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

Programme Educational Objectives (PEOs)

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

Programme Outcomes (POs)

Students shall be able to

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

New Scheme of M.Sc. (Chemistry) - 2018 onwards

First Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY101	Analytical Chemistry	3	1	0	3.5
2.	PCY102	Inorganic Chemistry	3	0	0	3.0
3.	PCY109	Stereochemistry and Photochemistry	3	0	0	3.0
4.	PCY201	Thermodynamics and Chemical Kinetics	3	1	0	3.5
5.	PCY206	Chemistry Lab-I	0	0	6	3.0
6.	PCY108	Chemical Biology (For non-medical group)	3	1	0	3.5
	PIM101	Basic Mathematics (For medical group)				
7.	PHU 002	Professional Communication	2	1	0	2.5
		Total	**17**	**4**	**6**	**22.0**

Second Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY215	Molecular Spectroscopy	3	1	0	3.5
2.	PCY202	Coordination Chemistry	3	0	0	3.0
3.	PCY203	Organic Reaction Mechanisms	3	0	0	3.0
4.	PCY104	Quantum Chemistry	3	1	0	3.5
5.	PCY209	Chemistry Lab-II	0	0	8	4.0
6.	PCYXXX	Elective-I	3	0	0	3.0
		Total	**15**	**2**	**8**	**20.0**

Third Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY307	Catalysis and Reagent	3	0	0	3.0
2.	PCY302	Symmetry and Group Theory	3	0	0	3.0
3.	PCY308	Interpretative Spectroscopy	3	1	0	3.5
4.	PCY309	Physical and Analytical Chemistry Lab	0	0	8	4.0
5.	PCYXXX	Elective – II	3	0	0	3.0
6.	PCYXXX	Computational Chemistry	2	0	2	3.0
	PCY391	Seminar/minor projects*	-	-	-	2.0
		Total	**14**	**1**	**10**	**21.5**

*May be undertaken/completed in academic or industry.

Fourth Semester

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCYXXX	Elective-III	3	1	0	3.5
2.	PCY402	Bioinorganic and Biophysical Chemistry	3	0	0	3.0
3.	PCY 491	Dissertation	-	-	-	12.0
		Total	**6**	**1**	**0**	**18.5**

Elective – I

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCY211	Medicinal and Pharmaceutical Chemistry	3	0	0	3.0
2.	PCY212	Synthetic and Natural Polymers	3	0	0	3.0
3.	PCYXXX	Supramolecular Chemistry	3	0	0	3.0
4.	PCYXXX	Material Chemistry	3	0	0	3.0
5.	PCY XXX	Green Chemistry	3	0	0	3.0

Elective - II

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCY321	Rearrangements and Retrosynthesis	3	0	0	3.0
2.	PCY322	Photophysical Chemistry	3	0	0	3.0
3.	PCYXXX	Environmental Chemistry	3	0	0	3.0
4.	PCYXXX	Organometallic Chemistry	3	0	0	3.0

Elective - III

S. No	Course No.	Course Name	L	T	P	Cr
1.	PCYXXX	Statistical Thermodynamics	3	1	0	3.5
2.	PCY401	Heterocyclic Chemistry and Natural Products	3	1	0	3.5
3.	PCYXXX	Inorganic Spectroscopy	3	1	0	3.5
4.	PPH423	Characterization Techniques	3	1	0	3.5

Total Number of Credits = 82.0

PCY101 ANALYTICAL CHEMISTRY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

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

Errors in Quantitative Analysis: Accuracy and precision of measurements, Determinate indeterminate, systematic and random errors in chemical analysis with examples, Absolute and relative errors; Source, effect and detection of systematic errors; Distribution of random errors, Normal error curve, Standard deviations, Rounding and expressing results of chemical computations.

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, Nernst equation, Concentration cells with and without liquid junction, Application of electrochemical cell (Lead Acid and Li-ion Batteries), Thermodynamics of reversible electrodes and reversible 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: The students should be able to interpret

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

Recommended Books:

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

Evaluation Scheme:

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

PCY102 INORGANIC CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s) : None

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

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

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

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

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

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

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

Recommended Books

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

Evaluation Scheme:

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

PCY109 STEREOCHEMISTRY AND PHOTOCHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddditions - antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions, Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements, Ene reaction.

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

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

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

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

Recommended Books

1. *Carey, F. A., and Sundberg, R. J., Advanced Organic Chemistry, (Part A): Structure and Mechanism, Springer (2007) 5th ed.*
2. *March, J., and Smith, M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms and structures, John Wiley (2007) 6th ed.*
3. *Depuy, C.H., and Chapman, O. L., Molecular Reactions and photochemistry Pearson Education, Limited, (1972).*
4. *Horsepool, W. H., Organic Photochemistry. A Comprehensive Treatment, Ellis Horwood, Chichester, U.K (1992).*
5. *Clayden, Greeves, Narren, and Wothers, Organic Chemistry, Oxford University Press (2001).*

Evaluation Scheme:

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

PCY201: THERMODYNAMICS AND CHEMICAL KINETICS

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

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

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.

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.

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.

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.

Course Learning Outcomes: After the completion of the course, the students should be able to:

1. explain the spontaneity of a process and the conditions required for a spontaneous process.
2. describe different methods to determine rate law and derive the rate law for various chemical reactions including fast reactions
3. explain collision and activated complex theory and determination of activation parameters for a reaction and homogeneous catalysis
4. explain importance of adsorption process, heterogeneous catalysis, Langmuir, and BET model
5. describe the concept of colloidal material, classification, synthesis and their stability for many practical uses

Recommended Books

1. *Atkins, P.W., Physical Chemistry, W.H. Freeman (1990).*
2. *Puri, B.R., Sharma, L.R., and Pathania, M.S., Principles of Physical Chemistry, Vishal Publishing Co. (2011) 45th ed.*
3. *Kapoor, K.L., A Text Book of Physical Chemistry, Vol. 3, Macmillan India (2005) 2nd ed.*
4. *Laidler, K.J., Chemical Kinetics, Dorling Kingsley (1998).*
5. *Rajaraman, J., and Kuriacose, J., Kinetics and Mechanism of Chemical Transformations, McMillan (2008).*
6. *Moroi, V., Micelles Theoretical and Applied Aspects, Springer (1986).*
7. *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

PCY206 CHEMISTRY LAB - I

L	T	P	Cr.
0	0	6	3.0

Prerequisite(s): None

Course Objective: To acquire skills for the purification, synthesis, quantification and extraction of organic and inorganic compounds.

Knowledge of Lab Safety and Software: Introduction to lab safety rules, Material safety datasheet, and norms, software (Excel, ACD/ ChemSketch)

Basic Purification Techniques: Distillation, Chromatography, Crystallization and melting point determination.

Basic Synthetic Techniques: Experiments based on stirring, refluxing, workup, filtration and extraction of natural products.

Organic Chemistry based Tests: Determination of acid, saponification and iodine value of fats and oils.

Volumetric and Gravimetric analysis: Basic concepts of quantitative analysis and methods of sampling. Volumetric analysis involving precipitation, complexometric and redox titrations. Gravimetric estimation of metals and ions in the mixture or from alloys.

Spectrophotometeric analysis: Estimation of certain ions/ transition metals/complexes/compounds by UV-Vis spectrophotometry, FTIR, atomic absorption spectrometry and flame photometry spectrometry.

Course Learning Outcomes: The students will acquire skills to

1. set up the apparatus for the purification, isolation, synthesis and characterization of certain compounds.
2. quantify ions by volumetric and gravimetric analysis.
3. operate and apply various spectroscopic techniques for identification and quantification.

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. *Pasto, D., Johnson, C. and Miller, M., Experiments and Techniques in Organic Chemistry, Prentice Hall (1991).*
4. *Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K., Vogel's Textbook of Quantitative Analysis, Pearson Education, (2007) 3rd ed.*
5. *Skoog, D. A., Holler, F. J., and Nieman, T. A., Principles of Instrumental Analysis, Thomson, (2006) 5th ed.*

Evaluation Scheme:

MST	EST
50	50

PCY108 CHEMICAL BIOLOGY

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

Prerequisite(s): None

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

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

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

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

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

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

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

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

Recommended Books

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

Evaluation Scheme:

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

PCY215 MOLECULAR SPECTROSCOPY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

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

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

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

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

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

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

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

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

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

Course Learning Outcomes: After the completion of the course, the students should be able to

1. explain the principle and instrumentation of microwave, infrared-vibration-rotation Raman and infra-red spectroscopy and interpret microwave, vibration-rotation Raman and infra-red spectra for chemical analysis.
2. explain the principle and instrumentation of electronic spectroscopy and analyze the electronic spectra of different species..
3. explain the principle and instrumentation of nuclear magnetic and electron spin resonance spectroscopy and apply the knowledge in characterizing the molecules and also their use in medical diagnostics.
4. explain the principle, instrumentation, and application of Mössbauer spectroscopy to study bonding in iron derived complexes.

Recommended Books

1. *Hollas, J.M., Modern Spectroscopy, John Wiley (1996) 3rd ed.*

2. *Windawi, H., and Floyd, F.L.H., Applied Electron Spectroscopy for Chemical Analysis (Chemical Analysis Vol. 63), John Wiley (1982).*
3. *Parish, R.V., NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Harwood (1991).*
4. *Chang,R., Basic Principles of Spectroscopy, McGraw-Hill (1971).*
5. *Ghosh, P.K., Introduction to Photoelectron Spectroscopy, **John Wiley** & Sons, New York (1983).*
6. *Carrington, A., and MacLachalan, A.D., Introduction to Magnetic Resonance, **Harper** and Row, New York, USA (1967).*

Evaluation Scheme:

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

PCY202 COORDINATION CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s) : None

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

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

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

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

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

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

Course Learning Outcomes: After the completion of the course, the students should be able to

1. explain the bonding in coordination complexes and
2. interpret the electronic spectra and magnetic properties
3. explain the formation and stability of the coordination complexes.
4. elucidate the kinetics and reaction mechanism of coordination complexes including redox reactions

Recommended Books

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

Evaluation Scheme:

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

PCY203 ORGANIC REACTION MECHANISMS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

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

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

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

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

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

Recommended Books

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

2. *Carey, F.A., and Sundberg, R.J., Advanced Organic Chemistry, (Part B), Springer (2007) 5th ed.*
3. *March, J., and Smith, M.B., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, John Wiley (2007) 6th ed.*
4. *Clayden, Greeves, Narren, and Wothers, Organic Chemistry, Oxford University Press (2001).*

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

PCY104 QUANTUM CHEMISTRY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

Evaluation Scheme:

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: Failures of classical mechanics, Postulates of quantum mechanics, State of a system, Probability amplitude, Probability density, Operators and observables, Eigen function and Eigen value, Hermitian operators, Commutators, Expectation value.

Discussion of solutions of the Schrodinger equation to some model systems *viz.*, Particle in a box, Harmonic Oscillator, The Rigid Rotor, The hydrogen atom.

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.

Approximate Methods: The variation theorem, Linear variation principle, Perturbational methods.

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

Course learning outcomes: After the completion of the course, the students should be able to

1. explain Schrodinger equation for various quantum chemical models such as, particle in a box, harmonic oscillator, rigid rotor models and their quantum chemical description.
2. explain the operator algebra and their physical significance
3. describe the electronic and Hamiltonian operators for H-like atoms and quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
4. describe the approximation methods to solve the Schrodinger equation of many electron systems and their application for to describe the concept of bonding

Recommended Books:

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

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

Evaluation Scheme:

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

PCY209 CHEMISTRY LAB- II

L	T	P	Cr
0	0	8	4.0

Prerequisite(s): None

Course Objective: To acquire skills to synthesize organic/inorganic compounds via single and multistep synthesis process, their characterization and applications.

Synthetic Organic Reactions: Involving oxidation, reduction, carbon carbon bond formation and rearrangement(s).

Multistep Organic Synthesis: Calculations, synthesis, purification and characterization of m-nitrobenzoic acid, (Route- Benzoic acid to methyl benzoate, methyl benzoate to m-nitromethylbenzoate, m-nitromethylbenzoate to m-nitrobenzoic acid)

Inorganic synthesis: Synthesis, separation and purification of following inorganic compounds, and their characterization by various techniques viz., TLC, UV-Vis, FT-IR, Magnetic moment measurement, conductivity measurements, and NMR techniques: Werner's complex, *cis* and *trans*-$[Co(en)_2Cl_2]^+$or *cis* and *trans*-$K_3[Fe(C_2O_4)_3]$, 1-Acetyl ferrocene and separation by TLC, $Hg[Co(SCN)_4]$, Cu(II) and Ni(II) complexes of Schiff base, $VO(acac)_2$, tris(8-hydroxyquilinato)aluminum(III) complex (by conventional and green method), bispyridine iodide nitrate(non-metal complex) and MnO_2/TiO_2/carbon nanomaterials.

Data Presentation Techniques: For chemistry literature, references, NMR, IR, UV-Vis and mass spectrometry, report writing.

Course Learning Outcomes: The students will acquire skills to

1. handle and use different organic and inorganic reagents.
2. set up organic and inorganic reactions and characterize products using spectroscopic techniques.
3. know the preparation, purification and characterization of different organic and inorganic compounds.

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. *Pasto, D., Johnson, C. and Miller, M., Experiments and Techniques in Organic Chemistry, Prentice Hall (1991).*
4. *Jolly, W. L., Synthesis and Characterization of Inorganic Compounds, Prentice Hall, (1970)1st ed.*
5. *Angelici, R. J., Synthesis and Techniques in Inorganic Chemistry, W B Saunderers Co. (1969).*

Evaluation Scheme:

MST	EST
50	50

PCY302 SYMMETRY AND GROUP THEORY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

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

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

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

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

Recommended Books

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

Evaluation Scheme:

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

PCY307 CATALYSIS AND REAGENTS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

Metal-Catalyzed Transformations in Organic Syntheses: Review of basic concepts in catalysis, Reactions of transition metal complexes, The Suzuki coupling, Heck reaction and other Pd-catalyzed reactions, Raney Nickel, Copper catalysis, Ruthenium catalyst, Rhodium catalyst, 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, Grignard's reagent, Jones reagent, Sarett's reagent, Pfitzer-Moffatt reagent, Ceric ammonium nitrate, Manganese oxide, Chromic acid, Silver oxide, Lithium dimethylcuprate, Lithium disopropylamide, Dicyclohexylcarbodimide, 1,3-Dithiane, Trimethylsilyl iodide, Tri-n-butyltin hydride, Triphenyltin hydride, Sodium acetoxy borohydride and other hydrides, n-Butyl lithium, Woodward and Prevost hydroxylation, Osmium tetroxide, DDQ, DCC, Selenium dioxide, Phase transfer catalysts, Crown ethers, Peterson's synthesis, Wilkinson's catalyst, Dehydrogentation by quinones, selenium dioxide, ferricyanide etc.

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

1. know the use of transition metal based and other catalysts for different organic reactions.
2. know the use of reagents for different reaction transformations.
3. be familiar with various coupling reactions and their applications in industry.

Recommended Books

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

Evaluation Scheme

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

PCY308 INTERPRETATIVE SPECTROSCOPY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): None

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

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

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

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

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

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

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

Course Learning Outcomes: The students will be able to

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

Recommended Books

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

Evaluation Scheme:

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

PCY309 PHYSICAL AND ANALYTICAL CHEMISTRY LAB

L	T	P	Cr
0	0	8	4.0

Prerequisite(s): None

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

Physical Chemistry Experiments

1. Determination of absolute viscosity of a given polymer.
2. To verify Freundlich and Langmuir Adsorption isotherms for adsorption of acetic acid/organic dyes on activated charcoal/nanomaterials.
3. Determination of rate constant of hydrolysis of an ester and to study the effect of temperature and ionic strength on reaction rate.
4. To study kinetics of inversion of cane sugar by optical rotation measurement.
5. To study the kinetics of degradation of organic pollutants by TiO_2 using UV-Vis spectrophotometer.
6. Application of Nuclear Magnetic Resonamce(NMR) spectroscopy as a quantification tool.
7. Use of Infra-red spectroscopy
   a) To analyse the intermolecular hydrogen bonding in alcohols
   b) To distinguish intra- and intra-molecular hydrogen bonding in *o*-nitro phenol and *p*-nitro phenol.
   c) To differentiate between acetic acid and thioacetic acid.

Analytical Chemistry Experiments

1. **Conductometry:** Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$), precipitation titration ($AgNO_3$ to AgCl) conductometrically.

2. **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 Ce^{3+}/Ce^{4+} system or Fe^{2+}/Fe^{3+} system.

3. **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.

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

Course Learning Outcomes: After the completion of the course, the students should be able to

1. be familiar with experimental techniques for controlling chemical reactions.
2. measure various physical and chemical properties of materials and the kinetics of a chemical reaction.
3. record and interpret the UV-Vis and IR spectra for structural analysis and kinetic studies.

4. develop experimental skills on conductivity meter, potentiometer, pH meter and voltammeter for different applications

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).*
4. *James, A.M., and Prichard, F.E., Practical Physical Chemistry, Longman, Harlow (1974) 3^{rd}ed*
5. *Ghosh, J.C., Experiments in Physical Chemistry, BharatiBhavan (1990).*

Evaluation Scheme:

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

PCYXXX COMPUTATIONAL CHEMISTRY

L	T	P	Cr
2	0	2	3.0

Prerequisite(s): Quantum Chemistry (PCY 104)

Course objective: The course will provide students with basic understanding of the various computational techniques and their application to chemistry and biology.

Introduction: Scope of computational chemistry, A brief outline of Semiempirical, *ab initio* and density functional theory, Vibrational frequency analysis, Thermochemistry, Limitations of computational techniques.

Orbitals: Slater-type orbitals (STO), Basis-sets, Effective core potentials (ECP), Superposition error, Molecular orbitals, Group orbitals, Natural orbitals, Spin natural orbitals.

Population analysis and Molecular properties: Mulliken and Natural bond orbital analysis, Density, electrostatic potential and dipole moment.

Application of these computational methods: Prediction of structural and electronic properties of molecules by using standard programs, Chemical properties and reactivity, Computation of potential energy surfaces. Analysis of thermochemistry for any chemical reactions.

Classical Molecular Dynamics: Introduction to non-bonded interactions, Electrostatic interactions, van der Waals interactions, Hydrogen bonding in molecular mechanics, Protein ligand interactions, Force fields, Force field models for the simulation of liquid water.

Molecular dynamics (MD) simulation methods, Conformational analysis by molecular mechanics and the applications of MD simulation on dynamical and structural studies of bio-molecules, Molecular Docking.

Laboratory Work:
Basics of Linux
Modeling chemical reactions using various software packages such as, Gaussian, ORCA, etc.
Computing the electronic structure, bonding and electronic properties of molecules by using the above mentioned programs.
Docking study and Molecular Dynamics simulation for biological systems using software packages such as, Amber, Gromacs, Autodock.

Assignment: Compulsory 4 weeks project on computational chemistry.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. run various quantum chemical and molecular dynamics software, such as Gaussian, ORCA, Gromacs/Amber.
2. explain chemical principles using computational modelling.
3. use those packages to solve different chemical and (bio)chemical problems.
4. analyze and interpret the outputs of these calculations to rationalize experimental outcomes or even making testable predictions.
5. use the molecular dynamics programs to explore the conformational changes of proteins with respect to time.

Recommended books:

1. *Cramer, C. J., Essentials of Computational Chemistry: Theories and Models, Wiley (2004) 2nd Ed.*
2. *F. Jensen., Introduction to Computational Chemistry,* John Wiley & Sons, 2007
3. *Leach, A., N, Molecular Modelling: Principles and Applications, Pearson (2001) 2nd Ed.*
4. *Koch, W., Holthausen, M. C., A Chemists Guide to Density Functional Theory, Wiley (2001) 2nd Ed.*
5. *Burdett, J. K., Whangbo, M. H., Albright, T, A, Orbital Interaction in Chemistry, Wiley (2013) 2nd Ed.*
6. *J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods. Gaussian Inc., 1996.*
7. *M. P. Allen and D. J. Tildesley, Computer Simulations of Liquids, Oxford, 1987*

Evaluation Scheme:

S.No.	Evaluation	Marks
1.	MST	20
2.	EST	30
3.	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)	50

PCY391 SEMINAR/ MINOR PROJECT

L	T	P	Cr
-	-	-	2.0

Prerequisite(s): None

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

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

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

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

Recommended Books/literature

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

Evaluation Scheme

REPORT	PRESENTATION
50	50

PCY401 HETROCYCLIC CHEMISTRY AND NATURAL PRODUCTS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

Aromatic Heterocycles: Classification (structural type), Criteria of aromaticity (bond lengths, Ring current and chemical shifts in ^{1}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 (CLOs): The students will be able to

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

Recommended Books

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

Evaluation Scheme

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

PCY 402: BIOINORGANIC AND BIOPHYSICAL CHEMISTRY

L	T	P	Cr.
3	0	0	3.0

Prerequisite(s): None

Course objective: The objective of this course is to provide exposure to the students of structure, function, folding and dynamics of proteins and metalloproteins.

Biophysical Chemistry: Conformations of proteins (Primary, Secondary, Ramachandran plot, Tertiary and Quaternary structure; Domains; Motif and Folds), Covalent and noncovalent interactions, Hofmeister series, Chaotropic and kosmotropic ions/cosolvents. Spectroscopic (CD, FTIR, NMR, Fluorescence) and calorimetric methods to study folding, stability, and dynamics of proteins, Thermal, Chemical, and pH-denaturations of proteins, Effect of denaturants on rates of folding and unfolding, Chevron plots. Ultrafast biological reactions, Folding intermediates and their detection test, Methods and techniques of chemical relaxation, Protein misfolding and its consequences.

Bioinorganic Chemistry: General terms, how and why does nature select inorganic elements? Inorganic Elements and evolution. Basic biological Coordination Chemistry. Kinetic and spectroscopic characteristics of bioinorganic systems. Systematic overview over tasks and examples of inorganic elements in biology. Non-redox active metals: Ion transport: membranes, energy, channels, pumps, Biomineralization.

Iron Containing Heme & Non-heme Metalloproteins: 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 and hemerythrins. Electron transfer and Respiration. Biochemistry of iron, Iron storage and transport by transferrin/ferritin. Model synthetic complexes of iron, Iron-sulfur proteins, Introduction to ferridoxins and rubredoxin. Biomimetic complexes of metalloenzymes.

Nonferrous Metalloproteins: Blue copper proteins, Zinc protein (carbonic anhydrase), Bio-inorganic chemistry of cobalt vitamin B_{12}, Photosynthetic reaction center. Metal deficiency and disease.

Metals in medicine: Anti-cancer agents, diabetes, arthritis, radionuclides and related applications.

Course Learning Outcomes: After the completion of the course, the students should be able to:

1. Describe the factors that govern the stability, folding, and dynamics of proteins.
2. Explain the kinetics, thermodynamics, and mechanism of protein folding and their implications in misfolding.
3. Describe the structure and biological functions of proteins and explain the role of metals in biology.
4. Explain the roles of metals in medicinal chemistry and toxic effects of metals.

Recommended Books:

1. Huheey, J.E., Keiter, E. A., and Keiter, R.L., Inorganic Chemistry, Pearson Education (2008).
2. Lippard, S.J., and Berg, J.M., Principles of Bioinorganic Chemistry, University Science Books *(1994).*
3. Voet, D., Voet, J.G., ad Pratt, C.W., Principles of Biochemistry, 4th Ed., John Wiley & Sons, Inc. (2013).
4. Nelson, D.L., Cox, M.M., Lehninger Principles of Biochemistry 6th Ed., W.H. Freeman (2013).
5. Cowan, J.A., Inorganic Biochemistry-An Introduction, Wiley-VCH (1997).
6. Cantor, C.R., and Schimmel, P.R., Biophysical Chemistry, Freeman (1980).
7. Van Holde, K.E., Johnson, W.C., and Ho, P.S., Principles of Physical Biochemistry, Pearson Education (1998).

Evaluation Scheme:

S. No.	**Evaluation**	**Marks**
1.	MST (Mid-Semester Test)	30
2.	EST (End-Semester Test)	50
3.	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)	20

PCY491 DISSERTATIONS

L	T	P	Cr
-	-	-	6.0

Prerequisite(s): None

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

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

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

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

Recommended Books/literature

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

Evaluation Scheme

DISSERTATION	PRESENTATION
60	40

PCY211 MEDICINAL AND PHARMACEUTICAL CHEMISTRY

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

Prerequisite(s): None

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

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

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

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

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

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

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

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

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

1. comprehend drug designing and development, their SAR and QSAR.
2. explain the mode of action of different drugs.
3. describe the role of drugs to inhibit the particular enzymes and treatment of disease.

Recommended Books

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

Evaluation Scheme

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

PCYXXX GREEN CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course objective: To introduce concepts of green chemistry and its importance/applications for a sustainable development.

Introduction: Toxicity of chemicals, chlorine and phosgene controversy.

Basic Principles of Green Chemistry: Prevention of Waste/By-Products, Maximum Incorporation of the Reactants into the Final Product, Prevention or Minimization of Hazardous Products, Designing Safer Chemicals, Energy Requirements for Synthesis, Selection of Appropriate Solvent, Selection of Starting Materials, Use of Protecting Groups, Use of Catalyst, Products Designed Should be Biodegradable, Designing of Manufacturing Plants, Strengthening of Analytical Techniques.

Designing a Green Synthesis: Choice of Starting Materials, Choice of Reagents, Choice of Catalysts, Choice of Solvents.

Green Chemistry in Day-to-Day Life: Dry Cleaning of Clothes, Versatile Bleaching Agent.

Green Reagent: Dimethylcarbonate, Polymer Supported Reagents.

Green Catalysts: Acid Catalysts, Oxidation Catalysts, Basic Catalysts, Polymer Supported Catalysts, biocatalyst.

Phase Transfer Catalysis in Green Synthesis: Introduction, Applications of PTC in Organic Synthesis, Oxidation Using Hydrogen Peroxide Under PTC Condition, Crown Ethers.

Microwave Induced Green Synthesis: Introduction, Applications - Microwave Assisted Reactions in Water, Microwave Assisted Reactions in Organic Solvents, Microwave Solvent Free Reactions (Solid State Reactions).

Ultrasound Assisted Green Synthesis: Introduction, Applications of Ultrasound.

Aqueous Phase Reactions: Introduction, Diels-Alder Reaction, Claisen Rearrangement, Wittig-Homer Reaction, Michael Reaction, Aldol Condensation, Knoevenagel Reaction, Pinacol Coupling, Benzoin Condensation, Claisen-Schmidt Condensation, Heck Reaction, Strecker Synthesis, Wurtz Reaction, Oxidations, Reductions, Polymerisation Reactions, Photochemical Reactions, Electrochemical Synthesis, Miscellaneous Reactions in Aqueous Phase.

Organic Synthesis in Solid State: Introduction, Solid Phase Organic Synthesis Without Using Any Solvent, Solid Supported Organic Synthesis.

Versatile Ionic Liquids as Green Solvents: Green Solvents, Reactions in Acidic Ionic, Liquids, Reactions in Neutral Ionic Liquids.

Synthesis Involving Basic Principles of Green Chemistry: Introduction, Synthesis of Ibuprofen and Styrene. Marine Antifoulant.

Recent literature examples of conventional Vs green synthesis.

Course Learning Outcomes: The students will acquire knowledge of

1. Concepts of green chemistry.
2. Applications of green chemistry for sustainable development.

Recommended Books

1. *Matlack, A. S., Introduction to Green Chemistry, CRC Press, (2010), 2nd ed.*
2. *Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).*
3. *Ahluwalia, V. K., and Kidwai, M., New Trends in Green Chemistry, Anamaya Publishers (2004).*
4. *Anastas, P. and Williamson, T. C., Green Chemistry Frontiers in Benign Chemical Synthesis and Processes, Oxford University Press (1999).*

Evaluation Scheme:

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

PCY 213 SUPRAMOLECULAR CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

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

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

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

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

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

Recommended Books

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

Evaluation Scheme

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

PCY XXX: MATERIAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course objective: The objective of this course is to provide basic knowledge of material characteristics and applications.

X-ray diffraction and crystal structure: Crystalline and Amorphous solid, Unit cell, Crystal systems, Bravais lattices, Single crystal, Indexing of lattice planes, Miller indices, Dislocations in solids, Point defects, Schottky and Frenkel defects, F-centre, Diffraction methods (X-ray, electron and neutron), Generation of X-rays (Cu-K and Mo-K), Bragg equation, Reciprocal lattice, Crystal structure analysis, Multiplicities, Systematically absent reflections, Structure factor, R value, Intensities and Electron density.

Electronic, Magnetic properties and Band theory of solids: Band theory of solids, Refinement of band theory, Band structures of Metals, Semi-conductors and insulators, Significance of band gap. Electrical conduction in metals, Superconductivity, Ferroelectric and Piezo-electric materials. Inorganic glasses, Glass transition temperature, Classification of magnetic materials and their examples, Curie and Curie-Weiss laws, Hysteresis.

Nanomaterials: Basic Concepts of Nanoscience and Nanotechnology, Types of nanomaterials, Optoelectronic and physicochemical properties, Band energetic and surface structural properties, Applications of nanomaterials.

Course Learning Outcomes: After the completion of the course, the students should be able to:

1. Describe Unit cells, lattice types, crystal system and point defects in solids.
2. Explain X-ray and electron diffraction for crystal structure analysis.
3. Explain electrical and magnetic properties of materials.
4. Elucidate the size-dependent physicochemical properties of nanomaterials.

Recommended Books:

1. West, A.R., Solid state chemistry and its applications, John Wiley and Sons (2004).
2. Smart, L.E., and Moore, E.A., Solid state chemistry: An introduction, Taylor & Francis *(2005).*
3. Chakrabarty, D.K., Solid state chemistry, New Age International (1996).
4. Ropp, R.C., Solid state chemistry, Elsevier (2003).
5. Pradeep, T., NANO: The Essentials, Tata McGraw-Hill (2007).
6. Lindsay, S. M., Introduction to Nanoscience, Oxford University Press (2010).

Evaluation Scheme:

S. No.	Evaluation	Marks
1.	MST (Mid-Semester Test)	25
2.	EST (End-Semester Test)	50
3.	Sessional (May include Project/Quizzes/Assignments/Lab Evaluation)	25

PCY321 REARRANGEMENTS AND RETROSYNTHESIS

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

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

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

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

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

Recommended Books

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

Evaluation Scheme

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

PCY322 PHOTOPHYSICAL CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

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

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

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

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

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

1. assess photochemistry and photophysical principles.
2. identify and characterize of transient intermediates by ultrafast modern techniques.
3. know the theory and application of photochemistry and photophysical principles of macromolecules.

Recommended Books:

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

Evaluation Scheme

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

PCY XXX ENVIRONMENTAL CHEMISTRY

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

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

Introduction: Environmental chemistry, Environmental composition, Chemical processes.

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

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

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

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

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

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

Air Pollution: Introduction and control methods

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

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

Recommended Books:

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

Evaluation Scheme

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

PCYXXX ORGANOMETALLIC CHEMISTRY

L	T	P	Cr
3	0	0	3.0

Prerequisite(s): None

Course Objective: To impart basic and advanced concepts in organometallic chemistry.

Main Group Organometallics: Introduction, Review of comparative aspects of synthetic methods, Reactivity and bonding in ionic, covalent, Electron deficient and electron rich organometallic compounds.

Structure and Bonding in Organometallic Compounds: 18 electron rule and its application to π-acceptor ligands, Limitations of 18 electron rule, Description of bonding models for π-acceptor ligands, including CO, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, Physical evidence and consequences of bonding.

Important Reactions of Organometallics: Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, Reactivity at metal-bound ligands.

Organotransition Metal Chemistry: σ-Bonded transition metal-alkyls, -aryls, -alkenyls (vinyls), -alkynyls (acetylides), Reactions in σ–organyls: homolytic cleavage, reductive elimination, electrophilic cleavage, insertion, β-metal hydrogen elimination, α-abstraction or α-elimination.

Transition Metal Organyls with Metal-Carbon Multiple Bonding: Transition metalcarbenes, -carbynes, -bridging carbenes/carbynes, Reactions of carbene/carbyne complexes: ligand substitution, nucleophilic, electrophilic attack, dismutation, ligand coupling reactions.

Organotransition Compounds with Multicenter Bonds (non-classically bonded): Concept of hapticity, Transition metal complexes of alkenes, Ziese salt, allenes, alkynes, allyls, butadienes; cyclic π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes; Reactions and bonding in ferrocene; Stereochemical non-rigidity in organometallic compounds and fluxional compounds, Bimetallic and cluster complexes.

Applications of Transition Metal-Organic Compounds in Catalysis: Hydroformylation, hydrogenation of olefins, Synthesis of chiral pharmaceuticals, olefins metathesis, Wacker process, polymerization (Zeigler-Natta Catalyst), Cyclooligomerisation of acetylene using nickel catalyst (Reppe catalyst), Polymer-bound catalysts and importance of organometallic compounds in certain biological systems.

Course Learning Outcomes: After the completion of the course, the students should be able to:

1. Describe the structure and bonding in main group and transition metal organometallic compounds.
2. Describe the reactivity and reaction mechanism of various organometallic compounds.
3. Describe the multicentre bonding in different organotransition metal compounds.
4. Apply the acquired knowledge to explain the catalysis by various transition metal-organic compounds.

Recommended Books:

2. *Huheey J. E., Keiter E. A. and Keiter, R. L., Inorganic Chemistry Principle of Structure and Reactivity, 4th Ed, Pearson Education Inc., (2003)*
3. *Douglas, B. E., McDaniel D. H. and Alexander J. J., Concepts and Models in Inorganic Chemistry, 3rd Ed., John Wiley & Sons, (2001)*
4. *Gupta B. D. and Elias A. J., Basic Organometallic Chemistry, 2nd Ed., University press (India) Pvt Ltd., (2013)*
5. *Crabtree, R. H., The Organometallic Chemistry of the Transition Metals, Wiley VCH, 6th Ed.,(2014).*
6. *Hill A. F., Organotransition Chemistry, The Royal Society of Chemistry, Cambridge, (2002)*
7. *Elschenbroich C. and Salzer, A., Organometallics, 2nd edition, Wiley VCH, (1992)*

Evaluation Scheme:

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

PCYXXX: STATISTICAL THERMODYNAMICS

L	T	P	Cr
3	1	0	3.5

Course objective: To acquire knowledge of statistical thermodynamics.

Statistical Thermodynamics: Thermodynamic probability and entropy, Ensembles and postulates, Micro canonical ensemble, Canonical ensemble and Grand Canonical ensemble, Fluctuations, Thermodynamic equivalence of ensembles, Second law of thermodynamics, Third law of thermodynamics. Partition function and its properties, Molar partition function, interpretation of thermodynamic laws, Thermodynamic properties in term of molecular partition function.

Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics.

Ideal Monoatomic Gas: Energy levels and canonical partition function, Thermodynamic functions.

Ideal Diatomic Gas: Rotational, Translational, Vibrational and Electronic partition functions for diatomic molecules. Virial coefficients.

Chemical Equilibrium: calculation of equilibrium constants in term of partition function. monoatomic solids.

Crystals: Lattice Models, theories of specific heat for solids: Einstein theory of the specific heat of crystals, the Debye theory of the heat capacity of Crystals.

Introduction to non-equilibrium thermodynamics.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. describe the various ensembles
2. correlate and differentiate Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics,
3. explain the partition function and the derivation of thermodynamic properties in terms of molecular partition function
4. theories of specific heat for solids.

Recommended Books

1. *Hill, T. L., An Introduction to Statistical Thermodynamics Dover Publications,(1986).*
2. *McQuarrie, D. A., Statistical Mechanics, University Science Books (2000).*

Evaluation Scheme:

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

PCYXXX INORGANIC SPECTROSCOPY

L	T	P	Cr
3	1	0	3.5

Prerequisite(s): PCY215 Molecular Spectroscopy

Course objective: To impart knowledge of applications of advanced spectroscopic techniques to understand the structure and bonding in inorganic complexes

Vibrational Spectroscopy: Theory of IR absorption, Types of vibrations, Observed number of modes of vibrations, Intensity of absorption bands, Theoretical group frequencies, Factors affecting group frequencies and band shapes (Physical state, Vibrational Coupling, Electrical effects, Resonance, Inductive effects, Ring strain) Vibrational-rotational fine-structure. Experimental method.
Application of vibrational spectroscopy to the following:
i) Distinction between
a) Ionic and coordinate anions such as NO_3^-, SO_4^{2-} and SCN^-
b) Lattice and coordinated water.
ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide.
iii) Modes of bonding of ambidentate ligands: ethylenediamine, diketonate, nitrosyl complexes

Nuclear Magnetic Resonance of Paramagnetic Substances in Solution:
Applications of NMR spectroscopy in co-ordination compounds using examples of metal nuclide ^{77}Se,^{113}Cd,^{119}Sn,^{125}Te,^{195}Pt, ^{199}Hg, contrast agents ,Shift reagent, Some application related to biochemical systems.

EPR: Introduction, Similarities between ESR and NMR, Behaviour of a free electron in an external Magnetic Field, Basic Principle of an Electron Spin, Spectrometer, Presentation of the spectrum, Hyperfine coupling in Isotropic Systems (methyl, benzene and Naphthalene radicals). Factors affecting the magnitude of g-values. Zero field splitting and Kramer's Degeneracy, Line width in solid state ESR, Double resonance technique in E.S.R. (ENDOR) Experimental method. Qualitative survey of EPR spectra of first-row transition metal ion complexes (d^1, d^2, d^3, low spin d^5, d^5, high spin d^6, d^7, d^9 system).

Applications of ESR to the following: 1. Bis-Salicylaldiimine - Copper –II 2. $CuSiF_6.6H_2O$ & $(NH_3)_5Co$-O-$Co(NH_3)_5$

Nuclear Quadrupole Resonance Spectroscopy: Basic concepts of NQR (Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies), Effect of magnetic field on spectra, Factors affecting the resonance signal (Line shape, position of resonance signal) Relationship between electric field gradient and molecular structure. Interpretation of NQR data, Structural information of the following: PCl_5, $TeCl_4$, $Na^+GaCl_4^-$, BrCN, HIO_3 and Hexahalometallates

Mössbauer Spectroscopy: Introduction, Principle, Conditions for Mössbauer Spectroscopy, parameters from Mössbauer Spectra, Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions MB experiment, Application of MB spectroscopy in structural determination of the following:
i) High spin Fe (II) and Fe (III) halides FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3$.6H2O. Low spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue. ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$ iii) Inorganic Sn(II) and Sn(IV) halides.

Photoelectron Spectroscopy: Introduction, photoelectron spectroscopy, Koopman's theorem, ESCA, chemical shift, X-ray photoelectron spectroscopy, molecular orbital diagrams of nitrogen and oxygen and their XPS spectra-ESCA, ultraviolet photoelectron spectroscopy (UPS), PES spectrum of N_2, O_2 and F_2, Photoelectron spectra for the isoelectronic sequence Ne, HF, H_2O, NH_3 and CH_4 vibrational structure in the N2 UPS spectrum, chemical shifts in XPS, exchange splitting and shake up process, Auger electron spectroscopy – basic idea.

Course learning outcomes: The students will be able to

1. interpret IR and Raman spectrum of inorganic complexes and assign mode of binding for ambidentate ligands
2. analyze the NQR data for chemical analysis
3. interpret EPR spectrum of coordination complexes and obtain idea about oxidation state of metal ion and ligand field
4. analyze the Mössbauer spectrum and obtain information about oxidation state as well as spin state of metal ion
5. understand the principle and instrumentation of PES and analyze the spectra for chemical analysis

Recommended Books

1. Physical methods in Inorganic Chemistry - R.S.Drago.
2. Modern Optical methods of Analysis - Eugens D.Olsen
3. Infrared spectra of Inorganic and coordination compounds - Kazuo Nakamoto
4. Introduction to Chemistry –Donald L.Pavia and G.M.Lampman.
5. Fundamentals of Molecular Spectroscopy-C.N.Banwel
6. Spectroscopy in Inorganic Chemistry - Rao & Ferraro Vol I & II
7. Advances in Inorganic and Radiation Chemistry Vol 6 & 8.
8. Quarterly reviews Vol 11 (1957)
9. Progress in Inorganic Chemistry Vol 8
10. Organic Spectroscopy-W. Kemp.
11. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
12. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.

Evaluation Scheme:

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