

Attainment of Programme Outcome

Master of Science (Chemistry)

CO, PO and PSO Mapping

Name of the Course: Inorganic Chemistry - I

Blueprint of the question paper	Section	Unit I	Unit II	Unit III	Unit IV	Unit V
	Section A	2	2	2	2	2
	Section B Any FIVE	2	2	1	1	1
	Section C Either OR	2	2	2	2	2
	Section D Any THREE	1	1	1	1	1

Semester – I			
Core I Inorganic Chemistry - I			
Course Code : 21PCHC11	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To explain the various photophysical and photochemical processes involved in inorganic compounds.
- To understand the atomic structure and periodical properties of elements.
- To explain the various concepts of acids and bases.

Unit I Inorganic Photochemistry

Photo-physical processes - Jablonski diagram - d-d and Charge-transfer reactions, Bimolecular deactivation and Energy transfer - Photochemical processes: Electron transfer reactions, Isomerisation and Substitution (Photoaquation, Photoanation Adamson's rules, Photorearrangement, Photo redox reactions) - Photochemistry of Cr(III) and Co(III) complexes-Photochemistry of Ruthenium Polypyridyls- Applications of Inorganic Photochemistry: Photochemical Conversion and Storage of Solar energy, Semiconductor electrodes.

Unit II Periodic properties and Ionic Bonding

Periodic properties of elements - Ionic radii, Ionization potential, Electron affinity, Electronegativity, Bond lengths, Bond strength, Bond angles, Bond order, Bond energies and lattice energy.

Ionic Bond - Properties of ionic substances - Lattice energy - Born-Haber cycle - Size effect: Ionic Radii - Factors affecting radii of ions - Covalent character predominantly in ionic bonds - Polarization - Fajan's rule - Results of polarization.

Reasoning related to chemical periodicity.

Unit III Molecular Structure and Bonding

Lewis electron dot diagrams - Hybridization, Octet rule - Resonance VSEPR theory - Walsh diagram (H_2O) - Bent's rule - Apicophilicity - Valence bond theory - MO theory of homo and heteronuclear diatomic molecules and poly atomic molecules (O_2 , N_2 , CO , HCl and BeCl_2) - Geometrical isomerism - Fluxionality - Types of chemical bonds (weak and strong) - Intermolecular forces.

Unit IV Acids and Bases

Acid base theories - Arrhenius, Bronsted- Lowry theory, Factors affecting strength of acids and bases - Lewis theory - Catalytic behaviour of acids and bases - The Hard soft interaction principle (HSIP), Proton affinity.

Non-aqueous solvents - Chemistry in liquid ammonia, liquid hydrogen fluoride, liquid sulphur dioxide - Super acids – Molten salts.

Calculation of the strength of acids and bases - Problems related to conjugate acid and bases-Identification of the stability of the complex using HSAB principle.

Unit V Lanthanides and Actinides

Occurrence, properties of the elements - Common and Uncommon Oxidation States - Absorption and Emission Spectra - Magnetic Properties - Separation of lanthanide elements - lanthanide and actinide contraction - Similarities between Actinides and Lanthanides - Coordination complexes and Organometallic compounds of lanthanides and actinides - Uses of lanthanide compounds as shift reagents.

Text Books

1. Rohatgi Mukherjee K.K. *Fundamentals of Photochemistry*. New age international (P) limited. 4th Edition 2021.
2. James E. Huheey, Ellen A. Keiter, Richard L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Harper Collins College Publishers. 4th Edition 2009.
3. Skoog D.A, West D.M, Holler F.J, Grouch S.R. *Fundamentals of Analytical Chemistry*, Thomson Asia Pvt. Ltd. 8th Edition, Third Reprint, 2005.
4. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic Chemistry*. ELBS, Oxford University Press. 1994.

Books for Reference

1. Lee J.D. *Concise Inorganic Chemistry*. Blackwell Science Ltd. 5th Edition, Reprint 2003.
2. Albert Cotton F, Geoffrey Wilkinson, Carlos A. Manic, Manfred Bochman. *Advanced Inorganic Chemistry*. Wiley Interscience Publication. 6th edition 1999.
3. James E. House. *Inorganic chemistry*. Elsevier Publications. 2008.
4. Keith F. Purcell, John C. Kotz. *Inorganic Chemistry*. Cengage India. 2010.
5. Hemant Kulshrestha, Ajay Taneja. *Upkar's CSIR-UGC NET/JRF/SET for Chemical Science*. Agra: Upkar Prakashan. Revised & Enlarged Edition.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	develop the idea about the photophysical and photochemical processes.	1,4	Ev
CO 2	produce semiconductor electrodes and solar cells based on laws of photochemistry.	7,8	Cr
CO 3	explain about the electron configuration, orbital stability and the reactivity	1	Ap
CO 4	demonstrate about the theories of VSEPR, Valence bond and Molecular Orbital.	1,4	Ap
CO 5	compare the chemistry of Non-aqueous solvents such as liquid ammonia, Liquid hydrogen fluoride, Liquid sulfur dioxide.	1,5	An
CO 6	compare the properties of elements present in Lanthanides and Actinides.	1,5	An

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Avg	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5	PSO-6	PSO-7	PSO-8	Avg
CO-1	3	3	3	3	3	2	3	2	3	3	3	3	3	3	2	2	1	2.5
CO-2	3	3	3	3	3	2	2	2	3	3	3	3	3	3	2	2	1	2.5
CO-3	2	2	3	3	3	2	1	2	2.3	3	3	3	3	3	2	2	1	2.5
CO-4	3	3	2	3	3	2	2	2	2.5	3	3	3	3	3	2	2	3	2.8
CO-5	3	3	3	3	3	2	2	2	3	3	3	3	3	3	2	2	3	2.8
CO-6	3	2	3	2	3	2	2	2	2.4	3	3	3	3	3	3	3	3	3.0
Average	3	3	3	3	3	2	2	2		3	3	3	3	3	2	2	1	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Attainment of Course Outcomes of the M.Sc. Chemistry Programme

Course Code	Name of the Course	Course Outcomes															
		Programme Outcomes (PO)								Programme Specific Outcomes (PSO)							
		PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	PSO -1	PSO -2	PSO -3	PSO -4	PSO -5	PSO -6	PSO -7	PSO -8
21PCHC11	Inorganic Chemistry - I	3	3	3	3	3	2	3	2	3	3	3	3	3	2	2	1
21PCHC12	Organic Chemistry - I	3	3	2.5	3	3	2	2	2	3	3	3	3	3	3	2	2
21PCHC13	Physical Chemistry - I	3	3	3	3	3	2	2	1.5	3	3	3	3	3	2	2	1
21PCHE11	A. Advanced Topics in Chemistry	3	3	2	3	3	3	2	2	3	3	2	2.5	3	3	2	2
21PCHE12	B. Food and Health Chemistry	3	3	2.5	2.5	3	3	2.5	2.5	3	3	2	3	3	3	3	2.5
21PCHC21	Inorganic Chemistry - II	3	2	2.3	2.3	2.3	2.3	2	2	3	2.2	2.2	2.3	3	3	2	2
21PCHC22	Organic Chemistry - II	2.5	2	2	2	2	3	2	2	2.5	2	2	3	3	3	3	3
21PCHC23	Physical Chemistry - II	3	2	2	2	2.2	3	2	2.3	2.5	2	3	2.2	2.3	2	1.2	
21PCHE21	A. Nanoscience and Technology	3	2	2	2	2	2.3	2.5	2	2.5	2	2.5	2.5	3	2.5	3	2
21PCHE22	B. Energy and Computational Chemistry	3	2.3	2	3	3	3	2.3	1.3	3	2	2	3	3	3	2	2
21PCHC31	Inorganic Chemistry - III	3	3	2	3	3	1.5	2	2	3	3	2	3	3	3	2.3	2.3
21PCHC32	Organic Chemistry - III	3	3	2	3	3	2	2	1.6	3	3	2	3	3	3	2.5	2.5
21PCHC33	Physical Chemistry - III	3	3	2	3	3	2	2	2	3	3	2	3	3	3	2.3	2.3
21PCHE31	A. Research Methodology	3	3	2	3	3	2	3	2	3	2.5	2	3	3	3	2.5	2.5
21PCHE32	B. Chemical Instrumentation	3	2.3	2	3	3	2	3	1.5	3	2.3	2	3	3	3	2.5	2.3
21PCHSS31	Course on Competitive Exams	3	2	2	3	3	2	3	2	3	2	2	3	3	2	3	2
21PCHC41	Inorganic Chemistry - IV	3	2.5	1	2.5	3	2	3	2	3	2	2	2	3	2.3	3	2.5

21PCHC42	Organic Chemistry - IV	3	2.5	1	3	3	2	3	1	3	2	2	2	3	2.5	3	2
21PCHC43	Physical Chemistry - IV	3	2.5	1.5	3	3	2	3	2	3	2.2	2	2	3	3	3	2
Average Correlation		3	2.6	2	2.8	2.8	2.3	2.4	1.9	3	2.5	2.2	2.7	3	2.7	2.4	2.1
Mean Overall Score		2.5	The POs and PSOs are strongly correlated with the COs of the programme														

Courses of the M.Sc. Chemistry Programme

Semester – I			
Core II	Organic Chemistry - I		
Course Code : 21PCHC12	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To acquire excellence in Organic Chemistry.
- To comprehend the various factors that operate in organic reactions.
- To appreciate the stereochemical aspects of a reaction.

Unit I Aromaticity and Ring System

Aromatic character – Huckel's rule – Aromatic, Antiaromatic and Non aromatic – Molecular orbital description of aromaticity, antiaromaticity and homoaromaticity- Alternate and Non-alternate hydrocarbons– Paratopic compounds - Aromaticity of azulene -Tropones – Annulene- Higher annulenes- Fullerenes – Sydnones – Structure, stereochemistry and synthesis of Adamantane, Diamantane and Cubane - Problems related to the classification of aromaticity (Aromatic, Antiaromatic and Non aromatic only)

Unit II Aliphatic Nucleophilic and Electrophilic Reactions

Aliphatic Nucleophilic Substitution: S_N1 , S_N2 and S_{Ni} mechanisms- Effect of substrate structure, effect of leaving group, effect of attacking nucleophile and effect of the reaction medium- Neighbouring group participation-substitution at vinylic and allylic carbons and reactivity - Ambient nucleophiles and Ambient substrates - Hydrolysis of esters.

Electrophilic substitution – SE_1 and SE_2 mechanism- effect of substrate structure and effect of leaving group.

Problems includes the basic concepts of Aliphatic Nucleophilic and Electrophilic reactions.

Unit III Reactive Intermediates and Rearrangements

Carbocation - Generation, stability, reaction, Mechanism of rearrangements involving carbocation as intermediate Beckmann, Wagner- Meerwein rearrangements.

Carbanion - Generation, stability, reaction, Mechanism of rearrangements involving carbanion as intermediate, Sommelet-Hauser and Favorskii rearrangements.

Carbenes - Generation, stability, structure, reactions and stereochemistry of carbenes - Wolff rearrangement, Carbylamine reaction and its synthetic applications.

Nitrenes - Generation, stability, reaction of nitrenes - Mechanism of rearrangements through Nitrene intermediate – Schmidt rearrangement - Hoffmann rearrangement.

Arynes -Generation, Structure, Stability, reactions and trapping of arynes – Cine substitution.Problems includes the basic concepts of reactive intermediates.

Unit IV Stereochemistry

Stereoisomerism- Introduction, classification, Principles of axial and planar chirality - Stereochemistry of allenes, spiranes and analogus- Atroisomerism in compounds other than biphenyl -optically activity and configurational nomenclature - Stereochemistry of Ansa Compound, Helicity- Topicity of ligands and faces– Homotopic, Enantiotopic, Diastereotopic - Nomenclature of stere heterotopic ligands and faces - Mechanism of racemisation involving free radicals and carbonium ions - Conformations of cyclic systems- monosubstitued, disubstitutedcyclohexanes [(1,2), (1,3), (1,4)], decalin, perhydrophenanthrene.

Problems related to Conformations.

Unit V Name Reactions

Reactions, Mechanism and Applications of Bouveault-Blanc reduction, Chichibabin reaction, Duff reaction, Etard reaction, Henery reaction, Nef reaction, Ritter reaction, Rosenmund reduction, Simmons-Smith reaction and Ullmann reaction.

Text Books

1. Ahluwalia V.K,Parshar R.K, *Organic Reaction Mechanism*.Narosa Publishing House. Fourth Edition 2013.
2. Mukherjee K.S, *Mechanism of Organic reactions*. Kolkota: Books and Allied Ltd. 2010.
3. Kalsi P.S.*Organic Reaction & Mechanism*.New Delhi: New-Age International Publishers. 4th Edition 2011.
4. Raj K Bansal. *Organic reaction mechanism*.New Delhi: New-Age International Publishers. 4th Edition 2012.
5. Kalsi P.S, *Stereochemistry: Conformation and Mechanism* New Delhi: New-Age International Publishers. 4th Edition 1997.

Books for Reference

1. March J.*Advanced Organic Chemistry*.New York: John-Wiley and Sons. Fourth Edition 1992.
2. Eliel E L.*Stereochemistry of Carbon Compounds*, New Delhi: Tata-McGraw Hill Publishing Company. 1975.
3. Nasipuri D. *Stereochemistry of Carbon Compounds*.New Delhi: New-Age International Publishers. 3rd Edition 2011.
4. Clayden, Greeves,Warren,Wothers.*Organic Chemistry*.New York: Oxford University Press. 2006.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	illustrate the basic of aromaticity	1	Un
CO 2	criteria for aromaticity and Huckel's $4n+2$ electron rule for benzene and non benzenoid aromatic compounds.	6	Ev
CO 3	Understand the various types and associate the neighboring group participation of aliphatic nucleophilic substitution reactions.	3	Un, Ap
CO 4	explain the generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals	2	Ap
CO 5	identify the stereochemistry notations, concept and its importance	1	Ap
CO 6	investigate the Name the reaction Mechanism and Applications	3	An

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Avg	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5	PSO-6	PSO-7	PSO-8	Avg
CO-1	2	3	1	3	3	2	3	2	2	3	3	3	2	3	2	2	1	2
CO-2	3	3	2	3	3	2	2	2	3	3	3	2	3	3	2	2	1	2
CO-3	3	3	3	3	2	2	1	2	2	3	3	3	3	3	2	2	1	3
CO-4	3	3	3	3	2	2	2	2	3	3	3	3	3	3	2	2	3	3
CO-5	3	3	3	3	3	2	2	2	3	3	3	3	3	3	2	2	3	3
CO-6	3	2	3	3	3	2	2	2	2.5	3	3	3	2	3	2	3	2	3
Average	3	3	2.5	3	3	2	2	2		3	3	3	3	3	3	2	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – I			
Core III	Physical Chemistry - I		
Course Code : 21PCHC13	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To achieve base knowledge about the concepts of physical chemistry.
- To solve Schrodinger equations for a particle moving in different dimensions.
- To demonstrate and prepare the polymer molecules by various methods.

Unit I Quantum Chemistry – I

Postulates of quantum mechanics - Operators and their algebra - Linear operator, Hermitian operators - Eigen functions and Eigen values - Orthogonality and Normalization Theorems - Schrodinger Wave equation (Time dependent and Time independent) - Solution of Schrodinger equations - Particle in a box (1D and 3D) - Hydrogen atom - Rigid rotor and Simple Harmonic Oscillator - Quantum mechanical tunnelling.

Problems based on i) Eigen functions & Eigen values

ii) Orthogonality & Normalization Theorems.

iii) Calculation of energy for particle moving 1-D and 3-D boxes.

Unit II Quantum Chemistry – II

Pauli exclusion principle - Slater determinant - Approximation methods - Variation theorem - Application of variation method to helium atom - Perturbation theory (First order) - Application to helium atom –HartreeFock - Self consistent field method (HF-SCF) to helium atom - Born-Oppenheimer approximations - MO and VB treatments of H₂ molecule - Huckel Molecular Orbital theory - Application to ethylene, butadiene and benzene.

Unit III Polymer Chemistry

Polymerization in homogeneous and heterogeneous phases - Kinetics and Mechanism of Free radical, Anionic and cationic polymerization - Molecular Weights - Methods of determination - Light scattering, Osmotic pressure and Viscosity methods - Glass transition temperature (T_g) - Factors affecting T_g - Conducting polymers - Factors affecting the conductivity of conducting polymers - Doping of Conducting polymers - Solitons, Polarons and Bipolarons.

Calculation of Molecular weight of the polymers.

Unit IV Photochemistry

Importance of photochemistry - Laws of photochemistry, Quantum yield and its determination - Physical properties of electronically excited molecules: excited state dipole moment, acidity constant and redox Potentials - Photophysical processes in electronically excited molecules: Jablonski diagram - Intersystem crossing, internal conversion, fluorescence,

phosphorescence and other deactivation processes - Photosensitisation, Chemiluminescence and Bioluminescence - Kinetics of Collisional quenching: Stern-Volmer equation - Deviation from Stern-Volmer equation - Experimental Techniques in Photochemistry: Chemical Actinometers.

Unit V Rotational Spectroscopy

Electromagnetic radiation - Quantization of energy - Regions of spectra - Width of spectral lines - Collision broadening, Doppler broadening, Heisenberg uncertainty principle - Intensity of spectral lines - Diatomic molecules as rigid rotors - Rotational energy levels, intensity of spectral lines, selection rules - Effect of isotopic substitution - Diatomic molecules as non-rigid rotors - Rotational transitions - Rotational spectra of linear and symmetric top polyatomic molecules.

Text books

1. Chandra A.K. *Introductory Quantum Chemistry*. Noida: Tata McGraw Hill. 4th edition, 1994.
2. Aruldas G. *Quantum Mechanics*. New Delhi: Prentice Hall of India Pvt. Ltd. 2006.
3. R. K. Prasad. *Quantum Chemistry*. New Delhi: New Age International Publishers. 4th edition, 2014.
4. Rohatgi Mukherjee K.K. *Fundamentals of Photochemistry*. New Age Publishers. 2017.
5. Banwell C.N. *Fundamentals of Molecular Spectroscopy*. Noida: McGraw Hill Education. 4th edition, 1994.

Books for Reference

1. McQuarrie D.A. *Quantum Chemistry*. Sausalito: University Science Books. 2008.
2. Levine I.N. *Quantum Chemistry*. New Jersey: Prentice Hall. 5th edition, 2000.
3. Atkins P.W. *Molecular Quantum Mechanics*. Clarendon. 1973.
4. Anatharaman R. *Fundamentals of Quantum Chemistry*. New Delhi: McMillan. 2001.
5. Atkins P.W. *Physical Chemistry*. ELBS edition. 3rd edition, 1987.
6. Ladd M. *Introduction to Physical Chemistry*. Cambridge. Oxford University Press. 2018.
7. Maron S.H., Lando J.B. *Fundamentals of Physical chemistry*. New York: MacMillan Publishers. 1974.
8. Bill Meyer F.W. *Text book of polymer science*. New York: John Wiley and sons. 3rd Edition. 1984.
7. Gowariker V.R., Viswanathan N.V., Jayadev Sreedhar. *Polymer Science*, New Delhi: New Age International (P) Limited, Publishers. 1st edition, Reprint, 2005.
8. Misra G.S. *Polymer science*. Wiley Eastern. 1986.
9. Barrow G.M. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill. 1964.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	Have a good foundation in understanding the physical and mathematical aspects of quantum mechanics.	1	Un
CO 2	apply the approximation methods to different atoms and find the dissociation energy and bond order for various molecules by applying Huckel molecular orbital theory.	4	Ap
CO 3	explain different types of methods of preparation of polymers.	5	Un
CO 4	prepare the polymer molecule and determine the molecular weight of polymer.	6	Cr
CO 5	deduce the experimental techniques involved in photochemical processes.	5	Ev
CO 6	classify the molecules according to their moment of inertia.	1	An

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Avg	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Avg
CO-1	3	3	3	3	3	2	3	2	3	3	3	3	3	3	2	2	1	2.5
CO-2	3	3	3	3	3	2	2	1	2.5	3	3	3	3	3	2	2	1	2.5
CO-3	3	3	3	3	3	2	1	2	2.5	3	3	3	3	3	2	2	1	2.5
CO-4	3	3	3	3	3	2	2	1	2.5	3	3	3	3	3	2	2	3	2.8
CO-5	3	3	3	3	3	2	2	2	3	3	3	3	3	3	2	2	3	2.8
CO-6	3	3	3	3	3	2	2	1	2.5	3	3	3	3	3	3	3	3	3.0
Average	3	3	3	3	3	2	2	1.5		3	3	3	3	3	2	2	1	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – I			
Elective IA. Advanced Topics in Chemistry			
Course Code : 21PCHE11	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To understand about molecular modelling and drug designing.
- To have in-depth knowledge about host-guest molecules.
- To create awareness about common diseases and their treatments.

Unit I Molecular modelling and Drug designing

Introduction Molecular modelling - Drug discovery: the Evolution and process - The role of Computer assisted drug design- Process of drug discovery- Bioassay- Lipinski's rule of five - Quantum mechanical simulations - *Ab Initio* methods, Semi Empirical methods- Molecular dynamics in drug design - Docking- types of searching methods in Docking, docking methods, the scoring function, docking using Auto Dock, Virtual screening, De novo design. Cheminformatics - SMILES (Simplified Molecular Input Line Entry Specification), Applications of Cheminformatics in Drug discovery.

Unit IISupramolecular Chemistry

Introduction - Development - Classification - Based on cavity and forces - Recent developments in Supramolecular compounds - Molecular self-assembly - Self-replicating molecular systems, Molecular self-assembly based on hydrogen bond and Metal coordinated self-assembly - Catenenes and Rotaxanes - Synthesis of crown ethers - Synthesis of Cryptands - Metal complexes with Crown ethers and Cryptands.

Unit III Green Chemistry

Twelve principles of greenchemistry - Green solvents - Supercritical CO₂ and H₂O - Microwave assisted reaction - Stille reaction, Suzuki reaction - Krohnke reaction -Hiyama reaction - Sonogashira reaction.

Introduction to Sonochemistry - Instrumentation - Types of Sonochemical reactions - Homogeneous reaction -Strecker reaction - Heterogeneous liquid-liquid reactions - Hydrolysis and Solvolysis - Heteogeneous solid-liquid reactions - Bouveault reactions, Barbier reaction of carbonyl compounds - Miscellaneous applications of ultrasound - Preparation of porous carbon powder - Sonochemical treatment of polluted water.

Unit IV Pharmaceutical Chemistry

Introduction - Drugs for common diseases due to insects & animals, Air borne diseases, Water borne diseases, Respiratory diseases & Diseases of the Nervous system. Pharmaceutical

Aids - Preservative, Anti-oxidants, Sequestrants - Colouring agents, Flavouring agents and artificial sweetening agents added in drugs - Different dosage forms of Drugs - Solid (Tablet), Semisolid (Paste, Cream), Liquid (Solution, Suspension, Emulsion) and Gaseous dosage form.

Unit V Environmental Chemistry

Environmental Segments - Natural cycles of environment: the hydrological, oxygen and nitrogen cycles - Chemical and Photochemical reactions in atmosphere: SO_2 , O_2 and O_3 chemistry, nitrogen oxides and organic compounds - Greenhouse effect - Ozone hole - El Nino phenomenon.

Microorganisms - Catalysts of aquatic chemical reactions - Acid-base and Ion exchange reactions in soil - Nitrogen pathways and NPK in soil - Waste classification and disposal - Solid waste management.

Text Books

1. Anand Solomon K. *Molecular modelling and Drug Design*. MJP publishers. 2016.
2. Kalsi P.S, Kalsi J.P. *Bioorganic, Bioinorganic and Supramolecular Chemistry*. New Age International Publishers. Second edition. 2010.
3. Ahluwalia V.K, Varma R.S. *Alternate Energy Processes in Chemical Synthesis: Microwave, Ultrasonic and Photo Activation*. Narosa Publishing House. New Delhi. 2008.
4. DE A.K. *Environmental Chemistr*. New age international publishers. 5th edition.

Books for Reference

1. Khopkar S.M. *Analytical chemistry of Macrocyclic and Supramolecular compounds*. Delhi: Narosa Publishing House. Second edition 2008.
2. Ahluwalia V.K, Rajender S. Varma. *Green Solvents for Organic synthesis*. Narosa Publishing House Pvt. Ltd. 2009.
3. Paul T. Anastas. *Text Book on Green Chemistry*. OUP. 2006.
4. Raghupati Mukhopadhyay, Sriparna Datta, Rajib Kumar Das. *Textbook of Pharmaceutical chemistry & Medicinal Chemistry*. Books and Allied (P) Ltd. First Edition 2011.
5. Jayashree Ghosh. *A Textbook of Pharmaceutical Chemistry*. New Delhi: S. Chand & Company Ltd. 1997.
6. Dr. Ravikrishnan A. *Environmental Science & Engineering*. Sri Krishna High tech Publishing Company Pvt. Ltd. Eleventh edition 2015.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	formulate molecular dynamics in drug design.	5	Ap
CO 2	perform docking using Autodock virtual screening and De nova designs.	5,4	Ap
CO 3	develop recent trends in the synthesis of crown ethers.	6	Cr
CO 4	design a green method for the synthesis of compounds using twelve principles of Green chemistry and sketch the natural cycles of environment such as the hydrological, oxygen and nitrogen cycles.	5,6	Cr
CO 5	Compare heterogeneous liquid- liquid and heterogeneous solid- liquid reactions and differentiate chemical and photochemical reactions occurs in atmosphere.	2,5	An
CO 6	synthesis the nanomaterial by ultra-sonication and acquire knowledge about common diseases due to insects, animals, air and water borne diseases.	1,6	Un

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Av g	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Av g
CO-1	3	3	2	2	3	3	2	2	2.5	3	3	2	2	3	3	2	2	2.5
CO-2	3	3	2	3	3	3	2	2	3	3	3	2	2	3	3	2	2	2.5
CO-3	3	3	2	3	3	3	2	2	3	3	3	2	3	3	3	2	2	3
CO-4	3	2	3	3	3	3	2	2	3	3	3	2	3	3	3	2	2	3
CO-5	3	2	3	3	3	3	2	2	3	3	3	2	3	3	3	2	2	3
CO-6	3	3	2	2	3	3	2	2	2.5	3	3	2	2	3	3	3	2	2.6
Average	3	3	2	3	3	3	2	2		3	3	2	2.5	3	3	2	2	
PO Mean									2.6	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – I			
Elective IB. Food and Health Chemistry			
Course Code : 21PCHE12	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To learn the importance of basic nutrients and maintain good health.
- Acquire knowledge about micro and macro nutrients to enhance our health.
- Aware of food adulterants affecting body health.

Unit I Health and its maintenance

Health - Mental health and Physical health - Food Pyramid - Types of Malnutrition - Causes and Remedies - Macro and Micro nutrients - Carbohydrates - Classification and their Biological functions - Proteins - Classification and their Biological functions - Vitamins - Classification and their Biological functions - Minerals (Fe, Ca, P, Na and K) and their Biological functions.

Unit II Drugs Metabolism

Introduction - Drug metabolism pathways - Phase I transformations - Oxidative reactions, The NIH Effect (Alkene epoxidation, Aliphatic hydroxylation, Oxidation of Carbon-Oxygen system and Oxidation of Carbon-Sulphur system), Reductive reactions (Carbonyl reduction, Reduction of Nitro group, Reductive Dehalogenation) and Hydrolytic reactions - Phase II transformations - Conjugation reaction (Glucouronic acid conjugation, Amino acid conjugation, Sulphate conjugation, Acetic acid conjugation and methyl conjugation) and Hard and Soft drugs.

Unit III Body Fluids

Blood Volume - Blood group - Functions of blood - Blood pressure - Anaemia - Blood sugar - Haemoglobin - Chemistry of respiration - Urine - Electrolyte balance. Enzymes - Types and their action - Hormones and their biological functions - Digestion in mouth, stomach, pancreas and intestine.

Unit IV Energy Metabolism

Introduction - Energy and metabolism - Measurement of energy - Energy cycle - Transformation of energy - Controlled energy in human metabolism - Covalent bond, Hydrogen bond and Phosphate bond. Controlled Reaction rates - Enzymes, Coenzymes and Hormones - Types of Metabolic reactions - Anabolism and catabolism - Energy metabolism - Basal metabolism, Methods of measuring BMR and Factors influencing BMR - Total energy requirement.

Unit V Food adulteration and Testing

Introduction - Legal aspects of food adulteration and prevention - Common Food adulterants in edible oils, ghee, coffee powder, chilli powder, turmeric powder, meat and milk - Harmful effects of the adulterants - Food Additives - Sweeteners, preservatives, flavours and colourants - Pesticide contaminants - Toxicants.

Text books

1. Ahluwalia V.K, Madhu Chopra. *Medicinal chemistry*. Ane Books Pvt. Ltd. Ane's Student edition, 2009.
2. Deb A.C. *Fundamentals of Biochemistry*. Calcutta: New Central Book Agency. 1994.
3. Alex V. Ramani. *Food chemistry*. Chennai. MJP Publishers. 2014.

Books for Reference

1. Ashutosh Kar. *Medicinal Chemistry*. New Delhi: Wiley Easterns Ltd. 1993
2. Jayashree Ghosh. *A text book of Pharmaceutical chemistry*. S. Chand & Co Ltd. 1999.
3. Satake M, Mido Y. *Chemistry for Health Science*. New Delhi: Discovery Publishing House. 2003.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	classify nutrients, proteins, vitamins and minerals.	1	An
CO 2	examine physical and mental health.	6	An
CO 3	explain various metabolism of drugs.	2	Un
CO 4	compare hard and soft drugs.	1	Ev
CO 5	measure blood pressure and sugar and detect various blood group for different persons.	8	An
CO 6	calculate body mass fluid and give the factors which affect BMF and test the adulterants present in food items.	3, 5	Ap

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Av g
CO-1	3	3	2	3	2	3	3	2	2.6	3	2	3	2	3	3	2	2	2.5
CO-2	3	2	3	2	3	2	1	3	2.3	3	3	2	3	3	3	3	3	2.8
CO-3	3	2	3	2	3	3	3	3	2.7	3	3	2	3	3	3	3	3	2.8
CO-4	2	3	2	3	3	2	3	2	2.5	2	3	2	3	2	3	3	2	2.5
CO-5	3	3	3	3	3	3	2	2	2.7	3	3	3	3	3	3	2	2	2.7
CO-6	3	3	2	2	3	3	3	3	2.7	3	3	2	3	3	3	3	3	2.8
Average	3	3	2.5	2.5	3	3	2.5	2.5		3	3	2	3	3	3	3	2.5	
PO Mean									2.6	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – II			
Core IV	Inorganic Chemistry –II		
Course Code : 21PCHC21	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To discuss the stability and bonding in Co-ordination compounds.
- To know the basics of organometallic chemistry.
- To demonstrate the principle and applications of IR, Raman and Mossbauer spectroscopies.

Unit I Stability of Co-ordination compounds

Coordination numbers and structures, Isomerism- Stability constants of complexes and their determination - Solubility method, Ion exchange method, Job's method and Bjerrum's method - Stabilisation of Unusual oxidation state - Irving William series and the spectrochemical series - Factors affecting stability constant: Charge, size & outer electron configuration of central metal ion; nature, Basicity & chelating ability of ligand atom; Size & number of chelate ring; Steric effect - Chelate and Macrocyclic effect.

Unit II Bonding in Co-ordination compounds

Valence bond theory - Crystal field theory for octahedral complexes ($[\text{TiF}_6]^{2-}$, $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$, $[\text{TiCN}_6]^{3-}$), Crystal field theory for tetrahedral complexes ($[\text{Zn}(\text{OH})_4]^{2-}$, $[\text{CoCl}_4]^{2-}$, $[\text{CuCl}_4]^{2-}$) and Crystal field theory for square planar complexes ($[\text{NiCN}_4]^{2-}$, $[\text{XeF}_4]^{2-}$) - Crystal Field Stabilisation Energy (CFSE) - Measurement of $10Dq$ or Δ_0 - Factors affecting magnitude of Δ_0 or $10Dq$ values - Consequences of crystal field splitting: ionic radii of transition metal ions, hydration energy, lattice energy - Unusual oxidation states and CFSEs - Jahn-Teller effect - Molecular orbital theory (sigma as well as pi bonding).

Unit III Organometallic chemistry I

Effective Atomic Number (EAN) - 16 and 18 electron rules - synthesis, structure and bonding in mono and polynuclear metal carbonyls, carbonylate ions, carbonyl hydride complexes - Isolobal fragments - Synthesis and reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes and arene complexes - Metallocenes and bonding in metallocenes. Calculation of Effective Atomic Number.

Unit IV Organometallic chemistry II

Reactions of organometallic complexes - Substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic displacement of coordinated ligands - Homogeneous Catalysis - Hydrogenation, Hydroformylation, Monsanto process, Wacker process, Alkene metathesis - Heterogeneous catalysis - Fischer-Tropsch process, Ziegler-Natta polymerization.

Unit V Spectroscopy I

IR and Raman Spectroscopy: Selection rules - Predicting number of active modes of vibrations - Applications of IR and Raman in the study of inorganic structures and coordination compounds - Application of isotopic substitution, detection of intra and intermolecular hydrogen bonding.

Mossbauer Spectroscopy: Principle, conditions for Mossbauer spectroscopy - Isomer shift - Quadrupole interactions - Magnetic interactions - Interpretation of spectra of iron and tin compounds.

Problems related to Mossbauer spectroscopy.

Text Books

1. Gopalan R, Ramalingam V. *Concise Coordination Chemistry*. Vikas Publishing House Pvt. Ltd., New Delhi. 2006.
2. James E. Huheey, Ellen A. Keiter, Richard L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Harper Collins College Publishers. 4th Edition 2009.
3. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic chemistry*, ELBS, Oxford University Press. 1994.
4. Gopalan R. *Textbook of Inorganic chemistry*. Universities press (India) Private Limited. 2012.
5. Skoog D.A, West D.M, Holler F.J, Grouch S.R. *Fundamentals of Analytical Chemistr.* Thomson Asia Pvt.Ltd.. 8th Edition, Third Reprint. 2005.

Books for Reference

1. Robert H. Crabtree. *The Organometallic Chemistry of the Transition Metals*. John Wiley & Sons, Inc., Publication. 6th Edition, 2006.
2. Gary L. Miessler, Donald A. Tarr. *Inorganic chemistry*. Pearson Publications. 3rd edition 2005.
3. Catherine Housecroft, Alan G. Sharpe. *Inorganic Chemistry*. Prentice Hall. 2007.
4. Albert Cotton F, Geoffrey Wilkinson, Carlos A. Manic, Manfred Bochman, *Advanced Inorganic Chemistry*. Wiley Interscience Publication. 6th edition 1999.
5. Wijesekara R.D. *Coordination Compounds: Bonding, Structure and Nomenclature*. New Delhi: Narosa Publishing House. 2008.
6. Soni P.L, Vandna Soni. *Coordination Chemistry: Metal complexes, Transition metal Chemistry with lanthanides and actinides*. New Delhi: Ane Books Pvt. Ltd. 2016.
7. Drago R.S. *Physical Methods in Inorganic Chemistry*. W.B. Saunders. 1977.
8. Ebsworth David E.A.V, Rankin Stephen Credock W.H. *Structural Methods in Inorganic Chemistry*. ELBS. IV edition 1988.
9. Hemant Kulshertha, Ajay Taneja, *Upkar's CSIR-UGC NET/JRF/SET for Chemical Science*. Agra: Upkar Prakashan. Revised & Enlarged Edition. 2021.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	judge about the stability and factors affecting the stability of the coordination complexes.	1, 2	Ev
CO 2	Measure Crystal Field Stabilisation Energy ($10Dq$ or Δ_0) of coordination complexes.	2, 4	Ev
CO 3	synthesis and can discuss about reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes and arene complexes	6, 7	Cr
CO 4	summarize the substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic reactions of organometallic complexes.	1, 4	Un
CO 5	predict about the number of active modes of vibrations in IR and Raman spectroscopy.	5	Un
CO 6	interpret the Mossbauer spectra of Iron and Tin complexes.	5, 7	Ev

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PSO -1	PSO -2	PSO -3	PSO -4	PSO -5	PSO -6	PSO -7	PS O-8	Av g
CO-1	3	2	2	3	2	3	3	1	2.4	3	2	2	3	2	2	2	2	2.3
CO-2	2	3	2	2	2	3	2	2	2.3	2	2	3	3	3	3	1	3	2.5
CO-3	3	2	2	2	3	2	2	2	2.3	3	2	2	2	3	3	2	2	2.4
CO-4	3	2	3	2	2	3	2	3	2.5	2	3	2	3	2	3	1	2	2.3
CO-5	2	1	3	3	3	3	2	3	3	2	2	3	2	3	3	2	1	2.3
CO-6	3	2	2	2	3	3	2	2	2.4	3	2	1	2	2	2	3	2	2
Average	3	2	2.3	2.3	2.3	2.3	2	2		3	2.2	2.2	2.3	3	3	2	2	2.5
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – II			
Core V	Organic Chemistry - II		
Course Code : 21PCHC22	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To support and advance the worldwide community of chemistry scholars.
- To enhance the basic and applied research framework in the Chemistry Department.
- To understand the principle behind thermal and photochemical organic reactions.

Unit I Reactions and Methods of Determination of their Mechanism

Essential requirements of chemical reaction- Mechanistic Classification of reaction- Thermodynamic requirements and Kinetic requirements for the reaction, Microscopic reversibility - Methods of Determining Mechanism: Non-kinetic methods: Identification of products, characterisation of intermediates, isotopic labelling, Stereochemical effect, Kinetic methods: Kinetic study, Isotope effects -Transition state theory - Hammond Postulate- Hammett equation- Linear Free Energy Relationship-Taft equation. Problems related to Hammett equation and Taft equation.

Unit II Molecular Rearrangements with Migrating Aptitude

Migration of Carbon – Wagner-Meerweinrearrangement, Benzil-Benzilic acid rearrangement and Dienone-Phenol rearrangement.

Migration of heteroatoms - Migration to electron deficient nitrogen, Beckmann rearrangement, Curtius rearrangement and Lossen rearrangement.

Migration to electron deficient oxygen – Baeyer-Villiger oxidation, Hydro peroxide rearrangement and Dakin reaction.

Migration to electron rich carbon – Neberrearrangement and Tiffenev-Demjanov rearrangement.

Aromatic rearrangements –Fries rearrangement and Hofmann-Martius rearrangement

Unit III Alkaloids and Flavonoids

Alkaloids –Introduction - General methods of extraction - Classification - Degradation studies - HEM, Emde and Von-Braun - Structural elucidation of papaverine, morphine, quinine and cocaine.

Flavonoids – Introduction- Properties - Reactions - Isolation- General methods for the elucidation of structure of flavones- Isoflavone, flavonols and Quercetin. Structural relationship between Flavone, Isoflavone and Flavonol.

Unit IV Organic Photochemistry

Photochemistry basic principles - Photochemistry of carbonyl compounds - Norrish Type I and II cleavage reactions, Photocycloadditions – Paterno-Buchi reaction, Photorearrangements-

Di- π -methane rearrangement, photo Fries rearrangement, Photoreduction of carbonyl compounds and aromatic hydrocarbons, Barton reaction, Photooxidation of alkenes and polyenes, Cis-Trans isomerisation of alkenes, Photochromism and Photoimaging.

Unit V UV - Visible and Infra - Red Spectroscopy

UV – Visible spectroscopy: Basic concepts, electronic energy levels, electronic transitions, selection rules, absorption laws and Instrumentation - Characteristic absorption of organic compounds, solvent effect - Applications of Woodward – Fisher rules for calculating absorption maximum in conjugated diene, triene, polyenes, α and β unsaturated carbonyl compounds, UV spectroscopy to problems in organic chemistry.

Optical rotatory dispersion and circular dichroism: Circular Birefringence and Circular Dichroism, Optical rotatory dispersion (ORD), Axial Helicity rule and Octant rule, Applications of Octant rule.

IR spectroscopy: Basic theory and Instrumentation - Characteristics of IR absorption of different functional groups - Factors influencing vibrational frequencies - Applications of Infra-red spectroscopy. Problems in spectroscopy.

Text Books

1. Kalsi P.S. *Organic Reaction & Mechanism*. New Delhi: New Age International Publishers. 4th Edition 2020.
2. Ahluwalia V.K, Parshar R.K. *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House. Fourth Edition 2019.
3. Mukherjee Kapoor Singh. *Mechanism of Organic reactions*. Kolkata: Books and Allied Ltd. 2021.
4. Raj K Bansal. *Organic reaction mechanism*. New Delhi: New Age International Publishers. 4th Edition 2012.
5. Gurdeep Chatwal. *Organic Chemistry of Natural Products Vol II*. Bombay: Himalaya Publishing House. 2011.
6. Jagdamba Singh, Jaya Singh. *Photochemistry and Pericyclic Reactions*. New Delhi: New Age international publishers. 4th edition 2019.
7. Sharma Y.R. *Elementary Organic spectroscopy*. New Delhi: S. Chand & Company. 5th Edition 2013.
8. Jag Mohan. *Organic spectroscopy Principles and Applications*. New Delhi: Narosa Publishing House. Second Edition 2011.

Books for Reference

1. Michael B Smith. *March's Advanced Organic Chemistry: Reactions, Mechanism and Structure*. New York: John-Wiley and Sons. 8th Edition 2019.
2. Jonathan Clayden, Nick Greeves, Stuart Warren, Wothers. *Organic Chemistry*. New York: Oxford University Press. 2nd Edition 2021.
3. Finar I.L. *Organic Chemistry, Volume I*. India: Pearson Education India. 6th Edition 2002.

4. Finar I.L. *Organic Chemistry, Volume II*. India: Pearson Education India. 5th Edition 2002.
5. Sykes P. *Guide Book to Mechanism in Organic Chemistry*. ELBS with Longmann. Sixth Edition 1997.
6. Norman R.O.C, Coxon J.M. *Principles of Organic synthesis*. Switzerland: Springer and Business Media, LLC. Third edition 1994.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO1	organize the various methods of determination of reaction mechanism	1	Cr
CO2	comprehend the various factors that operate in organic reactions	3	An
CO 3	analyse the migrating aptitude and rearrangements	4	An, Ap
CO 4	understand and determine the isolation and structural determination of alkaloids	2	Un, An
CO 5	discuss the Photochemistry of (n- π^*) transitions with particular reference to Norrish type I, Norrish II type reactions, Paterno - Buchi reactions & photochemistry of nitrites.	3	An
CO 6	understand the applicability of the spectroscopic techniques and Instruments	5	Un, Ap

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Av g
CO-1	3	2	2	2	1	2	2	3	2.1	3	2	3	2	2	2	2	3	2.4
CO-2	2	3	2	1	2	3	2	1	2	2	2	2	3	2	2	3	2	2.3
CO-3	3	2	2	1	3	2	1	2	2	3	2	2	2	3	3	2	3	3
CO-4	2	1	3	2	2	3	2	1	2	2	3	2	2	2	3	3	2	2.4
CO-5	2	1	3	3	3	2	2	2	2.3	2	2	2	3	3	3	3	3	3
CO-6	3	2	2	2	2	3	1	2	2.1	3	2	3	3	3	2	3	2	3
Average	2.5	2	2	2	2	3	2	2		2.5	2	2	3	3	3	3	3	
PO Mean									2.5	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – II			
Core VI	Physical Chemistry – II		
Course Code : 21PCHC23	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To learn the concepts of Group Theory and to demonstrate the various types of symmetry elements present in the molecules.
- To gain knowledge about the principles of surface chemistry and catalysis.
- To understand the principle and applications of IR and Raman spectroscopies and by applying the different kinds of spectroscopy, give the structure of molecules.

Unit I Group Theory - I

Symmetry elements and symmetry operations - Group postulates and types of group - Group multiplication table - Construction of multiplication table for C_{2v} , C_{3v} and C_{2h} - Point group - Schoenflies symbols - Matrix representations of symmetry operations - Reducible and irreducible representations - The Great Orthogonality theorem (GOT) - Properties of Reducible and irreducible representations - Construction of character tables for point groups (C_{2v} , C_{3v} and D_{2h}) by using the Great Orthogonality theorem.

Unit II Group Theory - II

Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Determination of Hybridisation of atomic orbitals in linear and non-linear molecules (AB_4 tetrahedral, AB_3 triangular planar, AB linear molecules) - Symmetries of vibrational modes in non-linear molecules (H_2O , NH_3 and BF_3) - Symmetries of vibrational modes in linear molecules (HCN , CO_2) - Symmetry selection rules for infrared and Raman spectra - Mutual exclusion principle.

Unit III Surface Chemistry & Catalysis

Surface phenomenon: Adsorption - Physisorption and chemisorption - Adsorption isotherms: Freundlich, Langmuir, Gibbs and BET adsorption isotherms - Measurement of surface area - Micelles and reverse micelles - Microemulsion - Solubilisation.

Catalysis: Homogeneous catalysis - Acid-base catalysis - Van't Hoff and Arrhenius complexes for Protropic and Protolytic mechanisms - Bronsted catalysis law - Hammett acidity function - Heterogeneous catalysis - Langmuir-Hinshelwood Mechanism - Langmuir-Rideal bimolecular mechanism - Enzyme catalysis: Michaelis-Menton Kinetics - Rate of enzyme catalyzed reaction - Factors influencing enzyme catalysis.

Unit IV Thermodynamics

Concepts of partial molar properties - Chemical Potential - Gibbs-Duhem equation - Gibbs-Duhem-Margulus equation - Partial Molar Volume and its significance - Determination of Partial Molar Volume - Method of Intercept and Apparent Molar Volume method - Concept of fugacity - Variation of fugacity with volume and pressure - Determination of fugacity by graphical method and compressibility factor method - Concept of Activity and activity coefficient - Determination of activity and activity coefficients for non-electrolytes from Gibbs-Duhem equation.

Unit V Vibrational and Raman Spectroscopy

Infrared spectroscopy -Polyatomic molecules - Fundamental vibrations and their symmetry - Overtone and combination frequencies - Concept of group frequencies - Fermi resonance and FT-IR.

Raman Spectroscopy -Rayleigh scattering - Raman Scattering - Classical and quantum theories of Raman effect - Rotational Raman spectra for linear and symmetric top molecules - Vibrational Raman spectra - Rotational fine structure - Polarization of light and the Raman effect - Technique and instrumentation - Laser Raman spectrometer - Structure determination from Raman and Infra-red spectroscopy.

Problems related to IR and Raman spectroscopy.

Text books

1. Raman K.V.*Group Theory and its Applications to Chemistry*. Tata McGraw Hill Co. 1994.
2. Rajaram K, Kuriacose J.C.*Thermodynamics for Students of Chemistry*.Jalandhar: S.L.N. Chand and Co. 2nd Edition 1986.
3. Gurdeep R.Chatwal, Sham K.Anand.*Spectroscopy*.Himalaya Publishing House. 2009.

Books for Reference

1. Cotton F.A.*Chemical applications of group theory*. Wiley. Third edition 2003.
2. Mark Ladd.*Symmetry and Group Theory in Chemistry*. New Delhi: Woodhead Publishing. 2013.
3. Antorpov L.*Theoretical Electrochemistry*. Moscow: Mir Publishers.
4. Bockris J O'M, Reddy A.K.N.*Modern Electrochemistry, Vol 1 & 2*. New York: Plenum Press.Second Edition. 1998.
5. McQuirrie D.A, Simon J.D.*Physical Chemistry: A Molecular Approach*.New Delhi: VivaBooksPvt. Ltd. 1999.
6. RajaramJ,Kuriacose J.C. *Thermodynamics for Students of Chemistry: Classical, Statistical and Irreversible*. New Delhi: Pearson Education. 2013.
7. Klotz I.M, Rosenberg R.M. *Chemical thermodynamics*. California: W.A.Benjamin Publishers.6th Edition1972.

8. Banwell C.N. *Fundamentals of Molecular Spectroscopy*. Noida: McGraw Hill Education. 4th Edition 1994.
9. Barrow G.M. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill. 1964.
10. Drago R.S. *Physical Methods in Inorganic Chemistry*. New Delhi: East West Press Ltd. 1971.
11. Straughan B.P, Walker S. *Spectroscopy, Volume 1, 2 & 3*. New York: London Chapman and Hall, A Halsted Press Book, John Wiley & Sons Inc. 1976.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	assign the symmetry elements and so that the point group of the given molecule.	2	An
CO 2	construct the character table for various point groups.	2	Cr
CO 3	apply the principles of group theory in determining hybridization and symmetries of vibrational modes in linear and non-linear molecules.	1	Ap
CO 4	compare the different types of adsorption isotherm and improve the surface area in catalysis.	4	Ev
CO 5	elaborate the theories and concepts of homogeneous and heterogeneous catalysed reactions and apply in project work.	6	Cr
CO 6	differentiate the given molecules whether they are IR active or Raman active and draw the structures of various molecules.	2	An, Cr

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Av g
CO-1	3	2	1	2	1	2	2	3	2	3	3	3	2	3	3	3	3	3
CO-2	2	3	1	2	2	3	2	3	2.3	2	2	3	3	3	2	3	3	2.2
CO-3	3	2	1	3	3	2	1	1	2	3	2	3	3	3	3	3	2	3
CO-4	2	1	3	2	2	3	2	3	2.3	1	3	3	3	3	3	3	3	2.4
CO-5	2	1	3	3	3	2	1	2	2.3	2	3	3	3	3	3	2	3	2.2
CO-6	3	2	3	2	2	3	3	2	2.5	3	2	2	3	3	3	3	3	3
Average	3	2	2.6	2	2.2	3	2	2.3			2.5	2	3	2.2	2.3	2	1.2	
PO Mean									2.5	PSO Mean								2.6
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – II			
Elective IIA. Nanoscience and Technology			
Course Code : 21PCHE21	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To introduce and give an insight into the fascinating area of Nanoscience.
- To synthesise the nanomaterials by eco-friendly methods and characterise the synthesized nanomaterials.
- To apply in different fields for the welfare of society.

Unit I Introduction to Nanotechnology

Introduction - Definition -Nanoscience and Nanochemistry-Terminology used in Nanotechnology - Nanostructures (Nanoparticles, Nano scale in one dimension, two dimension and three dimension) - Classification of nanoparticles - Properties of nanomaterials - Surface property, Physico-chemical, Electrical and electronic, Redox, Optical, Mechanical and Magnetic properties - Quantum Dot, Quantum well, Quantum wire and Nanocrystal.

Unit II Synthesis and characterisation

Synthesis of nanomaterials - Top down and Bottom up approach - Physical methods (Laser Ablation, Evaporation, Sputtering and Gas condensation) - Chemical methods (Thermolysis, Sonochemical approach and Sol-gel synthesis) - Biosynthesis (Elementary idea only) - Structural characterisation of nanomaterials - X-ray diffraction, Scanning Tunneling Microscopy and Atomic force microscopy.

Unit III Carbon nanotubes

Carbon nanotubes - Carbon allotropes (Diamond, Graphite, Carbon nanotubes) - Types of Carbon nanotubes - Synthesis of carbon nanotubes - Electric arc Discharge method, Laser method, Chemical vapour deposition method (CVD) - Purification methods, properties and applications of Carbon nanotubes.

Fullerenes - Synthesis and purification - Properties and applications of Fullerenes.

Unit IV Nanocomposites

Definition - Ceramic-matrix nanocomposites - Nanocomposites by mechanical alloying - Metal-matrix nanocomposites - Polymeric nanomaterials - Synthesis methods - Solution intercalation - Melt intercalation - Emulsion polymerization - In-situ polymerization - Properties of polymer nanostructured materials - Material properties - Thermoplastic nanocomposites - Nylon 6 nanocomposites - Thermoset nanocomposites - Epoxy nanocomposites - Elastomer nanocomposites - TPO nanocomposites.

Unit V Applications of Nanotechnology

Chemistry and Environment - Water purification - Energy storage - Rechargeable batteries, Hydrogen storage - Information and Communication - Heavy industry - Consumer goods (food, textiles and cosmetics) - Nano medicine - Medical applications of molecular nanotechnology (Nanorobots, Cell repair machines, nanonephrology).

Books for Reference

1. Shanmugam S. *Nanotechnology*. Chennai: MJP Publishers. 2011.
2. Parthasarathy B.K. *Nanostructure and Nanomaterials*. Delhi: Isha Books. 2007.
3. Uday Kumar. *Concepts in Nanochemistry*. New Delhi: Anmol Publications Pvt. Ltd. 2013.
4. Bandyopadhyay A.K. *Nano Materials*. New Age International Publishers, 2nd Edition 2012.
5. Viswanathan B. *Nano Materials*. New Delhi: Narosa Publishing House. 2013.
6. Khanna O.P. *A Text Book of Nanochemistry*. New Delhi: Astha Publishers & Distributors. 2014.
7. Guozhong Cao. *Nanostructures & Nanomaterials: Synthesis, Properties & Applications*. Imperial College Press. 2004.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	recall a thorough knowledge of basic underline disciplines of nanoscience and nanotechnology	4	Re
CO 2	explain the preparation, characterization and properties of nanomaterials	6	Un
CO 3	analyze the types and properties of carbon nanotubes	1	An
CO 4	assimilate existing and new concepts, methodology and researches and apply them in their academic research environment	7	Ev
CO 5	synthesise the nanomaterials by physical, chemical and biological methods. characterise the synthesized nanomaterials by various techniques.	6, 5	Cr
CO 6	apply the nanomaterials in energy storage, food and in day-to-day life.	8	Cr

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	1	2	2	2	3	3	2.3	3	2	3	2	3	2	3	2	2.5
CO-2	2	3	1	3	2	3	3	1	2.3	2	2	2	3	2	2	3	2	2.4
CO-3	3	2	3	2	3	2	3	3	3	3	2	3	2	3	3	2	2	2.5
CO-4	2	1	3	2	2	3	2	2	2	2	3	2	2	2	3	2	3	2.4
CO-5	2	1	3	3	3	3	2	2	2.4	2	2	2	3	3	2	3	2	2.4
CO-6	3	2	1	2	2	3	2	2	2.5	3	2	3	3	3	3	3	2	3
Average	3	2	2	2	2	2.3	2.5	2		2.5	2	2.5	2.5	3	2.5	3	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – II			
Elective IIB. Energy and Computational Chemistry			
Course Code : 21PCHE22	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To protect and improve the environment as a valuable asset against hazardous chemicals and energy resources.
- To acquire a realistic training of computational tools in career.
- To encourage the preferential use of renewable instead non-renewable energy.

Unit I Energy resources

Introduction - classification of energy resources- Renewable: Solar energy(Solar cells, Solar batteries, Solar heat collector and Solar water heater), Wind energy(Wind mills and Wind farms), Ocean energy (Tidal energy, Ocean thermal energy and geothermal energy) and Bio mass energy (bio fuel and Hydrogen fuel).

Non Renewable – Batteries- Construction, Working and Applications: Primary battery - Leclanche Cell , Alkaline battery, Lithium ion; Secondary battery - NICAD, Lead Acid , Nickel metal hydride cell - Fuel cell - Use of alternate energy sources - Energy Conversion process: Anaerobic digestion and bio gas.

Unit II Fuels and Combustion

Introduction - Classification of fuels - Calorific values - Solid fuel - Classification of coal by rank - Metallurgical coke and its manufacture (Otto Hoffmans method) - Liquid fuel - Petroleum - Synthetic petrol and its manufacture (Bergius process) - Knocking - Octane number and Cetane number. Gaseous fuel - Liquid Petroleum gas, Natural gas, Compressed natural gas - Ignition temperature - Explosive range - Analysis of flue gas (Orsat process).

Unit III Recent developments in catalysis

Introduction - Reactions over Solid - Acid catalyst (Alkylation, Cracking & Hydrocracking, Isomerisation) - Catalyst in Fine Chemical synthesis (Halogenation, Amination, Condensation, selective oxidation reactions) -Photocatalyst - Semiconductor as photocatalyst - Water splitting by Semiconductor Particle - Photocatalysis in the removal of Organic and Inorganic pollutants - Photocatalytic reduction of Dinitrogen -Photocatalysis of Organic reactions.

Unit IV Computational Chemistry

Introduction - Character set in C++ - Tokens - Keywords, identifiers and constants, variables, operators (Input/Output) - Cascading - Selection of statements - IF, IFELSE,

SWITCH, WHILE, DO.....WHILE, FOR, BREAK, CONTINUE and GOTO - Functions - Arrays - Classes - Pointers - Inheritance.

C++ programming for the determination of electronegativity of an atom - Lattice energy using Born - Lande equation - Normality, Molarity and Molality of solutions - Solubility of sparingly soluble salts - Molecular weights of organic compounds - Calculation of delocalisation energy values for aromatic systems.

Unit V Drawing Tools for Chemistry

Chemdraw: Introduction– Features and functionalities - search mode - Exploring the user interface and tool bars - Importing and exporting from chemdraw - Construction of following structures using Chemdraw: Carbohydrates, Aminoacids, Lipids, Nucleic acids.

Chem sketch: Introduction - Screen parts and their functions -Features - Chems sketch versus Chemdraw - 2D, 3D optimisation - Application.

Text Books

1. Ramesh Kumari. *Computers and their Applications to Chemistry*. New Delhi: Narosa Publishing House. Second Edition 2005.
2. Jain P.C, Monika Jain. *Engineering Chemistry*. New Delhi, Dhanpat Rai Publishing company Pvt.Ltd. 15th Edition 2011.

Books for Reference

1. Raman K.V. *Computers in Chemistry*. New Delhi: Tata McGraw-Hill Publishing Company Limited. 8th Edition 2005.
2. Viswanathan B, Sivasanker S, Ramaswamy A.V. *Catalysis: Principles and Applications*. Delhi: Narosa Publishing House. 4th Edition 2011.
3. Harish Kumar Chopra, Anupama Parmar. *A textbook of Engineering Chemistry*. New Delhi: Narosa Publishing House. 1st Edition 2008.
4. Gopalan R, Venkappayya D, Sulochana Nagarajan. *Engineering Chemistry II*. New Delhi: Vikas Publications. 2011.
5. Srinivasa V, Uma Mageswari S.D, Meena M. *Engineering Chemistry*. Scitech Publications. 2002.
6. [https:// www.acdlabs.com/resources/freeware/chemsketch/](https://www.acdlabs.com/resources/freeware/chemsketch/)
7. Bethany Halford. *Reflections on ChemDraw*. 2014.

Course outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	organise C++ programming for the determination of some Chemical properties.	4	An
CO 2	calculate the delocalisation energy for aromatic system.	6	Ev
CO 3	distinguish between renewable and non- renewable energy resources.	1	An
CO 4	explain the construction, working and applications of primary and secondary batteries.	7	Ap
CO 5	demonstrate the Orsat process for flue gas analysis. identify a catalyst used in fine chemical synthesis.	6, 5	Cr
CO 6	acquire knowledge about paints, dyes and pigments and their manufacture.	8	Ap

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Av g	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5	PSO-6	PSO-7	PSO-8	Av g
CO-1	3	2	2	2	3	3	2	1	2.3	3	2	2	2	2	3	1	1	2
CO-2	3	3	2	3	3	3	2	1	2.5	3	2	1	3	3	2	2	1	2.3
CO-3	3	2	1	2	3	3	3	1	2.3	2	1	2	2	3	2	1	1	2
CO-4	2	2	3	2	3	3	3	2	2.5	3	2	1	3	3	3	2	1	2.3
CO-5	2	3	3	3	3	2	3	2	3	2	2	2	2	3	2	1	1	2
CO-6	3	2	2	3	3	3	1	1	2.3	3	2	1	3	3	3	2	2	2.4
Average	3	2.3	2	3	3	3	2.3	1.3		3	2	2	3	3	3	2	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – III			
Core VII	Inorganic Chemistry - III		
Course Code : 21PCHC31	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To sketch the various crystal structures of the compounds.
- To explain the various electronic theories involved in conducting and semiconducting materials.
- To discuss the synthesis, properties and structures of inorganic rings, chains, cages and clusters.

Unit I Solid state I

Types of close packing – hcp and ccp packing efficiency, radius ratios – Methods of Single crystal growth–Bridgeman, Czochralski, Verneuil, Epitaxial growth of thin layers – Chemical vapour transport – Hydrothermal method –Dislocations in solids – Point defects – Schottky and Frenkel defects – Line defects – Surface Defects – Dislocations – Grain Boundary and Stacking Fault – Crystal structures of common ionic compounds NaCl, Na₂O, Zinc blende, Wurtzite, Nickel arsenide, CsCl, Rutile, CdI₂, CdCl₂, and CaF₂, Perovskite, K₂NiF₄, Spinel.

Unit II Solid state II

Electronic structure of solids – Band theory, free electron theory – Insulators and semiconductors and its types. Electrical properties (Thomson effect, Peltier effect, Seebeck effect, Hall effect) – Dielectric, Ferroelectric, Piezoelectric and Pyroelectric materials and their relationship and applications. Optical and electronic properties of semiconductors – Photovoltaic effect, Hall effect – p-n junction and n-p-n junction and their applications as Rectifiers and transistors – Solid electrolytes, superconductors, High-temperature superconductors, BCS theory, Cooper electrons– Meissner effect and levitation.

Unit III Inorganic chains, rings and cages

Chains – Chain catenation – Heterocatenation – Isopoly and heteropoly anions – Silicate minerals –Classification – Aluminosilicates – Sulphur nitrides – Intercalation compounds.

Rings – Borazines, Phosphazenes, Phosphazene polymers– Homocyclic and heterocyclic inorganic ring systems.

Cages – Synthesis, properties and structure of boranes [styx notation], heteroboranes, metalloboranes and carboranes, metallocarboranes, silicones – Wade's rule.

Unit IV Inorganic clusters

Introduction to clusters – Carbonyl clusters, anionic and hydrido clusters, carbide clusters, sulphur metal clusters – Structure and Bonding of Metal clusters: Dinuclear: Cu(II) carboxylate, Chromium(II) acetate and $[M_2Cl_8]^{4-}$ (M = Mo and Re) – Trinuclear: $[M_3(CO)_{12}]$ (M = Fe, Ru, Os) – Tetranuclear: $[M_4(CO)_{12}]$ (M = Co, Rh, Ir) – Hexanuclear clusters: $[Nb_6Cl_{12}]^{2+}$, $[Os_6(CO)_{18}]^{2-}$ and $[Mo_6Cl_8]Cl_4$ – Capping rule – Clusters rotation with CO shells – Chevrel phases – Isolobal relationships between main group and transition metal fragments – Zintl ions.

Unit V Spectroscopy II

Electronic spectroscopy – Microstates, Term symbols, selection rules – Orgel and Tanabe-Sugano diagrams – Charge transfer spectra – Electronic spectra for 1st row transition metal complexes – Calculation of Dq, B for octahedral d^2 and d^8 systems ($[V(H_2O)_6]^{3+}$, Ni(II) complexes) – Nephelauxetic ratio – Electronic spectra of lanthanide and actinide.

Photo electron spectroscopy – UVPES - Principle, spin-orbit coupling – XPES – Principle, chemical shift in XPES – Koopman's theorem – Applications of XPES and UVPES to inorganic spectra – Auger electron spectroscopy.

Text Books

1. West A.R. *Solid State Chemistry and its Application*. Asia: John Wiley & Sons. 2007.
2. James E. Huheey, Ellen A. Keiter, Richard L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Harper Collins College Publishers. 4th Edition 2009.
3. Gopalan R. *Textbook of Inorganic chemistry*. Universities Press(India) private limited. 2012.
4. Skoog D.A, West D.M, Holler F.J, Grouch S.R. *Fundamentals of Analytical Chemistry*. Thomson Asia Pvt.Ltd. Eighth Edition, Third Reprint 2005.
- 5.

Books for Reference

1. Wells A.F. *Structural Inorganic Chemistry*. Oxford University Press. 2012.
2. Azaroff L.V. *Introduction to solids*. Tata McGraw Hill publishing Ltd. 2000.
3. Kittel C. *Introduction to solid state physics*. Wiley Eastern Ltd. 7th Edition 2006.
4. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic chemistry*. ELBS, Oxford University Press. 1994.
5. Gary L. Miessler, Donald A. Tarr. *Inorganic Chemistry*. Pearson Publications. 5th Edition 2014.
6. Albert Cotton F, Geoffrey Wilkinson, Carlos A. Manic, Manfred Bochman. *Advanced Inorganic Chemistry*. Wiley Interscience Publication. 6th edition 1999.
7. Lee J.D. *Concise Inorganic Chemistry*. Blackwell Science Ltd. 5th Edition, Reprint 2003.
8. Drago R.S. *Physical Methods in Inorganic Chemistry*. Saunders College Publishing. 2nd Edition 1992.
9. Ebsworth David E.A.V, Rankin Stephen Credock W.H. *Structural Methods in Inorganic Chemistry*. ELBS. 1988.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	Predict the dislocations in the solids	4	Ev
CO 2	compare various techniques involved in single crystal growth.	4, 6	An
CO 3	calculate STYX notation for boranes and carboranes.	1	Ap
CO 4	coin the Isolobal relationships between main group and transition metal fragments.	1	Cr
CO 5	calculate the Microstates and Term symbols for Transition metal complex.	4	Ev
CO 6	discuss the applications of XPES and UVPES to inorganic spectra.	5, 7	An

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	1	2	3	1	2	3	2	3	3	2	3	3	2	2	2	3
CO-2	3	3	2	3	3	2	2	1	2.3	3	3	2	3	3	3	2	2	3
CO-3	3	2	1	2	3	1	1	3	2	3	2	2	3	3	3	2	2	3
CO-4	3	3	2	3	3	2	2	1	2.3	3	3	2	3	3	3	3	3	3
CO-5	3	2	2	3	3	1	1	3	2.3	3	2	2	3	3	3	2	2	3
CO-6	3	3	2	3	3	2	2	3	2.5	3	3	2	3	3	3	3	3	3
Average	3	3	2	3	3	1.5	2	2.3		3	3	2	3	3	3	2.3	2.3	
PO Mean									2.6	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

SEMESTER – III			
Core VIII	Organic Chemistry - III		
Course Code : 21PCHC32	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To study pericyclic reactions and their types with mechanism.
- To understand the stereochemistry of reactants, intermediates and products.
- To study the multi-step synthesis of various natural products.
- To learn the importance of steroids and terpenoids in natural products.

Unit I Aromatic Electrophilic and Nucleophilic Substitution Reaction

Aromatic Electrophilic substitution – Arenium ion mechanism – Selected reactions and Reactivity – Nitration – Nitrosation– Sulphonation – Halogenation – Friedel Craft’s alkylations and arylations – Vilsmeier Haack reaction – Jacobsen reaction – Houben Hoesch reaction.

Aromatic Nucleophilic Substitution – S_NAr mechanism – S_N1 (Aromatic) mechanism with evidences – Benzyne mechanism – Effect of substrate structure, leaving group, attacking nucleophile and solvent – Selected reactions – Von Richter and Smiles rearrangements.

Problems including the basic concepts of Aromatic Electrophilic and Nucleophilic Substitution Reaction.

Unit II Conformational Analysis

Conformation and reactivity of cyclic and acyclic compounds – Conformations of cyclohexanes– Ring inversion, monosubstituted cyclohexanes– Transition States and Intermediates, Conformational free energy, Determination of conformational energy, disubstituted cyclohexanes (1,2), (1,3) and (1,4) – Conformation of polysubstituted cyclohexanes – Trimethylcyclohexanes, Tetramethylcyclohexanes and Menthols – Conformational analysis of fused bicyclic systems– Decalin and perhydrophenanthrene– Curtin-Hammett principle.

Unit III Steroids and Terpenoids

Steroids: Occurrence, nomenclature, basic skeleton, isolation, structure determination and synthesis of Bile acids, Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Non-Steroid Hormones.

Terpenoids: Classification, nomenclature, occurrence, isolation – General methods of structure determination – Isoprene rule – Structure determination, stereochemistry and synthesis of the following representative molecules: Zingiberene, Camphor, Apitic Acid, α - pinene and squalene.

Unit IV Reagents in Organic Reactions

Synthetic applications of the following – Crown Ethers, Diazomethane, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone(DDQ), N,N-Dicyclohexylcarbodiimide (DCC), Di-isobutyl aluminium hydride (DIBAL), 1,3-dithiane, Fenton's reagent, Gilman, Jones reagent, Lithium diisopropylamide(LDA), Osmium tetroxide, Pyridinium chlorochromate (PCC), Phase Transfer Catalysts (PTC), Wilkinson's catalyst, Ziegler-Natta catalyst.

Unit V Pericyclic Reactions

Atomic and molecular orbitals – Woodward-Hoffmann rules – The Mobius and Huckel concept, FMO and correlation diagrams–Electrocyclic reactions – con and dis rotatory motions for $4n$ and $4n+2$ system (butadiene and 1,3,5-hexatriene) – Stereochemical course of electrocyclic reaction in terms of conservation of orbital symmetry –Cycloaddition – Suprafacial and antarafacial additions, [2+2] and [2+4] reactions (ethylene and butadiene) – Sigmatropic rearrangements with examples–C- and H-migration – [1,3], [3,3] & [1,5] shift – Claisen and Cope rearrangements.

Text Books

1. Mukherjee Kapoor Singh. *Mechanism of Organic reactions*. Kolkata: Books and Allied Ltd, 2021.
2. Kalsi P.S. *Organic Reaction & Mechanism*. New Delhi: New Age International Publishers, 4th Edition 2020.
3. Ahluwalia V.K, Parshar R.K. *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House. Fourth Edition 2019.
4. Somorendra Nath Sanyal. *Reactions, Rearrangements and Reagents*. Noida: Bharati Bhawan Publishers & Distributors. 2021.
5. Raj K Bansal. *Organic reaction mechanism*. New Delhi: New Age International Publishers. 4th Edition 2012.
6. Nasipuri D. *Stereochemistry of Carbon Compounds*. New Delhi: New Age International Publishers. 3rd Edition, 2018.

Books for Reference

1. Michael B Smith. *March's Advanced Organic Chemistry: Reactions, Mechanism and Structure*, New York: John-Wiley and Sons, 8th Edition, 2019.
2. Jonathan Clayden. Nick Greeves, Stuart Warren, Wothers. *Organic Chemistry*. New York: Oxford University Press. 2nd Edition 2021.
3. Ernest Eliel. *Stereochemistry of Carbon Compounds*. New Delhi: Tata-McGraw Hill Publishing Company. 2001.
4. Kalsi P.S. *Stereochemistry: Conformation and Mechanism*. New Delhi: New Age International Publishers. 8th Edition 2015.
5. Norman R.O.C, Coxon J.M. *Principles of Organic synthesis*. Switzerland: Springer and Business Media, LLC. Third edition 1994.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	familiarize the various types and Compare neighbouring group participation and Ambident nucleophiles of aromatic substitution reactions	2	Re
CO 2	discuss the Conformational analysis of cyclic molecules and the factors governing the reactivity of axial and equatorial substituents in cyclohexanes.	3	An
CO 3	study the synthesis and Elucidation of structure of steroids and terpenoids	4	Un, An
CO 4	learn the conversion of cholesterol to progesterone, estrogen and testosterone	5	Re
CO 5	acquire knowledge about the reagents specificity	3	Un
CO 6	to learn the concept of Cyclo addition, Electrocyclic and sigmatropic reaction mechanism	6	Cr

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Avg	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PSO-7	PSO-8	Avg
CO-1	3	2	2	3	3	1	2	2	2.3	3	3	2	3	3	3	2	2	2.6
CO-2	3	2	2	3	3	3	2	1	2.3	3	3	2	3	3	3	2	2	2.6
CO-3	3	3	2	3	3	3	2	3	2.3	3	3	2	3	3	3	3	3	2.9
CO-4	3	3	2	3	3	1	2	1	2.3	3	3	2	3	3	3	3	3	2.9
CO-5	3	2	2	3	3	3	2	1	2.3	3	3	2	3	3	3	2	2	2.6
CO-6	3	3	2	3	3	1	2	2	2.3	3	3	2	3	3	3	3	3	2.9
Average	3	3	2	3	3	2	2	1.6		3	3	2	3	3	3	2.5	2.5	
PO Mean									2.5	PSO Mean								2.8
Strength of PO Correlation				Strong					Strength of PSO Correlation						Strong			

Semester – III			
Core IX Physical Chemistry – III			
Course Code : 21PCHC33	Hrs / Week : 5	Hrs / Sem : 75	Credits : 4

Objectives:

- To achieve base knowledge about the concepts of physical chemistry.
- To solve Debye-Huckel theories for electrolytes.
- To demonstrate the Chemical information from spectroscopy.

Unit I Electrochemistry I

Debye-Huckel theory of inter-ionic attraction–Debye-Huckel Onsager equation and its validity– Debye-Falkenhagen and Wien effects – Activity coefficients of electrolytes – Debye-Huckel limiting law – Debye-Huckel Bronsted equation – Quantitative and qualitative verification of Debye-Huckel limiting law – Electrode-electrolyte interface – Structure of electrified interface: Helmholtz-Perrin model and Gouy-Chapman Diffuse charge model of the double layer – Electrocapillary phenomenon – Lipmann equation.

Unit II Electrochemistry II

Kinetics of electrode reaction – Polarization and over potential – Butler-Volmer equation for one step and multistep electron transfer reactions – Tafel equation – Significance of I_c and transfer coefficient – Diffusion over potential - Polarizable and non- polarizable electrodes – Ilkovic equation – Derivation of Ilkovic equation from Fick's laws of diffusion – Corrosion – Pourbaix diagrams – Evans' diagram – Bioelectrochemistry – Electrochemical mechanisms of nervous system.

Unit III Irreversible Thermodynamic Processes

Phenomenological laws and Onsager reciprocal relations – Entropy production due to heat flow – Entropy production in chemical reactions – Entropy production and entropy flow in open system – Transformation properties of fluxes and forces – Principle of microscopic reversibility and Onsager reciprocal relations – Verification of Onsager relations – Electro kinetic effect – Thermomolecular pressure difference and Thermomechanical effect. Applications of irreversible thermodynamics to biological and non-linear thermodynamics of Irreversible processes.

Unit IV Nuclear Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance Spectroscopy – Theory of PMR spectra – Chemical shift – Factors affecting chemical shift – Solvents used in NMR – Solvent shift – Hydrogen bonding – Relaxation times and spin-spin interactions - Theory of Spin-spin splitting – Magnitude of

coupling – Coupling constant, J – Factors influencing coupling constant –Calculation of coupling constants– First-order spectra of complex systems – NMR of simple AX and AMX type molecules – Double resonance technique.

Unit V Electronic Spectroscopy and Photoelectron spectroscopy

Electronic spectroscopy – Electronic spectrum of diatomic molecules – Born-Oppenheimer approximation – Sequences and progressions – The Frank-Condon principle – Dissociation energy and dissociation products – The forttrat diagram – Predissociation.

Photoelectron spectroscopy – Principle – XPES, UVPES and Chemical information from photoelectron spectroscopy – Applications of ESCA.

Text books

1. Glasstone S. *An Introduction to Electrochemistry*. New Delhi:East West Press Pvt. Ltd. 1956.
2. Puri, Sharma, Pathania. *Principle of Physical Chemistry*. Vishal Publications. 48th Edition 2020.
3. Gurdeep R. Chatwal, Sham K. Anand. *Spectroscopy*. Himalaya Publishing House. 2009.

Books for Reference

1. Antorpov L. *Theoretical Electrochemistry*. Moscow:Mir Publishers. 2nd Edition 1977.
2. Bockris J O'M, Reddy A K N. *Modern Electrochemistry*. New York:PlenumPress.Vol. 1 & 2, Second Edition 1998.
3. McQuirrie D.A, Simon J.D. *Physical Chemistry. A Molecular Approach*. New Delhi: Viva Books Pvt. Ltd.1999.
4. Rajaram J, Kuriakose J C. *Kinetics and Mechanism of Electrochemical Transformations*. New Delhi: Ch-13, Macmillan India Ltd. 1993.
5. Banwell C.N. *Fundamentals of Molecular Spectroscopy*. Noida: McGraw Hill Education.4th Edition1994.
6. Barrow G M. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill. 1964.
7. Drago R.S. *Physical Methods in Inorganic Chemistry*. New Delhi: East West Press Ltd. 1971.
8. Straughan B.P, Walker S. *Spectroscopy*. New York: London Chapman and Hall, A Halstet Press Book, John Wiley & Sons Ins. Volume 1, 2 & 3.1975.

Course Outcomes:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO1	Outline the behavior of electrolytes in solutions.	4	An
CO2	Predict the structure of the electrode surface and the applications of electrode process.	2	Cr
CO 3	investigate the corrosion and polarization studies.	1	Ev
CO 4	Justify electrochemical mechanisms of biological systems.	4	Ev
CO 5	Categorise the principle and applications of NMR and EPR spectroscopy.	4	An
CO 6	judge the structure of molecules by applying various spectroscopic techniques.	2	Ev

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	1	2	3	2	2	2	2	3	3	2	3	3	2	2	2	2.5
CO-2	3	3	2	3	3	1	2	1	2.3	3	3	2	3	3	3	2	2	3
CO-3	3	2	2	3	3	2	3	2	2.4	3	2	2	3	3	3	2	2	2.5
CO-4	3	3	2	3	3	1	2	1	2.3	3	3	2	3	3	3	3	3	3
CO-5	3	2	2	3	3	2	1	3	2.3	3	2	2	3	3	3	2	2	2.5
CO-6	3	3	2	3	3	3	2	1	2.3	3	3	2	3	3	3	3	3	3
Average	3	3	2	3	3	2	2	2		3	3	2	3	3	3	2.3	2.3	
PO Mean									2.5	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – III			
Elective III	A. Research Methodology		
Course Code : 21PCHE31	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To provide resources to the students to stimulate basic research interest and other creative endeavours that promote entrepreneurial culture.
- To explain about various thermal and electrochemical instrumentation techniques.
- To learn about all the hyphenated techniques used for the separation of compounds.
- To interpret the results of analysis with accuracy.

Unit I Research methodology

Introduction of research–Selection of a research topic – Surveying the literature– Sources– primary source and secondary source – Identification of research problem – Actual investigation and analysis of experimental results – Reporting the results in the form of communication, paper – Dissertation and thesis writing– Project proposals to funding agency – Impact factor, citations and h-index –Publication and Indexing: Scopus, Web of Science and Google scholar – Concepts of IPR and Plagiarism.

Unit II Thermo and electro analytical methods

Thermoanalytical Methods –Principle, instrumentation and applications of Thermogravimetry (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC).

Electroanalytical Techniques –Coulometry– Principle, Instrumentation and Applications. Voltammetry– Types (Stripping voltammetry, Cyclic voltammetry, Amperometry) – Principle, instrumentation and applications

Unit III Spectroscopic & Surface techniques

Principle, instrumentation and applications of Atomic Absorption Spectroscopy, Atomic Fluorescence Spectroscopy and Atomic Emission Spectroscopy.

Principle, instrumentation and applications of Energy dispersive spectroscopy (EDAX), Transmission electron microscopy (TEM), Scanning electron microscope (SEM) and Scanning Probe Microscopes.

Unit IV Data Analysis

Errors in chemical analysis – Classification of errors –Methods for determination of accuracy– Improving accuracy of analysis – Comparison between precision and accuracy –

Significant figures – Mean, median, mode and standard deviation – Confidence interval – Propagation of measurement uncertainties – Comparison of results – “t” test, “F” test and “chi” square test – Rejection of results – Presentation of data – Correlation analysis and correlation coefficient – Linear regression – Related Problems.

Unit V Research and Teaching Methodology

Teaching – Objectives of Teaching - Phases of Teaching – Teaching methods: Lecture Method, Discussion Method, Discovery Learning, Inquiry, Problem Solving Method, Project method, Seminar – Integrating ICT in Teaching: Individualized Instruction, Ways for Effective Presentation with Power Point – Documentation – Evaluation: Formative, Summative & Continuous and comprehensive Evaluation – Later Adolescent – Psychology: Meaning, Physical, Cognitive, Emotional, Social and Moral Development – Teaching Later Adolescents.

Text Books

1. Gurdeep R. Chatwal, Sham K. Anand. *Instrumental Methods of Chemical Analysis*. Mumbai: Himalaya Publishing House. 5th edition 2014.
2. Skoog D.A, West D.M.F, Holler J, Crouch. S.R. *Fundamentals of Analytical Chemistry*. Thomson Asia Pvt. Ltd. Eighth Edition, Third Reprint 2005.
3. Banwell C.N, *Fundamentals of molecular spectroscopy*. Noida: McGraw Hill Education, 4th Edition 1994.

Books for Reference

1. Anderson J, Durston B.H, Poole. M. *Thesis and Assignment Writing*. New Delhi: Wiley Eastern. 1986.
2. Sharma B.K. *Instrumental Methods of Chemical Analysis*. Goel Publishing House, 23rd Edition 2004.
3. Willard H, Merrit Jr. L, Dean. A. *Instrumental methods of analysis*. CBS Publishers and Distributors. 2004.
4. Rajammal P. Devadas. *A Handbook of Methodology of Research*. Chennai: S.R.K. Vidyalyaya Press. 1976.
5. Dominoswki R.L. *Research Methods*. Prentice Hall. 1981.
6. Ebel H.F, Bliefert C, Russey W.E. *The Art of Scientific Writing*. Weinheim: VCH. 1988.
7. Joseph A, *Methodology for Research*. Bangalore: Theological Publications. 1986.
8. Douglas A. Skoog, James Holler F, Stanley R. Crouch. *Instrumental Analysis*. New Delhi, Cengage Learning India Private Limited. Eighth Indian Reprint 2011.
9. Asim K. Das, Mahua Das. *Fundamental Concepts of Inorganic Chemistry*. New Delhi: CBS Publishers & Distributors Pvt. Ltd. Volume 7, First Edition Reprint 2019.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	select the research topic and able to survey the literature. improve the accuracy of data in chemical analysis.	4, 3	Ev
CO 2	submit the project proposals to the funding agency.	8	Ap
CO 3	explain about the principle, instrumentation and applications of TGA, DTA and DSC.	5,6	Un
CO 4	compare principle, instrumentation and applications of potentiometry, coulometry and voltammetry.	5	An
CO 5	describe different types of Atomic spectroscopy.	1,5	Un
CO 6	Interpret data using TEM, SEM, XRD and EDAX techniques.	5,7	Ev

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Av g	PS O-1	PS O-2	PS O-3	PS O-4	PS O-5	PS O-6	PS O-7	PS O-8	Av g
CO-1	3	3	2	3	3	2	3	2	2.6	3	3	2	3	3	2	3	3	2.6
CO-2	3	3	2	3	3	2	3	2	2.6	3	3	2	3	2	2	3	3	2.6
CO-3	3	2	2	2	3	1	2	1	2	3	2	2	3	3	3	2	2	2.5
CO-4	3	2	2	2	3	1	2	1	2	3	2	2	3	3	3	2	2	2.5
CO-5	3	2	2	2	3	2	2	1	2.3	3	2	2	3	3	3	2	2	2.5
CO-6	3	3	2	3	3	1	3	2	2.5	3	3	2	3	3	3	3	3	2.9
Average	3	3	2	3	3	2	3	2		3	2.5	2	3	3	3	2.5	2.5	
PO Mean									2.6	PSO Mean								2.7
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester–III			
Elective:III B. Chemical Instrumentation			
Course Code:21PCHE32	Hrs/Week:4	Hrs/Sem:60	Credits:4

Objectives:

- To impart the students with basic principles and concepts in Instrumental techniques.
- To understand the nature and Choice of methods of measurements.
- To learn the limits of detection and amplification.
- To demonstrate the concepts of Operational amplifiers.

Unit I Measurement and Instrumentation

Introduction - The nature of a measurement - Choice of a method of measurement - Control of variables - Basic design patterns - General properties of modules - Propagation of uncertainty - Single channel design - Limit of detection and amplification - Automatic operation and computer control.

Unit II Operational amplifiers

The operational amplifiers – Limitations on amplifier performance – Mathematical operations - Differentiation - Integration - Measurement of current and voltage - Precise control of current and voltage.

Unit III Signal-to-Noise Optimisation

Sensitivity and detection limits – Noise – Minimising Noise in a system – Signal averaging - Modulation: Chopping - Demodulation: Phase sensitive detection - Other methods of Optimising Signal-to-Noise ratio.

Unit IV Digital Electronics

Binary logic concepts - Logic gates – Multivibrators - Counters - Wave shaping – Analog to digital convertors – Instruments and Digital computers.

Unit V Instrumentation for Optical Absorption Spectrometry

Visual Photometers - Filter Photometers – Spectrophotometer – Double beam Spectrophotometer - Recording Spectrophotometers - Optimal value of adjustable parameters – Multiple internal reflection assembly – Rapid scanning spectrometer – Non-

dispersive Photometers – Photo metric titration equipment – Fourier transform Spectrometers.

Textbooks

1. Strobel H.A. *Chemical instrumentation – A systematic approach to Instrumentation Analysis*. Phillipines: Addison-Wesley Publishing Company Inc. 2nd Edition 1973.

Books for Reference

1. Jeffery G.H, Bassett J, Mendham J, Denney R.C. *Vogel's Textbook of Qualitative Chemical Analysis*. Essex: Longman Scientific and technical. 5th Edition 1989.
2. Skoog D.A, Holler F.J, Crouch S.R. *Principles of Instrumental Analysis*. Belmont CA: Thompson Brooks/Cole. 6th Edition 2007.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO1	Demonstrate automatic operation and computer control	1,5	Ap
CO2	Precise control of current and voltage.	6,8	Ap
CO3	Differentiate modulation and demodulation	5	An
CO4	Point out limitation on amplifier performance	1	Cr
CO5	predict binary logic concepts, logic gates and multi-vibrators	7	Un
CO6	Distinguish visual, filter and spectrophotometers and interpret the optimal value of adjustable parameters	7,8	Ap

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	2	3	3	2	3	2	2.5	3	2	2	3	3	2	3	2	2.5
CO-2	3	2	2	2	3	1	2	1	2	3	2	2	2	3	3	2	2	2.4
CO-3	3	2	2	2	3	1	2	1	2	3	2	2	2	3	2	2	2	2.3
CO-4	3	2	2	2	3	1	2	1	2	3	2	2	2	3	2	2	2	2.3
CO-5	3	3	2	3	3	2	3	2	3	3	3	2	3	3	3	3	3	3
CO-6	3	3	2	3	3	2	3	2	3	3	3	2	3	3	3	3	3	3
Average	3	2.3	2	3	3	2	3	1.5		3	2.3	2	3	3	3	2.5	2.3	
PO Mean									2.5	PSO Mean								2.6
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester III	
Self-Study Course Course on Competitive Exams	
Code: 21PCHSS31	Credits: 2

Objectives:

- To provide a platform to the students for building the fundamentals of basic mathematics for competitive examinations preparation strategy.
- Establish a framework to help students acquire knowledge and expertise necessary to secure employment opportunities in the government sector.

UNIT I

Number System (Including divisibility) – HCF and LCM (Including Factors, Multiples and Prime Factorization).

(Chapter: 1 & 2, pages 1 – 46)

UNIT II

Fractions and Decimals – Square and Square roots, Cube and Cube Roots, Indices and Surds.

(Chapter: 3 & 4, pages 47 – 94)

UNIT III

Time, Work and Wages (Including Pipes & Cistern) – Time, Speed and Distance (Including Trains, Boats and Stream, Circular Motion, Races and Games.

(Chapter: 15 & 16, pages 317 - 374)

UNIT IV

Permutations & combinations and Probability.

(Chapter: 18, pages 391 - 416)

UNIT V

Set Theory (Including Venn Diagram) – Data Analysis and Data Interpretation (Including Caselet, Table, Line Graph, Bar Graph, Mixed Bar).

(Chapter: 24 & 27, pages 559 – 570, 615 – 648)

Text Books:

1. Er. Deepak Agarwal, Gupta D.P. *Rapid Quantitative Aptitude with Shortcuts and Tricks for Competitive Exam*. Disha Publication.

Books for Reference

1. Dr. Aggarwal R.S. *Quantitative Aptitude for Competitive Examinations* S. Chand Publication.

2. Rajesh Verma, *Fast Track Objective Arithmetic*. Arihant Publication.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	solve real life problems requiring interpretation and comparison of various representations of ratios	2	Ap
CO 2	distinguish between proportional and non-proportional situations and when appropriate apply proportional reasoning	1, 2	An
CO 3	solve problems applying probabilistic reasoning to make decisions	2	Ap
CO 4	evaluate claims based on empirical, theoretical and subjective probabilities	1, 4	Re
CO 5	solve problems using high speed mental calculations	7	Ap
CO 6	understand the basic concepts of logical reasoning skills	1, 2	Un

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
CO-2	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
CO-3	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
CO-4	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
CO-5	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
CO-6	3	2	2	3	3	2	3	2	3	3	2	2	3	3	2	3	2	2.5
Average	3	2	2	3	3	2	3	2		3	2	2	3	3	2	3	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – IV			
Core X	Inorganic Chemistry - IV		
Course Code : 21PCHC41	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To explain the various photophysical and photochemical processes involved in inorganic compounds.
- To understand the chemistry involved in energy sources of life and functions of enzymes.
- To discuss the theory of various types of nuclear reactions.
- To study in detail NMR, NQR and ESR spectroscopies.

Unit I Bioinorganic chemistry I

Energy sources of life – Non-photosynthetic process – Metalloporphyrins – Cytochromes A,B,C – Dioxygen binding – Interaction between Heme and Dioxygen , Binding of Dioxygen – Myoglobin – Structure and Functions of Hemoglobin – Electron transfer : Rubidoxins and Ferridoxins – Respiration: Blue copper proteins – Photosynthesis: PS-I, PS-II– Photosynthesis with mechanism of Chlorophyll.

Unit II Bioinorganic chemistry II

Enzymes – Zinc enzymes: Carboxypeptidase A, Carbonic anhydrase, Inhibition and poisoning of enzymes illustrated by Xanthane oxidase, aldehyde oxidase, Copper enzyme: Superoxide dismutase, Toxicity of Metals and the role of Metallothionines – Nitrogen fixation – *Invitro* and *Invivo* conditions. Iron storage and transport proteins: Transferrin, Hemosiderin, Ferritin and Siderophores.

Unit III Nuclear Chemistry

Nuclear Reactions – Types, Q value, Cross Section of reactions – Direct nuclear reaction – transmutation reactions: Stripping and pickup – high energy reactions: neutron evaporation and spallation –Theory of nuclear fission– Nuclear Fusion and stellar energy – The Pinch effect – Generation of electricity from nuclear fusion – Nuclear waste disposal – Artificial Disintegration and its methods – Devices used for radioactive measurements i) Countering Techniques such as G.M Ionization and Proportional counters ii) Tracer techniques (Neutron activation analysis).

Unit IV Reaction mechanism in Coordination Complexes

Labile and inert complexes – Thermodynamic and kinetic stability of complexes – mechanism of substitution reactions of metal complexes – D, Id, A and Ia mechanisms – Substitution reactions in octahedral and square planar complexes, acid-catalyzed reactions,

base-catalyzed reactions – Trans effect and its influence, water exchange, anation, isomerization reactions. Redox reactions: Inner and outer sphere electron transfer mechanism – Template reactions.

Unit V Spectroscopy III

NMR –Principle, ^{31}P , ^{19}F and ^{15}N NMR - Applications of spin-spin coupling to structure determination: P_4S_3 , BrF_5 , Pentacyanohydridorhodate(III) ion, SF_4 , TiF_4 , H_3PO_3 , H_3PO_2 – Comparison between ^1H and ^{15}N - NMR of $^{15}\text{NH}_3$ – Comparison between ^1H , ^{31}P and ^{19}F - NMR of H_2PF_3 and HPF_2 –Double resonance – NMR of fluxional molecules such as PF_5 , $(\eta^1\text{-C}_5\text{H}_5)_2(\eta^5\text{-C}_5\text{H}_5)_2\text{Ti}$, $(\eta^5\text{-C}_5\text{H}_5)_2\text{Fe}_2(\text{CO})_4$ and PCl_2F_3 .

EPR – Principle–Fine structure– Interaction between nuclear spin and electron spin (hyperfine coupling) – Hyperfine splitting of systems with $I=1/2$, 1 & $3/2$ – Zero field splitting &Kramer's degeneracy – EPR spectrum deduction for $[\text{Co}(\text{H}_2\text{O})^{2+}]$, $[\text{Cr}(\text{H}_2\text{O})^{2+}]$, $[(\text{NH}_3)_5\text{Co-O-O-Co}(\text{CN})_5]^{5+}$, $[(\text{NH}_3)_5\text{Co-O-O-Co}(\text{NH}_3)_5]^{5+}$ – Covalency of M-L bonding in bis(salicylalimine)copper(II) complex by EPR study – Jahn-Teller distortion in Cu(II) complexes.

Text Books

1. James E. Huheey, Ellen A. Keiter, Richard L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Harper Collins College Publishers. 4th Edition 1993.
2. Rohatgi Mukherjee K.K. *Fundamentals of Photochemistry*. New age international limited. 2006.
3. Arnikar H.J. *Essentials of Nuclear Chemistry*. Wiley Eastern Ltd. 4th Edition 2000.

Books for Reference

1. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic chemistry*. ELBS, Oxford University Press. 1994.
2. Gary L. Miessler, Donald A. Tarr. *Inorganic chemistry*. Pearson Publications, Third edition 2014.
3. Catherine Housecroft, Alan G. Sharpe. *Inorganic Chemistry*. Prentice Hall. 4th Edition 2012.
4. Albert Cotton F, Geoffrey Wilkinson, Carlos. A. Manic, Manfred Bochman. *Advanced Inorganic Chemistry*. Wiley Interscience Publication. 6th edition 1999.
5. Purcell K.F, Kotz J.C. *Inorganic Chemistry*. WB Saunders Company. 1977.
6. Robert H. Crabtree. *The Organometallic Chemistry of the Transition Metals*. John Wiley & Sons Inc. Publication. 6th Edition 2014.

7. Lee J.D. *Concise Inorganic Chemistry*. Blackwell Science Ltd. 5th Edition, Reprint 2003.
8. Samuel Glasstone. *Source Book of Atomic Energy*. East West Pvt. Ltd. 1969.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	demonstrate about the energy sources of life using photosynthetic and non-photosynthetic processes	1,4	Ap
CO 2	illustrate the inhibition and poisoning of xanthane oxidase and aldehyde oxidase.	1,4	Ap
CO 3	describe about tracer technique and counter technique in nuclear chemistry.	5,7	An
CO 4	sketch the electron transfer mechanism for inner and outer sphere complexes.	3,4	Ap
CO 5	catagorise the principle and applications of NMR, NQR and EPR spectroscopy.	5,8	An
CO 6	demonstrate the structural information from NMR and EPR spectra.	5,8	Ap

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PS O- 1	PS O- 2	PS O- 3	PS O- 4	PS O- 5	PS O- 6	PS O- 7	PS O- 8	Av g
CO-1	3	2	1	2	2	2	3	1	2	3	2	2	2	2	2	2	3	2.3
CO-2	3	3	1	2	3	2	3	2	2.4	3	2	2	2	3	2	3	2	2.4
CO-3	3	3	2	2	3	2	3	3	3	3	2	2	2	3	2	3	2	2.4
CO-4	3	3	1	3	3	2	3	2	2.5	3	2	1	2	3	2	3	3	2.4
CO-5	3	2	1	3	3	2	3	1	2.3	3	2	3	2	3	3	3	2	3
CO-6	3	2	2	3	3	2	3	3	3	3	2	2	2	3	3	3	3	3
Average	3	2.5	1	2.5	3	2	3	2		3	2	2	2	3	2.3	3	2.5	
PO Mean									2.5	PSO Mean								2.6
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

SEMESTER – IV			
Core XI Organic Chemistry - IV			
Course Code : 21PCHC42	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To understand the stereochemistry of reactants, intermediates and products.
- To understand the stereo-chemical aspects and its applications in organic synthesis.
- To learn the advanced spectroscopic techniques for analysis of organic compound.

Unit I Addition and Elimination Reaction

Addition reaction – Addition to C=C bonds – Electrophilic, nucleophilic and free-radical additions - Additions to conjugated systems – Carbene addition to double bonds – Hydration of olefins. Reactions – Birch reduction – Hydroboration – Michael reaction – Diels-Alder reactions - Mannich reaction – Meerwein-Ponndorf reduction – Reformatsky, Claisen, Stobbe, Darsen, Wittig, Thorpe and Benzoin condensations.

Elimination reactions – E1, E2 and E1CB mechanisms – Orientations – Hofmann and Saytzeff rules – Mechanism and orientation in pyrolytic elimination – Chugaev reaction – Cope elimination – Dehydration of alcohols – Dehydrohalogenation – Elimination versus substitution.

Unit II Retrosynthetic Analysis

Synthon – Synthetic equivalent – Functional group inter conversions – Use of protecting groups for alcohols, amines, acids, carbonyl compounds – Use of activating and blocking groups – Robinson annulation reaction – Carbon skeletal complexity – Role of key intermediates in organic synthesis – Retrosynthetic analysis of the following compounds – Twistane, cis-Jasmone, Baclofen, Brufen, Trihexyl phenidyl, Bisabolene, α -onocerin, isonootkatone, cascarillic acid, camphor.

Unit III Heterocycles and Nucleic acids

Heterocycles: Nomenclature, reactivity, aromaticity, spectral properties – Synthesis and electrophilic and nucleophilic substitution reactions of Indole, Oxazole, Thiazole, Pyrimidine, Pyrazine – Fused ring heterocycles.

Nucleic acids: Nucleic acids and nucleotides – Structure of nucleic acids – Base pairing in DNA – The Watson-Crick model – Nucleic acid and heredity – Replication of DNA – Structure and synthesis of RNA – Transcription – RNA and protein biosynthesis – Translation – DNA sequencing – DNA synthesis.

Unit IV NMR and C¹³ Spectroscopy

PMR spectroscopy – Basic principle – Number of signals – Chemical shift Chemical shift parameters and Internal Standards – Factors influencing chemical shift – Spin-spin coupling in AX, ABX, AMX type molecules – Coupling Constant – Geminal, vicinal and long

range coupling – Nuclear Overhauser Effect (NOE) – FT-NMR – C^{13} NMR – 2D NMR – 2D-pulse sequences COSY – NOESY – INEPT and DEPT.

Unit V Mass Spectroscopy

Mass spectrometry – Basic principles–Instrumentation–Techniques of Ion production – EI, CI, FD, FAB, ESI-MS, MALDI-MS–Base peak – Molecular ion and parent ion– Metastable ion – Isotope ion – Daughter ion –Factors affecting fragmentation and governing reaction pathway– Factors governing reaction pathway–Nitrogen rule –Fragmentation pattern of various classes of organic compounds – Hydrocarbons, alcohols, amines, aldehyde, ketone, ether, ester, acids, phenols, amides – Mc-Lafferty rearrangement.

Combined Spectroscopy problems for UV, IR, NMR, C^{13} and Mass Spectroscopy

Text Books

1. Ahluwalia V.K, Parshar R.K. *Organic Reaction Mechanism*. New Delhi: Narosa Publishing House. Fourth Edition 2019.
2. Mukherjee Kapoor Singh. *Mechanism of Organic reactions*. Kolkata: Books and Allied Ltd. 2021.
3. Kalsi P.S. *Organic Reaction & Mechanism*. New Delhi: New Age International Publishers. 4th Edition 2020.
4. Raj K Bansal. *Organic reaction mechanism*. New Delhi: New Age International Publishers, 4th Edition 2012.
5. Gurdeep Chatwal. *Organic Chemistry of Natural Products Vol II*. Bombay: Himalaya Publishing House, 2011.
6. Agarwal O.P. *Natural Products Volume I & II*. Meerat: Krishna Prakashan Media (P) Ltd. 2017.
7. Sharma Y.R. *Elementary Organic spectroscopy*. New Delhi: S. Chand & Company. 5th Edition 2013.
8. Jag Mohan. *Organic spectroscopy Principles and Applications*. New Delhi: Narosa Publishing House. Second Edition 2011.

Books for Reference

1. Finar I.L. *Organic Chemistry, Volume I*. India: Pearson Education India. 6th Edition, 2002.
2. Finar I.L. *Organic Chemistry, Volume II*. India: Pearson Education India. 5th Edition, 2002.
3. Warren Stuart. *Designing Organic Synthesis: A Programmed Synthon approach*. New York: John Wiley & Sons, 2013.
4. Jonathan Clayden, Nick Greeves, Stuart Warren. *Wothers Organic Chemistry*, New York: Oxford University Press, 2nd Edition 2021.
5. Norman R.O.C, Coxon J.M. *Principles of Organic synthesis*. Switzerland: Springer and Business Media, LLC. 3rd Edition 1994.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	describe various reactions involved in addition to C=C bonds	3	Un
CO 2	demonstrate/apply the concepts involved in elimination reaction	5	Ap
CO 3	study about the outline of retrosynthetic analysis with some examples	6	An
CO 4	outline Salient features of fragmentation pattern of organic compounds, Appraise the different retrosynthetic compounds	4	Ap
CO 5	explain the nomenclature, reactivity and spectral properties of heterocyclic compounds	5	An
CO 6	know about the NMR spectroscopy, distinguish spin-spin coupling and application to organic structure ^{13}C spectroscopy	7	Ap

	PO									PSO								
	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	Avg	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5	PSO-6	PSO-7	PSO-8	Avg
CO-1	3	2	1	2	3	2	3	1	2.3	3	2	1	2	3	3	2	2	2.3
CO-2	3	3	1	2	3	2	3	3	3	3	2	2	2	3	2	3	2	2.4
CO-3	3	3	2	3	3	2	3	1	3	3	2	2	2	3	2	3	3	3
CO-4	3	3	1	3	3	2	3	1	2.4	3	2	2	2	3	3	3	2	3
CO-5	3	2	1	3	3	2	3	1	2.3	3	2	1	2	3	3	3	3	3
CO-6	3	2	1	3	3	2	3	1	2.3	3	2	1	2	3	3	3	2	2.4
Average	3	2.5	1	3	3	2	3	1		3	2	2	2	3	2.5	3	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		

Semester – IV			
Core XII	Physical Chemistry - IV		
Course Code : 21PCHC43	Hrs / Week : 4	Hrs / Sem : 60	Credits : 4

Objectives:

- To understand the theories and applications of chemical kinetics.
- To elucidate the structure of chemical compounds by electron spin resonance spectroscopy.
- To gain knowledge about the principles of radiation chemistry and phase equilibrium.

Unit I Chemical Kinetics

Theories of reaction rates – Arrhenius theory – Hard-sphere collision theory of gas phase reactions – Potential energy surfaces – Activated complex theory for ideal gas reactions (formation in terms of partition functions) – Relation between activated complex theory and hardsphere collision theory – Thermodynamic formulation – Activated complex theory (Enthalpies and entropies of activation) – Unimolecular reactions – Lindemann, Hinshelwood, RRK, RRKM and Slater theories – Kinetic isotopic effect.

Unit II Chemical and Phase Equilibria

Chemical equilibrium – Definition, Nature and characteristics – Law of mass action – De Donder's treatment of chemical equilibria – Thermodynamic relations for chemical affinity – Homogeneous equilibria – Heterogeneous equilibria – Linear free energy relationship (Hammett equation).

Phase rule – Conditions for equilibrium between phases – Gibbs phase rule – Derivation – One component system – Liquid Helium system – Two component system – Sodium sulphate-Water system–Three component system – Acetic acid-Chloroform-Water system.

Unit III Statistical Thermodynamics

Aim of statistical thermodynamics – Ensembles (Canonical, micro canonical and grand canonical ensembles) – Microstates and macrostates – Stirling's approximation – Maxwell-Boltzmann distribution law – Types of statistics – Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics – Comparison of B.E. and F.D. statistics with Boltzmann statistics – Partition function – Molecular, Translational, Rotational, Vibrational, Electronic and Nuclear partition functions – Thermodynamic properties E, H, S, A, G, Cv and Cp in terms of partition function – Thermodynamic properties of ideal mono atomic gas – Calculation of entropy of monatomic gases (Sackur-Tetrode equation) – Debye theory of heat capacity of solids – Statistical thermodynamics of Ortho and Para Hydrogen.

Unit IV Radiation Chemistry

Introduction –Differences between radiation chemistry and photochemistry – Sources of High energy radiation– Interaction with matter: Primary effects due to charged particles, Radiation Tracks Spurs and δ -rays – Interaction of γ -radiation with matter: Photoelectric effect, Compton Scattering and Pair Production – Units for measuring radiation absorption – Radiation Dosimetry – Units of radiation energy – Chemical Dosimetry – Radiolysis of water: Mean LET in water radiolysis, Ionic Products, Free radical products and Hydrated electrons – Applications of radiation chemistry.

Unit V EPR and Mossbauer Spectroscopy

Electron Spin Resonance Spectroscopy – Basic principles – Factors affecting “g” value – Hyperfine splitting –Deuterium, methyl, benzene, naphthalene, anthracene, o-, p- and m-xylene, p-benzosemiquinone radicals –McConnel equation: Calculation of electron density – Fine structure in ESR – Zero field shifting and Kramer`s degeneracy – Double resonance – ELDOR and ENDOR.

Mössbauer spectroscopy – Theory and Principle of Mössbauer spectroscopy – Isomer shift – Quadrupole interactions – Magnetic hyperfine interaction – Doppler shift – Recoil energy – Chemical applications.

Text Books

1. Gupta M.C. *Statistical Thermodynamics*. Wiley Easter Ltd. 1990.
2. Kuriacose, Rajaram. *Kinetics and Mechanism of Chemical Transformation*. Delhi: Macmillan & Co. 1993.
3. Banwell C.N. *Molecular spectroscopy*. New Delhi: TATA McGraw Hill Co. 1997.

Books for Reference

1. Lee J.F, Sears F.W, Turcotte D.L. *Statistical Thermodynamics*. 1972.
2. Donald McQuarrie. *Statistical Thermodynamics*. New Delhi: Viva Books Private Ltd. Indian Edition 2003.
3. Ferrell L. Hill. *Introduction to Statistical Thermodynamics*. London: Addison-Wesley Publishing Company, INC. 1962.
4. Frost A.A, Pearson R.G. *Kinetics and Mechanism*. Wiley Eastern Pvt. Ltd. 1970.
5. Laidler K.J. *Chemical Kinetics*. New Delhi: TATA McGrawHill Co. Third edition 1984.
6. Spinks J.W.T, Woods R.J. *Introduction to Radiation Chemistry*. John Wiley & Sons. 2nd Edition 1976.
7. Hughes G. *Radiation Chemistry*. Oxford University Press. 1973.
8. Drago R.S. *Physical Methods in Inorganic Chemistry*. New Delhi: East West Press Ltd. 1971.
9. Chang R. *Basic Principles of Spectroscopy*. New Jersey: Englewood Cliffs. 1978.
10. Straughan B.P, Walker S. *Spectroscopy*. New York: London Chapman and Hall, A Halstet Press Book, John Wiley & Sons Ins. Volume 1,2, 3. 1975.
11. Barrow G.M. *Introduction to Molecular Spectroscopy*. Tata McGraw Hill Edition. 1993.

12. Gurdeep R Chatwal, Sham K Anand. *Spectroscopy*. Himalaya Publishing House. 2009.
13. Gupta M.C. *Statistical Thermodynamics*. New Delhi: New Age International Pvt. Ltd. 1995.
14. Moore W.J. *Physical Chemistry*. Orient Longman. 5th Edition 1976.
15. Castellan G.W. *Physical Chemistry*. Addison Wesley. 3rd Edition 1983.

Course Outcomes:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO 1	examine the theories and concepts of chemical kinetics for homogeneous and heterogeneous catalysed reactions.	1	Ap
CO 2	sketch the phase diagram for one, two and three component systems	5	An
CO 3	apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.	4	Ap
CO 4	understand the applications of radiation chemistry in different fields.	1	Un
CO 5	interpret electron spin resonance and Mössbauer spectroscopies.	4	Ev
CO 6	judge the structure of molecules by performing hyperfine splitting technique.	5	Ev

	PO									PSO								
	PO -1	PO -2	PO -3	PO -4	PO -5	PO -6	PO -7	PO -8	Av g	PSO -1	PSO -2	PSO -3	PSO -4	PSO -5	PSO -6	PSO -7	PSO -8	Avg
CO-1	3	3	1	2	3	2	3	2	2.4	3	2	1	2	3	3	2	1	2.2
CO-2	3	2	2	2	3	2	3	2	2.3	3	2	3	2	3	2	3	2	2.5
CO-3	3	3	2	3	3	2	3	1	3	3	3	2	2	3	2	3	2	2.5
CO-4	3	3	1	3	3	2	3	2	3	3	2	1	2	3	3	3	2	2.4
CO-5	3	2	2	3	3	2	3	2	2.5	3	2	3	2	3	3	3	2	2.6
CO-6	3	2	1	3	3	2	3	1	2.3	3	2	1	2	3	3	3	2	2.4
Average	3	2.5	1.5	3	3	2	3	2		3	2.2	2	2	3	3	3	2	
PO Mean									2.5	PSO Mean								2.5
Strength of PO Correlation				Strong						Strength of PSO Correlation						Strong		