Scheme and Syllabus

B.Sc. (Chemistry) Honours / B.Sc. (Chemistry) Honours with Research

4^{th} Year

School of Chemistry & Biochemistry
Thapar Institute of Engineering & Technology, Patiala

Scheme of B.Sc. (Chemistry) Honours

Seventh Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY101	Analytical Chemistry	3	1	0	3.5
2.	PCYXXX	Inorganic and Organometallic Chemistry	3	0	0	3.0
3.	PCY109	Stereochemistry and Photochemistry	3	0	0	3.0
4.	PCY308	Interpretative Spectroscopy	3	1	0	3.5
5.	PCY309	Physical and Analytical Chemistry lab	-	-	8	4.0
		Total	12	2	8	17.0

Eighth Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY202	Coordination Chemistry	3	0	0	3.0
2.	PCY203	Organic Reaction Mechanisms	3	0	0	3.0
3.	PCY402	Bioinorganic and Biophysical Chemistry	3	0	0	3.0
4.		Elective-I	3	0	0	3.0
5.	PCY209	Chemistry Lab-II	-	-	8	4.0
	PCYXXX	Seminar	-	-	-	4.0
		Total	12	0	8	20.0

Elective – I

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY211	Medicinal and Pharmaceutical Chemistry	3	0	0	3.0
2.	PCY213	Supramolecular Chemistry	3	0	0	3.0
3.	PCY218	Material Chemistry	3	0	0	3.0

Total Number of Credits = 37.0

Scheme of B.Sc. (Chemistry) Honours with Research

Seventh Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY101	Analytical Chemistry	3	1	0	3.5
2.	PCYXXX	Inorganic and Organometallic Chemistry	3	0	0	3.0
3.	PCY109	Stereochemistry and Photochemistry	3	0	0	3.0
4.	PCY308	Interpretative Spectroscopy	3	1	0	3.5
5.	PCYXXX	Minor Research Project	-	-	-	2.0
		Total	12	2	0	15.0

Eighth Semester

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY202	Coordination Chemistry	3	0	0	3.0
2.	PCY203	Organic Reaction Mechanisms	3	0	0	3.0
3.	PCY402	Bioinorganic and Biophysical Chemistry	3	0	0	3.0
4.		Elective-I	3	0	0	3.0
5.	PCYXXX	Dissertation	-	-	-	12.0
		Total	12	0	0	24.0

Elective – I

S. No.	Course No.	Course Name	L	T	P	Cr
1.	PCY211	Medicinal and Pharmaceutical Chemistry	3	0	0	3.0
2.	PCY213	Supramolecular Chemistry	3	0	0	3.0
3.	PCY218	Material Chemistry	3	0	0	3.0

Total Number of Credits = 39.0

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

PCYXXX INORGANIC AND ORGANOMETALLIC 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) 6^{th} ed.*
2. *Huheey, J.E., Keiter, E.A. and Keiter, R.L., Inorganic Chemistry, Pearson Education, (2002) 4^{th} ed.*
3. *Greenwood, N.N., and Earnshaw, A., Chemistry of the Elements, Butterworth-Heinemann, (1997) 2^{nd} ed.*
4. *Lee, J.D., Concise Inorganic Chemistry, ELBS, (1996) 5^{th} ed.*
5. *Sharpe, E., Inorganic Chemistry, Pearson Education (2003) 3^{rd} 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 -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

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.

4. record and interpret the UV-Vis and IR spectra for structural analysis and kinetic studies.evelop 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) 3rded*
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 Minor Research 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 work on a research problem in any of the departmental research laboratory according to their interest. Progress of work will be monitored continuously and evaluated at the end of semester by a committee formed by HSCBC 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

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

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, 4^{th} Ed., John Wiley & Sons, Inc. (2013).
4. Nelson, D.L., Cox, M.M., Lehninger Principles of Biochemistry 6^{th} 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

PCYXXX DISSERTATION

L	T	P	Cr
-	-	-	12.0

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 one year project work in any of the research laboratory in school of chemistry and biochemistry and has to submit the dissertation. Evaluation will be as per institute policy / external expert.

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

1. analyze current literature 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, -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

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 218 : 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

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