# Syllabus of M.Sc – Chemistry

## PCY101 ANALYTICAL CHEMISTRY

L	Т	Р	Cr
3	1	0	3.5

### **Prerequisite(s):** None

Course objective: To introduce concepts of various analytical techniques.

**Errors in Quantitative Analysis:** Accuracy, Precision, Sensitivity, Specificity, Standard deviation, Classification of errors and their minimization, Significant figures, Criteria for rejection of data, Q-test, T-test and F-test, Control chart, Sampling methods, Sampling error, Statistical data treatment, Standard reference materials, Introduction to chemical metrology.

**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 Outcome: The students will acquire knowledge of

- 1. Data handling/ statistical treatment of data.
- 2. Principles of optical methods like AES, AAS, Plasma and Electric Discharge Spectroscopy, Spectrofluorimetry, Nephelometry and Turbidimetry.
- 3. Potentiometric, Coulometric, and Voltametric methods of analysis.
- 4. Chromatographic Techniques and applications.

- 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) 7<sup>th</sup>ed.

- 3. Christian, G.D., Analytical Chemistry, Wiley (2007) 6<sup>th</sup>ed.
- 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) 8<sup>th</sup>ed.

## PCY102 INORGANIC CHEMISTRY

L	Т	Р	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. Photophysical properties of Lanthanide complexes.

Nuclear Chemistry: Nuclear reactions, Radio Analytical Techniques and Activation analysis.

**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, Homogeneous and Heterogeneous Catalysis, Hydrogenation, Carbonylation and Polymerization.

Course outcome: 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) 6<sup>th</sup>ed.

- 2. Huheey, J.E., Keiter, E.A. and Keiter, R.L., Inorganic Chemistry, Pearson Education, (2002) 4<sup>th</sup> ed.
- *3. Greenwood, N.N., and Earnshaw, A., Chemistry of the Elements, Butterworth-Heinemann, (1997)* 2<sup>*nd*</sup> *ed.*
- 4. Lee, J.D., Concise Inorganic Chemistry, ELBS, (1996) 5<sup>th</sup> ed.
- 5. Sharpe, E., Inorganic Chemistry, Pearson Education (2003) 3<sup>rd</sup> 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 Organotransition Metal Chemistry, University Science Books (1989).

## PCY103 STEREOCHEMISTRY AND PHOTOCHEMISTRY

L	Т	Р	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.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, Energy level of  $\pi$ -molecular orbitals, Annulenes, Antiaromaticity,  $\psi$ -Aromaticity, Homo-aromaticity, PMO approach.

**Stereochemistry:** Conformational analysis of Cycloalkanes and Decalins, Effect of conformation on reactivity, Conformation of sugars, Steric-strain due to unavoidable crowding. Elements of symmetry, 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. Asymmetric synthesis.

**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, Fluxional tautomerism, Ene reaction.

**Photochemistry:** Introduction, Photochemistry of Alkenes: Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, 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, Photochemistry of Aromatic Compounds: Isomerisations, Additions and Substitutions. Photo-Fries reactions of Anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions.

## Course Outcome: 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) 5<sup>th</sup> ed.
- 2. *March, J., and Smith, M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms and structures, John Wiley (2007)* 6<sup>th</sup> 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).

## PCY104 QUANTUM CHEMISTRY

L	Т	Р	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:** Introduction, Schrodinger equation and the Postulates of Quantum Mechanics. Discussion of solutions of the Schrodinger equation to some model systems *viz.*, Particle in a box, The Harmonic Oscillator, The Rigid Rotor, The Hydrogen atom.

**Approximate Methods:** The Variation Theorem, Linear Variation Principle, Perturbation Theory (first order and non-degenerate). Applications of Variation Method and Perturbation Theory to the Helium atom.

**Angular Momentum:** Ordinary angular momentum, Generalized angular momentum, Eigen functions for angular momentum, Eigen values of angular momentum, Operator using ladder operators, Addition of angular momenta, Spin, Antisymmetry and Pauli exclusion principle.

**Electronic Structure of Atoms:** Electronic configuration, Russell-Saunders terms and Coupling Schemes, Slater-Condon parameters, Term Separation Energies of the  $p^n$  Configuration, Term Separation Energies for the  $d^n$  Configurations, Magnetic Effects: Spin-orbit Coupling and Zeeman Splitting, Introduction to the methods of Self-consistent field, The Virial Theorem.

**Born-Oppenheimer Approximation:** Hydrogen molecule ion. LCAO-MO and VB treatments of the Hydrogen molecule; Electron Density, Forces and their role in Chemical Binding. Hybridization and valence MOs of  $H_2O$ ,  $NH_3$  and  $CH_4$ . Huckel Theory of Conjugated Systems, Bond Order and Charge Density Calculations, Applications to Ethylene, Butadiene, and Cyclobutadiene.

Course Outcome: 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 manyelectron 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) 5<sup>th</sup> ed.
- 2. Chandra, A.K., Introduction to Quantum Chemistry, Tata McGraw Hill (2004) 4<sup>th</sup> ed.
- 3. Atkins, P., and Friedman, R., Molecular Quantum Mechanics, Oxford University Press (2005) 4<sup>th</sup> ed.
- 4. Prasad, R.K., Quantum Chemistry, Wiley Easter (1992).
- 5. *McWeeny*, *R.*, *Coulson's Valence*, *Oxford University Press* (1980) 3<sup>rd</sup> ed.

## PCY105 ELECTROCHEMISTRY AND THERMODYNAMICS

L	Т	Р	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 series, Electrochemical cells, Concentration cells with and without liquid junction, Application of electrochemical cell, Thermodynamics of reversible electrodes and reversible cells. Zeta potential, Redox indicators, Debye-Huckel treatment of dilute

electrolyte solutions, Derivation of Debye-Huckel limiting law, Extended Debye-Huckel law, Photoelectrochemical cells.

**Classical Thermodynamics:** Concepts involved in first, second and third law of thermodynamic, Thermodynamic equation of state, Maxwell relations, Free energy and entropy of mixing, Partial molar quantities, Gibbs-Duhem equation. Equilibrium constant, Temperature-dependence of equilibrium constant. Phase rule for one and two component system, Thermodynamic description of phase transitions. Ideal and non-ideal solutions, Activity and activity coefficient, Mean ionic activity coefficient, Ionic strength, Determination of activity and activity coefficient by Debye Huckel law, Concept of fugacity and determination of fugacity.

**Statistical Thermodynamics:** The concepts of Ensemble, Thermodynamic probability and entropy, 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, Calculation of equilibrium constants in term of partition function. Monoatomic solids, Theories of specific heat for solids.

**Course Outcome:** 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) 6<sup>th</sup> ed.
- 2. Puri, B.R., Sharma, L.R., and Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co. (2011) 45<sup>th</sup> ed.
- 3. Kapoor, K.L., A Text Book of Physical Chemistry, Vol. 3, Macmillan India (2005) 2<sup>nd</sup> ed.
- 4. Laidler, K.J., Chemical Kinetics, Dorling Kingsley (2007).
- 5. Rajaraman, J., and Kuriacose, J., Kinetics and Mechanism of Chemical Transformations, McMillan (2008).

## PCY106 INORGANIC CHEMISTRY LAB

L	Т	Р	Cr
0	0	6	3.0

Prerequisite(s): None

**Course Objective:** To impart the knowledge of various analytical techniques for inorganic compounds.

**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:** Covering the examples of cation and anion estimation, Mixture of cations present in the same solution.

**Spectrophotometeric determination:**  $NO_3^-$  in water sample,  $K_2Cr_2O_7$  in the presence of KMnO<sub>4</sub> and Fe(III) using 8-hydroxyquinoline.

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

Atomic absorption Spectrometry: Ni, Zn and Fe.

**Course outcome:** 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) 3<sup>rd</sup> ed.*
- 2. Skoog, D.A., Holler, F.J., and Nieman, T.A., Principles of Instrumental Analysis, Thomson, (2006) 5<sup>th</sup> ed.

## PCY107 CHEMICAL BIOLOGY

L	Т	Р	Cr
3	1	0	3.5

**Prerequisite(s):** None

**Course Objective:** To introduce structure, function and organization of various bio-molecules present in the living cell.

**Introduction:** 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.

**Cell Structure and Functions:** Structure of prokaryotic and eukaryotic cells, Intracellular organelles and their functions.

Amino Acids, Peptides and Proteins: Classification of amino acids and their properties, Polypeptides, Primary Structures - amino acid sequencing, Sequence determination, Chemical and Enzymatic hydrolysis of proteins to peptides, Secondary structures - forces responsible for holding of secondary structures,  $\alpha$ -helix,  $\beta$ -sheets, Super secondary structure, Ramachandran Plot, Triple helix structure of collagen, Tertiary structure of protein-folding and domain structure, Quaternary structure. **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:** Carbohydrates of glycoproteins and glycolipids, Role of sugars in biological recognition, Blood group substances, Carbohydrate metabolism - Kreb's cycle, Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, Pentose Phosphate pathway.

**Lipids:** Properties of lipid aggregates-micelles, Bilayers, Liposomes and their biological functions, Biological membranes, Fluid Mosaic model of membrane structure.

**Vitamins:** General characteristics, Classification, Role of Vitamins, Fat and water soluble vitamins, Deficiency of vitamins and diseases.

**Biocatalysis:** Enzymes classification and nomenclature, Enzyme Kinetics, Mechanisms of enzyme catalysis, Active sites, Activators and inhibitors, Coenzyme, Isozymes.

Course Outcome: The students will acquire knowledge of

- 1. Molecular structure of proteins, DNA, RNA, Carbohydrates, Lipids and Vitamins.
- 2. Organization and working principles of various components present in living cell.

## **Recommended Books**

- 1. Jain, J.L., Jain, S., and Jain, N., Fundamentals of Biochemistry, S. Chand (2005).
- 2. Stryer, L., Berg, J.M., and Tymoczko, J.L., Biochemistry, W.H. Freeman (2004) 4<sup>th</sup> ed.
- 3. Voet, D., and Voet, J.G., Biochemistry, John Wiley (1995) 2<sup>nd</sup> ed.
- 4. Conn, E.E., and Stump, F., Outlines of Biochemistry, John Wiley (2006) 5<sup>th</sup> ed.
- 5. Nelson, D.L., and Cox, M.M., Principles of Biochemistry, W.H. Freeman (2004) 4<sup>th</sup> ed.

## PCY201 MOLECULAR SPECTROSCOPY

L	Т	Р	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, Natural line width and natural line broadening, 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, Nuclear and electron spin interaction and Effect of external field, Applications.

**Vibrational Spectroscopy:** Infrared Spectroscopy– Simple harmonic oscillator, Vibrational energies of diatomic molecules, Zero point energy, Force constant and bond strengths; Anharmonicity, Vibration-rotation spectroscopy, P, Q, R branches, Breakdown of Oppenheimer approximation; Vibrations of polyatomic molecules, Selection rules, Normal modes of vibration, Group frequencies, Overtones, Hot bands, Factors affecting the band positions and intensities, Metal-ligand vibrations, Normal co-ordinate analysis.

**Raman Spectroscopy** - Classical and quantum theories of Raman effect, Pure rotational, Vibrational and Vibrational-Rotational Raman spectra, Selection rules, Mutual exclusion principle, Resonance Raman spectroscopy, Coherent anti Stokes Raman spectroscopy (CARS).

**Electronic Spectroscopy:** Energies of atomic and molecular orbitals, Vector representation of momenta and vector coupling, Spectra of hydrogen atom and alkali metal atoms. Vibronic transitions, Vibrational progressions and geometry of the excited states, Franck-Condon principle, Electronic spectra of polyatomic molecules, Emission spectra, Radiative and non-radiative decay, Internal conversion, Spectra of transition metal complexes, Charge-transfer spectra.

**Magnetic Resonance Spectroscopy:** Nuclear Magnetic Resonance Spectroscopy - Nuclear spin, Nuclear resonance, Saturation, Shielding of magnetic nuclei, Chemical shift and its measurements, Factors influencing chemical shift, Deshielding, Spin-spin interactions, Factors influencing coupling constant 'J', Classification (ABX, AMX, ABC, A<sub>2</sub>B<sub>2</sub> etc.), Spin decoupling, Basic ideas about instrument, NMR studies of nuclei other than proton - <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P, FT-NMR, Advantages of FT-NMR, Use of NMR in medical diagnostics.

**Electron Spin Resonance Spectroscopy** - Basic principles, Zero field splitting and Kramer's degeneracy, Factors affecting the 'g' value, hyperfine coupling constants, Spin, Hamiltonian, Measurement techniques, 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 Outcome: 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) 3<sup>rd</sup> 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).

## **PCY202 COORDINATION CHEMISTRY**

L	Т	Р	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  $\pi$ -donor ligands, Back-bonding, 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 absolute configuration in optically active metal chelates and their stereochemical information. Stereochemistry and IUPAC nomenclature of coordination compounds.

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

**Metal-ligand equilibrium in solution:** Stepwise and overall formation constants and their determination, trends in stepwise constants, Factors affecting the stability of metal complexes, Chelate effect and its thermodynamic origin.

**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 hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Reactions without metal ligand bond cleavage.

Redox reactions, Electron transfer reactions, mechanism of one electron transfer reactions, Electron transfer reaction in biological systems, Inorganic photochemistry, ligand field photochemistry of  $d^n$  complexes, Photochemistry of carbonyl compounds, 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 Outcome: 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) 6<sup>th</sup> ed.
- 2. Huheey, J.E., Keiter, E. A., and Keiter, R. L., Inorganic Chemistry, Pearson Education (2002) 4<sup>th</sup> ed.
- 3. Greenwood, N.N., and Earnshaw, A., Chemistry of the Elements, Butterworth-Heinemann (1997) 2<sup>nd</sup> ed.
- 4. Lever, A.B.P., Inorganic Electronic Spectroscopy, Elsevier Science (1985) 2<sup>nd</sup> ed.
- 5. Banerjea, D., Coordination Chemistry, Asian Books Private Limited (2007) 2<sup>nd</sup> ed.
- 6. McCleverty, J.A., and Meyer, T.J., Comprehensive Coordination Chemistry II, Vol. 9, Elsevier (2004) 1<sup>st</sup> ed.

### **PCY203 ORGANIC REACTION MECHANISMS**

L	Т	Р	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  $-S_N^2$ ,  $S_N^1$ , 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  $S_N^1$  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. Ambident nucleophile, Regioselectivity.

Electrophilic – Bimolecular mechanisms –  $S_E^2$  and  $S_E^{i}$ . The  $S_E^{1}$  mechanism, Electrophilic substitution accompanied by double bond shifts.

**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, Reimer-Tiemann, Kolbe-Schmidt reactions, Bischler-Napieralski, Pechmann, Houben, Hoesch, Hoffmann-Martius reaction. Nucleophilic – Aromatic nucleophilic substitution mechanism (SNAr, SN1 and Arynes), Reactivity and reactions, Bucherer reaction, Ullmann reaction, Chichibabin reaction.

Addition Reaction: Addition to carbon-carbon multiple bonds, Mechanism of additions involving Electrophiles, Nucleophiles and Free radicals, Addition to conjugated systems, Orientation and reactivity,

Hydration, Hydroxylation, Hydroboration, Ozonolysis, Expoxidation, Hydrogenation of double bond, Birch reduction.

Addition to carbon-hetero multiple bonds, Addition to carbon oxygen double bond, Structure and reactivity, Hydration, Addition of ROH, RSH, CN, Hydride ion, LiAlH<sub>4</sub>, NaBH<sub>4</sub>, Meerwin-Pondrof, Wolf-Kishner, Aldol, Perkin, Claisen, Benzoin, Benzil-benzilic acid, Mannich, Dieckmann, Michael, Strobe, Darzen, Witting, Doebner, Knoevenagel and Reforematsky reactions.

## **Elimination Reactions:** $\beta$ -Elimination – E<sub>2</sub> and E<sub>1</sub>, $\alpha$ -elimination

Course Outcome: 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) 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) 6<sup>th</sup> ed.
- 4. Clayden, Greeves, Narren, and Wothers, Organic Chemistry, Oxford University Press (2001).

## PCY204 INDUSTRIAL AND GREEN CHEMISTRY

L	Т	Р	Cr
3	0	0	3.0

#### **Prerequisite(s):** None

Course objective: To impart knowledge industrial chemistry and applications of Green Chemistry.

**Industrial Organic Syntheses:** The raw material and basic processes, Chemical processes used in industrial organic synthesis, Petrochemicals, Production of methanol, Ethanol, Acetaldehyde, Acetic acid, Isopropyl alcohol, Ethylene glycol, Glycerine, Acetone, Phenol, Formaldehyde, Ethyl acetate, 1,3-butadinene and styrene.

**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**: Principles of Green Chemistry, Concept of atom economy, Tools of Green Chemistry: Alternative feedstocks/starting materials, Reagents, Solvents, Product/target molecules, Catalysis and process analytical chemistry. Evaluation of chemical product or process for its effect on human health and environment, Evaluation of reaction types and methods to design safer chemicals. Evaluating the effects of Chemistry: Toxicity to humans, Toxicity to wildlife, Effects on local environment, Global environmental effects. Planning a green synthesis.

**Applications of Green Chemistry:** Green synthesis of Ibuprofen, Design and application of surfactants for carbon dioxide for precision cleaning in manufacturing and service industries, Polyester regeneration technology, Microbes as environmentally benign synthetic catalysts, Environmentally safe marine antifoulant, Use of molting agents to replace more toxic and environmentally harmful insecticides, Carbon dioxide as blowing agent, Oxidant activators to replace chlorine based delignification process in paper and pulp industry, Biodegradable polyaspartate polymers for inhibitors and dispersing agents, Recent applications in green chemistry.

Course Outcome: The students will acquire knowledge of

- 1. Importance, industrial production procedures of gases, basic organic chemicals, detergents, insecticides and sugars.
- 2. Concepts and applications of Green Chemistry.

- 1. Howard, W.L., Introduction to Industrial Chemistry, Wiley-Interscience (1986).
- 2. Weissermel, K., and Arpe, H.J., Industrial Organic Chemsitry, VCH (1997) 3<sup>rd</sup> ed.
- 3. Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).
- 4. Anastas, P., and Williamson, T. C., Green Chemistry Frontiers in Benign Chemical Synthesis and Processes, Oxford University Press (1999).
- 5. Ahluwalia, V. K., and Kidwai, M., New Trends in Green Chemistry, Anamaya Publishers (2004).

## PCY205 ORGANIC CHEMISTRY LAB

L	Т	Р	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<sub>f</sub> values, Column chromatography.

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

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

**Polarimetry:** Determination of enantiomeric composition by using a polarimeter.

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

Determination of melting point and mixed melting point, Acid value and saponification value of an oil sample.

Course Outcome: The students will acquire knowledge of

- 1. Chromatographic separation and identification of organic compounds.
- 2. Purification, Crystallization, and different Distillation processes.
- 3. Determination of enantiomeric composition by polarimeter.
- 4. Synthesis, purification and characterization of aspirin, Schiff's base, Diels-Alder adduct.

- 1. Leonard, J., Lygo, B., and Procter, G., Advanced Practical Organic Chemistry, Blackie Academic (1995) 2<sup>nd</sup> 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).

### PCY206 PHYSICAL CHEMISTRY LAB

L	Т	Р	Cr
0	0	6	3.0

### **Prerequisite(s):** None

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

Determine the relative and absolute viscosity of a given liquid, Determine the surface tension of n-propyl alcohol, n-butyl alcohol and n-heptane, Calculate the parachor value for  $> -CH_2$  group and atomic parachors of C and H, Determination of refractive indices of given liquids and find out the composition of a mixtures of liquid, To verify Freundlich and Langmuir Adsorption isotherms for adsorption of acetic acid on activated charcoal, Determination of partition coefficient of benzoic acid between toulene and water, Determination of the rate constant of hydrolysis of an ester; the effect of (a) Change of temperature and activation energy measurement (b) Ionic strength of the media, To study kinetics of inversion of cane sugar by optical rotation measurement, Determination of Quantum Yields of a photochemical reaction, Determination of radioactivity in a surface soil, cement and fly ash, Half life determination of radioisotopes <sup>137</sup>Ba, Determination of the solubility of a sparingly soluble salt with the help of radio isotopes, Cyclic Voltammetry study of Fe<sup>+2</sup>/Fe<sup>+3</sup>system.

Course Outcome: 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).

#### PCY 301 CHEMICAL KINETICS AND SURFACE CHEMISTRY

L	Т	Р	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, Laws of photochemistry, 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 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).

## PCY302 SYMMETRY AND GROUP THEORY

L	Т	Р	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, Selection rules- Infra Red and Raman spectra.

Course Outcome: 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) 3<sup>rd</sup> 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).

## PCY303 CATALYSIS AND REAGENTS

L	Т	Р	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-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 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 and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast. Protecting groups. Discussion of synthetic strategies and tactics.

Course Outcome: 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) 3<sup>rd</sup> ed.
- 2. Carruthers, W., Some Modern Methods of Organic Synthesis, Cambridge University Press (1987).

## PCY304 ORGANIC STRUCTURE ANALYSIS

L	Т	Р	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, Ethers, Phenols 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, FT-IR.

**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, Spinspin 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, Nuclear magnetic double resonance, Contact shift reagents, Solvent effects. Continuous wave and FT-NMR. Resonance of other nuclei – F and P.

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

Course Outcome: 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<sup>th</sup> ed.
- 4. Silverstein, R.M., and Webster, F.X., Spectrometric Identification of Organic Compounds, John Wiley & Sons, Inc. (2005) 7<sup>th</sup> 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).

## PCY305 ANALYTICAL CHEMISTRY LAB

	L	Т	Р	Cr
	0	0	3	1.5
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## **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, Determination of the strength of strong and weak acids in a given mixture 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.

**pH metry:** 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 determine formal potential and diffusion coefficient of  $Fe(CN)_6^{3-}$ , To study the electrochemistry of  $Co(NH_3)_6^{3+}$  by cyclic voltammetry.

**Course Outcome:** 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) 3<sup>rd</sup> ed.
- 2. Das, R.C., and Behra, B., Experimental Physical Chemistry, Tata McGraw-Hill (1983).
- 3. Ghosh, J.C., Experiments in Physical Chemistry, Bharati Bhavan (1990).

### **PCY306 INORGANIC SYNTESIS LAB**

L	Т	Р	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<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-hydroxyquilinato)aluminum(III) complex.

Course Outcome: 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 the characterization of coordination complexes.

- 1. Jolly, W.L., Synthesis and Characterization of Inorganic Compounds, Prentice Hall, (1970)1<sup>st</sup> 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).

### PCY307 ORGANIC SYNTHESIS LAB

L	Т	Р	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, <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. Microwave Synthesis: Alkylation of diethyl malonate with benzyl chloride. Three Component Coupling: Synthesis of dihydropyrimidinone.

**Multistep synthesis:** Preparation of methylbenzoate from benzoic acid. Synthesis of mnitromethylbenzoate from methylbenzoate. Demethylation of m-nitromethylbenzoate to get mnitrobenzoic 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 Outcome: 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.

- 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).

## PCY401 HETROCYCLIC CHEMISTRY AND NATURAL PRODUCTS

L	Т	Р	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 <sup>1</sup>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, Thiiranes, Azetidines, Oxetanes and Thietanes.

**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 Outcome: 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.

- 1. Gilchrist, T.L., Heterocyclic Chemistry, Prentice Hall (1997) 3<sup>rd</sup> 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. <u>Koskinen</u>, A., Asymmetric Synthesis of Natural Products, Wiley (1993).
- 6. Apsimon J., Total synthesis of Natural Products (1-7) Wiley Interscience (1973-1988).

## PCY402 ADVANCED TOPICS IN CHEMISTRY

L	Т	Р	Cr
3	1	0	3.5

#### **Prerequisite(s):** None

Course objective: To impart knowledge of biophysical, bioinorganic, and solid state chemistry.

**Biophysical Chemistry:** Structures and biophysical properties of biomolecules, Primary, Secondary and Tertiary structures of proteins, Hofmeister series, Chaotropic and kosmotropic ions and cosolvents. Spectroscopic (CD, FTIR, Fluorescence) and calorimetric methods to study folding, Stability, and Dynamics of proteins, Thermal, Chemical, and pH-denaturations of proteins, Kinetic and thermodynamic controlled reactions, Two-state thermodynamic models for reversible and irreversible biological reactions, Noncovalent interactions, Hydrogen bonding, Electrostatic and hydrophobic interactions, Electrostatic folding/unfolding free energy, Conformational stability of proteins, Water structure and its interaction with biomolecules, Ultrafast biological reactions, Methods and techniques of chemical relaxation, Folding intermediates and their detection test, Protein misfolding and its consequences, Spectroscopic (NMR, CD, FTIR, and fluorescence), Calorimetric, and bioinformatics methods to study the Protein-surfactant, Protein-denaturant, and Protein-drug interactions.

**Bioinorganic Chemistry:** Heme and non-heme proteins, Haemoglobin and myoglobin as oxygen carriers, Bohr effect, Coordination chemistry of Fe(II) in haemoglobin and oxyhaemoglobin, Relaxed and tense (R & T) configurations of haemoglobin, Electronic formulations and mode of bonding of dioxygen in haemoglobin. Structure and functions of cytochromes, Hemerythrins and Hemocyanins. Biochemistry of iron, Iron storage and Transport, and ferritin, Transferrin. Model synthetic complexes of iron and copper, Introduction to ferridoxins, Blue copper proteins, Zinc protein (carbonic anhydrase), and Iron-sulfur proteins, Bio-inorganic chemistry of cobalt vitamin B12, Metal deficiency and disease, Toxic effects of metals.

**Solids State and Advanced Materials:** Diffraction methods (X-ray, electron and neutron), Structure of simple lattices and X-ray intensities, Structure factor and its relation to intensity and electron density, X-ray structure analysis, 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, Origin of magnetic dipoles in solids, Paramagnetic spin systems, Spontaneous magnetization, Ferrimagnetic materials.

Course Outcome: 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) 4<sup>th</sup> ed.
- 2. Lesk, A.M., Introduction to Protein Science, Oxford University Press, (2010) 2<sup>nd</sup> ed.
- *3. Cowan, J.A., Inorganic Biochemistry-An Introduction, Wiley-VCH (1997)*  $2^{nd}$  *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).

PCY MEDICINAL AND PHARMACEUTICAL CHEN	<b>AISTF</b>	RY		
	L	Т	Р	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. Quantitative structure activity relationship (QSAR): History and development. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: Lipophilicity, Partition coefficient, electronic ionization constants, Steric, Shelton and surface activity parameters and redox potentials. 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. Mention of uses of pharmacokinetics in drug development process.

**Pharmacodynamics:** Introduction, Elementary treatment of enzyme stimulation, Enzyme inhibition, Sulphonamides, Membrane active drugs, Drug metabolism, Xenobiotics, Biotransformation, Significance of drug metabolism in medicinal chemistry.

Antineoplastic Agents: Introduction, Cancer chemotherapy, Special problems, Role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.

**Cardiovascular Drugs:** Introduction, Cardiovascular diseases, Drug inhibitors of peripheral sympathetic function, Central intervention of cardiovascular output. Direct acting arteriolar dilators.

Local Antiinfective Drugs: Introduction and general mode of action.

**Psychoactive Drugs:** Introduction, Neurotransmitters, CNS depressants, General anaesthetics, Mode of action of hypnotics, Sedatives, Anti-anxiety drugs, Benzodiazipines, Buspirone, Neurochemistry of mental diseases. 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 Outcome: 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) 12<sup>th</sup> 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) 7<sup>th</sup> ed.
- 4. Brunton, L.L., Chabmer, B.A., and Knollmann, B.C., Goodman and Gilman's Pharmacological Basis of Therapeutics, Ed. McGraw-Hill (2011) 12<sup>th</sup> ed.
- 5. Silverman, R.B., The Organic Chemistry of Drug Design and Drug Action, Elsevier (2004) 2<sup>nd</sup> ed.
- 6. Lednicer, D., Strategies for Organic Drug Synthesis and Design, John Wiley & Sons. (2008) 2<sup>nd</sup> ed.

## PCY---SYNTHETIC AND NATURAL POLYMERS

L	Т	Р	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, Catalysts in polymerization.

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

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, 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 Outcomes: 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. 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).

## PCY --- SUPRAMOLECULAR CHEMISTRY

L	Т	Р	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- $\pi$ , anion- $\pi$ ,  $\pi$ - $\pi$  and vander waal interactions, Supramolecular Chemistry in Life, Ionophores, Porphyrin and other tetrapyrrollic macrocycles, Coenzymes, Neurotransmitters, 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, Host-guest interactions, Preorganisation and complimentarity, Lock and key analogy, Binding of cationic, Anionic, Ion pair and neutral guest molecules.

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

**Molecular Devices:** Molecular Electronic devices, Molecular wires, Molecular rectifiers, Molecular switches and Molecular logic gates.

Examples of recent developments in supramolecular chemistry from current literature.

Course Outcome: 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

- 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).

## **PCY---BIOFUELS**

L	Т	Р	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 outcomes:** The students will acquire the knowledge of biofuel production technologies, and their applications.

- 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).

#### **PCY--- REARRANGEMENTS AND RETROSYNTHESIS**

L	Т	Р	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, Chemoselectivity, Reversal of polarity (umpolung), Cyclisation reactions, Amine synthesis.

Course Outcomes: 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.

- 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, Bharati Bhavan (2004).
- 4. Chemistry Education: Research and Practice in Europe, 2002, Vol. 3, No. 1, pp. 33-64.

## **PCY--- PHOTOPHYSICAL CHEMISTRY**

L	Т	Р	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, Importance of electron jump between perpendicular orbital's, heavy atom effect, 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.

**Theory of Photoreactions:** Visualization of reactions on excited state surfaces, Minima, Funnels and conical intersections.

**Identification of Minima on Excited State Surfaces:** Surface touching, Cleavage of s and p bonds, Diradicals, Salem diagrams, Photochemical generation and excited state reactions of reactive intermediates (carbenes, nitrenes, radicals, diradicals, and carbocations).

**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<sub>2</sub> photocatalysis, Photosynthesis (plants), Intermediates in photoreactions, Identification and characterization through modern techniques, Flash photolysis, CIDNP, Photoacoustic, Stepscan IR.

**Course Outcomes:** 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:**

1. Lakowicz, J. R., Principles of Fluorescence Spectroscopy, Springer, New York (2006), 3<sup>rd</sup> 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).

## PCY--- BIOPOLYMER AND PROTEIN CHEMISTRY

-	-	-		-	_	 L	Т	Р	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, Biocomposites and biomaterials, Biological attacks on polymeric materials and degradation mechanisms in polymeric materials, Degradation products in different environments, Environmental issues when using polymers, Recovery/reuse of plastics.

**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 (Myoglobin, Hemoglobin, Lysozyme, Ribonuclease A, Carboxypeptidase, Transferrin, Ferritin, and Chymotrypsin), 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, Protein misfolding and disease, Thermodynamics of protein folding by spectroscopic and calorimetric methods, Ultrafast folding dynamics study by laser flash photolysis, Methods and techniques of chemical relaxations, Protein conformational study by NMR and fluorescence spectroscopy, Measurement of hydrodynamic radii by dynamic light scatter, Single molecule protein folding study by atomic force microscopy.

Course Outcome: 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) 2<sup>nd</sup> ed.

### **PCY--- ENVIRONMENTAL CHEMISTRY**

L	Т	Р	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  $pE^{\circ}$ .

**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.

Humic material – Formation, Composition, Structure determination using spectroscopy, Properties.

**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.

**Microbiological Processes:** Classification of microbes, Microbiological carbon cycle, Microbiological sulfur cycle.

Air Pollution: Introduction and control methods

Course outcomes: 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.

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