, T.L., *Heterocyclic Chemistry*, Prentice Hall (1997)
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 Vol.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/Quizes/Assignments/Lab Evaluation)
30	50	20

## PCY402: ADVANCED TOPICS IN CHEMISTRY

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>1</b>	<b>0</b>	<b>3.5</b>

**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 (CLO):

The students will acquire knowledge of:

1. Factors that govern the stability, folding, and dynamics of proteins.
2. Kinetics, thermodynamics, and mechanism of protein folding.
3. Structure and biological functions of proteins and the role of metals in biology.
4. 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).
2. Lesk, A.M., *Introduction to Protein Science*, Oxford University Press, (2010).
3. Cowan, J.A., *Inorganic Biochemistry-An Introduction*, Wiley-VCH (1997).
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

## PCY211: MEDICINAL AND PHARMACEUTICAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

**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, Bioisosterism, 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, Benzodiazepines, Buspirone. Antipsychotic drugs - the neuroleptics, Antidepressants, Butyrophenones, Serendipity and drug development, Stereochemical aspects of psychotropic drugs.

**Antibiotics:** Cell wall biosynthesis, Inhibitors,  $\beta$ -lactam rings, Antibiotics inhibiting protein synthesis.

### Course Learning Outcome (CLO):

The students will acquire knowledge of:

1. Drug designing and development, their SAR and QSAR.
2. Mode of action of different drugs.
3. 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).
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).
4. Brunton, L.L., Chabmer, B.A., and Knollmann, B.C., *Goodman and Gilman's Pharmacological Basis of Therapeutics*, Ed. McGraw-Hill (2011).
5. Silverman, R.B., *The Organic Chemistry of Drug Design and Drug Action*, Elsevier (2004).
6. Lednicer, D., *Strategies for Organic Drug Synthesis and Design*, John Wiley & Sons. (2008).

**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

**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 (CLO):**

The student will have knowledge of:

1. Different mechanisms of polymerization.
2. Number, weight and viscosity average molecular weights with various techniques

3. Processing of thermoplastic and thermosetting polymers.
4. concept of conducting polymers and their applications.

**Recommended Books:**

1. Gowariker, 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/Quizes/Assignments/Lab Evaluation)
30	50	20

## PCY213: SUPRAMOLECULAR CHEMISTRY

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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- $\pi$ , anion- $\pi$ ,  $\pi$ - $\pi$  and van der Waal interactions, Ionophores, Porphyrin and other tetrapyrrolic 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 complementarity, 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 (CLO):

The students will acquire knowledge of:

1. Molecular recognition and nature of bindings involved in biological systems
2. Structure of supramolecules of various types in solution and solid state
3. 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

## PCY214: BIOFUELS

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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 (CLO):

The students will acquire the knowledge of 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/Quizes/Assignments/Lab Evaluation)
30	50	20



## PCY321: REARRANGEMENTS AND RETROSYNTHESIS

L	T	P	Cr
3	0	0	3.0

**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-Meerwein, 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 (CLO):

The students will acquire knowledge of

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

## PCY322: PHOTOPHYSICAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

**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 Photophysical 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<sub>2</sub> photocatalysis, , Flash photolysis.

### Course Learning Outcomes (CLO):

The student will have knowledge of:

1. Photochemistry and photophysical principles.
2. Identification and characterization of transient intermediates by ultrafast modern techniques.
3. Theory of photoreaction.
4. application of photochemistry and photophysical principles on simple and macromolecules.

### References Books:

1. Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*, Springer, New York (2006).
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/Quizes/Assignments/Lab Evaluation)
30	50	20

## PCY323: BIOPOLYMER AND PROTEIN CHEMISTRY

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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, Colligative 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 (CLO):

The students will acquire knowledge of:

1. Physico-chemical properties, and molecular architecture of biopolymers.
2. Folding, stability, and dynamics of protein.
3. Dynamics by using fast kinetic methods (Stopped flow and laser flash photolysis).

### 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).

### Evaluation Scheme:

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

<b>PCY432: ENVIRONMENTAL CHEMISTRY</b>				
	<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
	<b>3</b>	<b>0</b>	<b>0</b>	<b>3.0</b>

**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  $pE^\circ$ .

**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 (CLO):**

Students will be able to learn:

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).
2. Rao C.S., *Environmental Pollution Control Engineering*, New Age International Publishers, New Delhi (2006).
3. Sindhu P.S., *Environmental Chemistry*, New Age International Publishers (2002).
4. De A.K., *Environmental Chemistry*, New Age International Publishers (2008).

**Evaluation Scheme:**

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