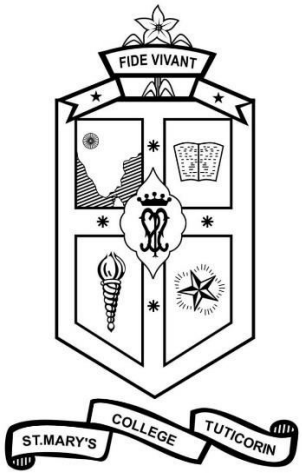
ST. MARY'S COLLEGE (AUTONOMOUS)

Re-accredited with A+ Grade by NAAC

Thoothukudi – 628001, Tamil Nadu

(Affiliated to Manonmaniam Sundaranar University)



Syllabus

M.Sc. Chemistry

School of Physical Sciences

Outcome Based Curriculum

(w.e.f. 2021)

Preamble

M.Sc. Chemistry program provides broad foundation in chemistry to the students in doing analyses and in solving analytical problems. The students will gain the integrating knowledge to apply in a variety of discipline.

Vision

To enhance the knowledge of the students and mould them for their better future.

Mission

- To create sound knowledge of chemistry.
- To make the students to understand the life time applications in chemistry.
- To enrich the subject related skills of the students and apply the same in their life.

Programme Outcomes

PO. No.	At the end of the M.Sc. Program, the students will be able to
PO-1	obtain in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods in Science
PO-2	understand their subject areas more clearly and develop skills to critically reflect upon the theory they learn.
PO-3	adopt the scientific methods and hypothesis testing in designing and execution of experiments.
PO-4	think critically, work independently and focus in research oriented activities.
PO- 5	inculcate an ability to engage in life-long learning to improve professional competency.
PO-6	extend and understand the impact of science on society.
PO-7	apply their professional ability for entrepreneurship and self-employment.
PO-8	understand and commit to professional ethics and social responsibility.

Program Specific Outcomes

PSO No.	Students of M. Sc. Chemistry will be able to	PO Addressed
PSO 1	Gain complete knowledge about all fundamental aspects and the importance of the elements of chemistry.	**PO - 1**
PSO 2	Understand the background of organic reaction mechanisms, complex chemical structures, molecular rearrangements and separation	**PO - 1, 6**
PSO 3	Appreciate the coordination chemistry and structure of molecules, properties of compounds, structural determination of complexes using	**PO - 1, 4**
PSO 4	Gather attention about the physical aspects of atomic structure, dual behaviour, reaction pathways with respect to time, various energy transformations, molecular assembly in nano-level, significance of electrochemistry, molecular segregation using their	**PO - 1, 6**
PSO 5	Learn about the potential uses of analytical, industrial and green	**PO - 3**
PSO 6	Demonstrate the ability to synthesise, separate and characterize the compounds using published reactions, protocols, standard laboratory equipments by eco-friendly chemical processes.	**PO - 2**
PSO 7	Broaden their professional foundations through various activities	**PO - 5,7**
PSO 8	Get enormous job opportunities at all level of chemical, pharmaceutical, food products and life oriented material	**PO - 5,8**

ST.MARY'S COLLEGE (AUTONOMOUS), THOOTHUKUDI

Master of Science (Chemistry)

Course structure (w. e. f. 2021)

Semester - I

Subject	Course code	Title of the paper	Contact Hours /week	Credits	Max. marks		
					CIA	ESE	Total
Core I	21PCHC11	Inorganic Chemistry - I	5	4	40	60	100
Core II	21PCHC12	Organic Chemistry - I	5	4	40	60	100
Core III	21PCHC13	Physical Chemistry - I	4	4	40	60	100
Elective I	21PCHE11/ 21PCHE12	A. Advanced Topics in Chemistry / B. Food and Health Chemistry	4	4	40	60	100
Core Practical I	21PCHCR1	Inorganic Chemistry Practicals - I	4	-	-	-	-
Core Practical II	21PCHCR2	Organic Chemistry Practicals - I	4	-	-	-	-
Core Practical III	21PCHCR3	Physical Chemistry Practicals - I	4	-	-	-	-
			30	**16**	**160**	**240**	**400**

Semester - II

Subject	Course code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core IV	21PCHC21	Inorganic Chemistry - II	4	4	40	60	100
Core V	21PCHC22	Organic Chemistry - II	5	4	40	60	100
Core VI	21PCHC23	Physical Chemistry - II	5	4	40	60	100
Elective II	21PCHE21 / 21PCHE22	A. Nanoscience and Technology / B. Energy and Computational Chemistry	4	4	40	60	100
Core Practical I	21PCHCR1	Inorganic Chemistry Practicals - I	4	4	40	60	100
Core Practical II	21PCHCR2	Organic Chemistry Practicals - I	4	4	40	60	100
Core Practical III	21PCHCR3	Physical Chemistry Practicals - I	4	4	40	60	100
			30	**28 + 2**	**280**	**420**	**700**

Semester - III

Subject	Course code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core VII	21PCHC31	Inorganic Chemistry - III	5	4	40	60	100
Core VIII	21PCHC32	Organic Chemistry - III	4	4	40	60	100
Core IX	21PCHC33	Physical Chemistry - III	5	4	40	60	100
Elective III	21PCHE31/ 21PCHE32	A. Research Methodology / B. Chemical Instrumentation	4	4	40	60	100
Core XVII Practical IV	21PCHCR4	Inorganic Chemistry Practicals - II	4				
Core Practical V	21PCHCR5	Organic Chemistry Practicals - II	4				
Core Practical VI	21PCHCR6	Physical Chemistry Practicals - II	4				
Self-study Course / MOOC / Internship (Optional)	21PCHSS1/ 21PCHM31 /21PCHI31	Course on Competitive Exams	-	+2		(100)	(100)
			30	**16 + 2**	**160**	**240**	**400**

Semester - IV

Subject	Course code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core X	21PCHC41	Inorganic Chemistry - IV	4	4	40	60	100
Core XI	21PCHC42	Organic chemistry - IV	4	4	40	60	100
Core XII	21PCHC43	Physical Chemistry - IV	4	4	40	60	100
Core Practical IV	21PCHCR4	Inorganic Chemistry Practicals - II	4	4	40	60	100
Core Practical V	21PCHCR5	Organic Chemistry Practicals - II	4	4	40	60	100
Core Practical VI	21PCHCR6	Physical Chemistry Practicals - II	4	4	40	60	100
Core Project	21PCHP41	Project	6	6	40	60	100
			30	**30**	**280**	**360**	**700**

Master of Science (Chemistry)

Components	Credit per Semester	No. of Courses	Total Credits
Core	**4**	**12**	**48**
Elective	**4**	**3**	**12**
Practical	**4 (Non-Semester)**	**6**	**24**
Project	**6**	**1**	**6**
Total credits			**90**

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.

Course outcome:

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

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

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 Kulsherstha, Ajay Taneja. *Upkar's CSIR-UGC NET/JRF/SET for Chemical Science*. Agra: Upkar Prakashan. Revised & Enlarged Edition.

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.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	simulate the nomenclature of different compounds	1, 7	Ev
CO 2	illustrate the basic of aromaticity	5	Un
CO 3	criteria for aromaticity and Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds.	6	Ev
CO 4	understand the various types of aliphatic nucleophilic substitution reactions	5	Un
CO 5	explain neighbouring group participation in aliphatic Electrophilic substitution.	5	Ap
CO 6	explain the generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals	6	Ap
CO 7	learn the concept stereochemistry and its importance	7	Re
CO 8	identify the stereochemistry notations	1,7	Ap

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

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: SN_1SN_2 and SN_i 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 stereoheterotopic ligands and faces - Mechanism of racemisation involving free radicals and carbonium ions - Conformations of cyclic systems - monosubstitued, disubstituted cyclohexanes [(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.

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.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	Have a good foundation in understanding the physical and mathematical aspects of quantum mechanics.	1	Un
CO 2	Know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.	4	An
CO 3	Apply the approximation methods to different atoms and find the dissociation energy and bond order for various molecules by applying Huckel molecular orbital theory.	7	Ap
CO 4	Explain different types of methods of preparation of polymers.	6	Un
CO 5	Prepare the polymer molecule and determine the molecular weight of polymer.	6	Cr
CO 6	Predict the rate of collisional quenching.	6	Cr
CO 7	Deduce the experimental techniques involved in photochemical processes.	7	Ev
CO 8	Classify the molecules according to their moment of inertia.	1	An

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

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 – Hartree Fock - Self consistent field method (HF-SCF) to helium atom - Born-Oppenheimer approximations - MO and VB treatments of H_2 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. Aruldhas G. Quantum Mechanics. New Delhi: Prentice Hall of Indian 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 Willey and sons.3rd Edition
7. Gowarikar 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.

Semester – I			
Elective I	**A. 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.

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.	6,8	Cr
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.	5,6	Cr
CO 5	compare heterogeneous liquid- liquid and heterogeneous solid- liquid reactions	2	An
CO 6	acquire knowledge about common diseases due to insects, animals, air and water borne diseases.	1,8	Un
CO 7	synthesise the nanomaterials by ultrasonication.	7	Cr
CO 8	sketch the natural cycles of environment such as the hydrological, oxygenand nitrogen cycles.	6	Cr
CO 9	differentiate chemical and photochemical reactions occurs in atmosphere.	1,5	An

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

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 II Supramolecular 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 CO_2 and H_2O - 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_3chemistry, 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 Activatio*n. 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.

Semester – I			
Elective I	**B. 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.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSOs 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.	8	An
CO 6	detect various blood group for different persons.	3, 6	Ev
CO 7	calculate body mass fluid and give the factors which affect BMF.	4	Ap
CO 8	test the adulterants present in food items.	8	Cr

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

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 - Basel 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.

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.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	judge about the stability and factors affecting the stability of the coordination complexes.	1,2	Ev
CO 2	categorise the ligands into strong and weak by Irving William series and the spectrochemical series.	2,3	An
CO 3	discuss the various features of Valence bond, Crystal field and Molecular orbital theories.	1,7	An
CO 4	measure Crystal Field Stabilisation Energy (10Dq or Δ_0) of coordination complexes.	4	Ev
CO 5	synthesise and discuss reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes and arene complexes	2,3	Cr
CO 6	summarise the substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic reactions of organometallic complexes.	2,3	Un
CO 7	predict about the number of active modes of vibrations in IR and Raman spectroscopy.	2,6	Un
CO 8	interpret the Mossbauer spectra of Iron and Tin complexes.	2,5	Ev

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

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 ($[TiF_6]^{2-}$, $[Ti(H_2O)_6]^{3+}$, $[TiCN_6]^{3-}$), Crystal field theory for tetrahedral complexes ($[Zn(OH)_4]^{2-}$, $[CoCl_4]^{2-}$, $[CuCl_4]^{2-}$) and Crystal field theory for square planar complexes ($[NiCN_4]^{2-}$, $[XeF_4]^{2-}$) - 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.. 8thEdition, 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 Kulsherstha, Ajay Taneja, *Upkar's CSIR-UGC NET/JRF/SET for Chemical Science*. Agra: Upkar Prakashan. Revised & Enlarged Edition. 2021.

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.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO1	organize the various methods of determination of reaction mechanism	6	Cr
CO2	comprehend the various factors that operate in organic reactions	3	An
CO 3	use relevant concepts and terminology in a correct fashion	8	Re
CO 4	understand the isolation and structural determination of alkaloids	5	Un
CO 5	determine structure and stereochemistry of Morphine and quercetin	6	Cr
CO 6	gain knowledge of photochemical organic reactions	5	Ap
CO 7	discuss the Photochemistry of (n-π*) transitions with particular reference to Norrish type I, Norrish II type reactions, Paterno - Buchi reactions & photochemistry of nitrites.	8	An
CO 8	understand the applicability of the spectroscopic techniques	4	Un

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

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-Meerwein rearrangement, 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, Hydroperoxide rearrangement and Dakin reaction.

Migration to electron rich carbon – Neber rearrangement 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, Photorearrangemts - Di-π-methane rearrangement, photo Fries rearrangement, Photoreduction of carbonyl compounds and aromatic hydrocarbons, Barton reaction, Photooxidation of alkenes an 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 – Fieser 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 Dichorism, Opticalrotatory dispersion (ORD), Axial Haloketone 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: Spinger and Business Media, LLC. Third edition 1994.

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.

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.	1	An
CO 2	construct the character table for various point groups.	7	Cr
CO 3	apply the principles of group theory in determining hybridization and symmetries of vibrational modes in linear and non-linear molecules.	5	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.	4	Cr
CO 6	discuss in detail about partial molar properties.	1	Ap
CO 7	identify vibrational course structure and rotational fine structure of electronic band and differentiate the molecules whether they are IR active or Raman active.	1	Ap
CO 8	illustrate different types of electronic spectroscopy and draw the structures of various molecules.	4	Un

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

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. McQurrie D.A, Simon J.D. *Physical Chemistry*: *A Molecular Approach*. New Delhi: Viva Books Pvt. Ltd. 1999.
6. Rajaram J,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 Edition 1972.
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 Halstet Press Book, John Wiley & Sons Ins. 1976.

Semester – II			
Elective II	**A. 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.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs 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	aware of challenges, risks and promises of nano technological development	6	Cr
CO 6	synthesise the nanomaterials by physical, chemical and biological methods.	6	Cr
CO 7	characterise the synthesized nanomaterials by various techniques.	5	Ev
CO 8	apply the nanomaterials in energy storage, food and in day-to-day life.	8	Ap

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

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 - Nanocompsites by mechanical alloying - Metal-matrix nanocomposites – Poymer 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.

Semester – II			
Elective II	**B. 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.

Course outcomes

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

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

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, IF …..ELSE, 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, Amino acids, Lipids, Nucleic acids.

Chem sketch: Introduction - Screen parts and their functions - Features - Chemsketch 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/
7. Bethany Halford. *Reflections on ChemDraw*. 2014.

Semester – I & II			
Core Practical I	**Inorganic Chemistry Practicals – I**		
Course Code : 21PCHCR1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Microscale Qualitative analysis of inorganic mixture containing two familiar and two less familiar cations - Pb, Cu, Bi, Cd, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Te, Se, Mo, Ce, Zr, V, Ti and Li.
2. Complexometric titrations – Estimation of Cu, Zn, Cd, Ni and Mg by EDTA titration in presence of either Pb or Ba.

Course Work

Green synthesis of nanomaterials by using

a) Ultra-sonicator
b) Magnetic stirrer

Reference

1. Svehla. G. *Vogel's Qualitative Inorganic Analysis*. Pearson Education. 7th edition 2012.
2. Guozhong Cao. *Nanostructures & Nanomaterials: Synthesis, Properties & Applications.* Imperial College Press. 2004.

Semester – I & II			
Core Practical II	**Organic Chemistry Practicals - I**		
Course Code : 21PCHCR2	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Microscale Qualitative Analysis of an organic binary mixture

i) Pilot separation
ii) Bulk separation
iii) Determination of melting and boiling points
iv) Analysis of organic compounds
v) Derivatization
vi) Recrystallisation

2. Single stage preparation of Organic compounds

1. Preparation of Benzoic acid from benzyl Chloride.
2. Preparation of Resacetophenone from resorcinol.
3. Preparation of dibenzalacetone from benzaldehyde.
4. Preparation of 2, 4, 6-tribromoaniline from aniline.
5. Preparation of Tetrahyrocarbazole from cyclohexanone.
6. Preparation of Picric acid from phenol.
7. Preparation of phenol-formaldehyde resin from phenol and formaldehyde.
8. Preparation of di-β-naphthol from β-naphthol.

3. Course work

Isolation experiments of alkaloids

1. Isolation of lycopene from riped tomotoes.
2. Isolation of piperine from pepper.

Books for Reference

1. Furniss B.S, Hannaford A.J, Smith P.W.G, Tatchell A.R. *Vogel's Textbook of Practical Organic Chemistry*. Pearson Education Ltd. V Edition 2008.
2. Gnanapragasam, Ramamurthy. *Organic Chemistry Lab Manual*. Chennai: S. Vishwanathan Printers, Publishers (P) Ltd. Second Edition 2007.
3. Ragupathi Mukhopadhyay, Pratul Chatterjee. *Advanced Practical Chemistry*. Books and Allied (p) Ltd. Third Edition 2007.
4. Bidhan Chandra Ray, Satyanarayan Das. *A textbook on Chemistry Practical*. London: New Central Book Agency Ltd. 2014.
5. Sananda Chatterjee. *A Chemical Analyser's Guide: A Practical Approach to Chemist & Laboratory Guide.* New Delhi: Dominant Publishers. 2014.

Semester – I & II			
Core Practical III	**Physical Chemistry Practicals - I**		
Course Code : 21PCHCR3	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

I Conductometry

1. Determination of solubility product of a sparingly soluble silver salt.
2. Determination of dissociation constant of a weak acid.
3. Conductometric Titrations
   i) Estimation of HCl and CH_3COOH in a mixture (vs NaOH)
   ii) Estimation of HCl and NH_4Cl in a mixture (vs NaOH)
   iii) Estimation of CH_3COOH and CH_3COONa in a mixture (vs NaOH)
   iv) Estimation of CH_3COOH and CH_3COONa in a mixture (vs HCl)

II Distribution

i) Distribution of Benzoic acid between Toluene and Water.
ii) Distribution of I_2 between benzene and water.

III Thermometry

Determination of solution enthalpy
i) Oxalic acid – Water
ii) Ammonium oxalate – Water
iii) Naphthalene – Toluene

Course Work

i) Study of Kinetics of primary salt effect on $K_2S_2O_8$
ii) Removal of dyes from effluent.

Books for Reference

1. Viswanathan B, Raghavan P.S. *Practical Physical Chemistry*. Viva Books. 2017.
2. Michell J. Sienko, Robert A. Plane, Stanley T. Martu, *Experimental Chemistry.* International Student Edition. 1984.
3. David P. Shoemaker, Carl W. Garland, Joseph W. Nibler. *Experiments in Physical Chemistry*. McGraw Hill International. 1988.
4. Peter Mathews G. *Experimental Physical Chemistry*. Oxford University Press. 1986.
5. Sananda Chatterjee. *A Chemical Analyser's Guide: A Practical Approach to Chemist & Laboratory Guide*. New Delhi: Dominant Publishers. 2014.

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.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	demonstrate about Electrical properties and applications of semiconductors.	1,4	Ap
CO 2	discuss about the High temperature super conductors and their applications in Levitation.	4,7	An
CO 3	compare various techniques involved in single crystal growth.	6,8	An
CO 4	sketch the Crystal structures of some Ionic compounds.	1,2	Cr
CO 5	distinguish between Homocyclic and heterocyclic inorganic ring systems.	1,3	An
CO 6	calculate STYX notation for boranes and carboranes.	4	Ap
CO 7	coin the Isolobal relationships between main group and transition metal fragments.	6,8	Cr
CO 8	calculate the Microstates and Term symbols for Transition metal complex.	4,8	Ev
CO 9	discuss the applications of XPES and UVPES to inorganic spectra.	5,6	An

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

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, Na_2O, Zinc blende, Wurtzite, Nickel arsenide, CsCl, Rutile, CdI_2, $CdCl_2$, and CaF_2, Perovskite, K_2NiF_4, Spinels.

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, Seeback 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.

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, Reprint2003.
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.

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.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	familiarize the various types of aromatic substitution reactions.	2	Re
CO 2	compare neighbouring group participation and Ambident nucleophiles in aromatic Electrophilic substitution.	4	Ev
CO 3	discuss the Conformational analysis of cyclic molecules and the factors governing the reactivity of axial and equatorial substituents in cyclohexanes.	5	An
CO 4	discuss optical rotatory dispersion and how it is used for the determination of structure of chiral molecules.	6	Ap
CO 5	study the synthesis and Elucidation of structure of steroids and terpenoids.	6	Re
CO 6	learn the conversion of cholesterol to progesterone, estrogen and testosterone.	8	Un
CO 7	acquire knowledge about the reagents specificity.	4	An
CO 8	know about the NMR spectroscopy.	6	Un
CO 9	distinguish spin-spin coupling and application to organic structure ^{13}C spectroscopy.	2	An

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

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 – Vilsmeir 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) an (1,4) – Conformation of poylsubstituted 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, Progestrone, 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 Edition2019.
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.3rdEdition, 2018.

Books for Reference

1. Michael B Smith. *March's Advanced Organic Chemistry: Reactions, Mechanism and Structure*, New York: John-Wiley and Sons, 8thEdition, 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.8thEdition 2015.
5. Norman R.O.C, Coxon J.M. *Principles of Organic synthesis*.Switzerland: Spinger and Business Media, LLC.Third edition1994.

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.

Course Outcomes:

CO No.	Upon completion of this course, students will be able to	PSOs 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.	7	Cr
CO 3	investigate the corrosion and polarization studies	7	Ev
CO 4	analyse Onsager relations and Electro kinetic effect	1	An
CO 5	Justify electrochemical mechanisms of nervous system	6,7	Ev
CO 6	Categorise the principle and applications of NMR and EPR spectroscopy.	6,8	An
CO 7	differentiate the various types of electronic spectroscopy and draw the structures of various molecules.	4	An
CO 8	judge the structure of molecules by applying various spectroscopic techniques.	5	Ev

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

Unit I Electrochemistry I

Debye-Huckel theory of inter-ionic attraction–Debye-Huckel Onsager equation and its validity– Debye-Falkenhagen and Wein effects – Activity coefficinets of electerolytes – 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 – Evan's 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 fortrat 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: Plenum Press. Vol. 1 & 2, Second Edition 1998.

3. McQurrie 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 Edition 1994.

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.

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.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	select the research topic and able to survey the literature.	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.	3,6	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
CO 7	improve the accuracy of data in chemical analysis.	5	Ev
CO 8	defend teaching methods.	6,7	Ev

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

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, 23rdEdition 2004.
3. Willard H, Merrit Jr. L, Dean. A. *Instrumental methods of analysis.* CBS Publishers and Distributers. 2004.
4. Rajammal P. Devadas. *A Handbook of Methodology of Research.*Chennai: S.R.K. Vidyalaya 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 & Distributers Pvt. Ltd. Volume 7, First Edition Reprint 2019.

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.

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.	6	Ap
CO7	control noise level in a system.	1,7	Cr
CO8	interpret the optimal value of adjustable parameters	7,8	Ev

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

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 uncertainity - 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 Noiseinasystem – Signal averaging - Modulation: Chopping - Demodulation: Phase sensitive detection-Other methods of Optimising Signal-to-Noise ratio.

Unit IV DigitalElectronics

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

Unit V Instrumentation for Optical Absorption Spectrometry

VisualPhotometers-FilterPhotometers-Spectrophotometer-DoublebeamSpectrophotometer - Recording Spectrophotometers - Optimal value of adjustable parameters – Multiple internal reflection assembly – Rapid scanning spectrometer – Non-dispersive Photometers – Photometric titration equipment – Fourier transform Spectrometers.

Textbooks

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

Books forReference

1. Jeffery G.H, Bassett J, Mendham J, Denney R.C. *Vogel's Text book of Qualitative chemical analysis.* Essex: Longman Scientific and technical. 5th Edition1989.
2. Skoog D.A, Hollar F.J, Crouch S.R. *Principles of Instrumental analysis.* Belmont CA: Thompson Brooks/Cole. 6th Edition 2007.

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.

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	2,6	Ap
CO 2	distinguish between proportional and non-proportional situations and when appropriate apply proportional reasoning	6	An
CO 3	solve problems applying probabilistic reasoning to make decisions	2	Ap
CO 4	evaluate claims based on empirical, theoretical and subjective probabilities	6,4	Re
CO 5	create and use visual displays of data	4	Cr
CO 6	solve problems using high speed mental calculations	6	Ap
CO 7	understand the basic concepts of logical reasoning skills	1,4	Un
CO 8	acquire satisfactory competency in use of data analysis	7	Un

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

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.

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.

Course Outcome:

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

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

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 mechanismin 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 $^{15}NH_3$ – 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, $(ή^1\text{-}C_5H_5)_2$ $(ή^5\text{-}C_5H_5)_2Ti$, $(ή^5\text{-}C_5H_5)_2Fe_2(CO)_4$ and PCl_2F_3.

EPR – Principle–Fine structure– Interaction between nuclear spin and electron spin (hyperfine coupling) – Hyperfine splitting of systems withI=1/2, 1 &3/2– Zero field splitting &Kramer's degeneracy – EPR spectrum deduction for $[Co(H_2O)^{2+}]$, $[Cr(H_2O)^{2+}]$ $[(NH_3)_5Co\text{-}O\text{-}O\text{-}Co(CN)_5]^{5+}$, $[(NH_3)_5Co\text{-}O\text{-}O\text{-}Co(NH_3)_5]^{5+}$ – Covalency of M-L bonding in bis(salicylaldimine)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. 6thEdition 2014.
7. Lee J.D. *Concise Inorganic Chemistry*. Blackwell Science Ltd. 5thEdition, Reprint 2003.
8. Samuel Glasstone. *Source Book of Atomic Energy.* East West Pvt. Ltd. 1969.

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.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	to describe various reactions involved in addition to C=C bonds	2	Ap
CO 2	to demonstrate/apply the concepts involved in elimination reaction	2	Ap
CO 3	study about the outline of retrosynthetic analysis with some examples	7	An
CO 4	appraise the different retrosynthetic compounds	5	Ev
CO 5	to learn the concept of cycloaddition, electrocyclic and sigmatropic reaction mechanism	6	Cr
CO 6	explain the nomenclature, reactivity and spectral properties of heterocyclic compounds	3	Un
CO 7	demonstrate the synthesis and reactivity of heterocyclic compounds	2	Ap
CO 8	outline salient features of fragmentation pattern of organic compounds	8	Ev

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

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-Pondorf 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 interconversions – 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 –Reterosynthetic analysis of the following compounds – Twistane, cis-Jasmone, Baclofan, Brufen, Trihexylphenydyl, 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 C^{13} 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: HimalayaPublishing 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: Spinger and Business Media, LLC.3rd Edition 1994.

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.

Course Outcomes:

CO No.	Upon completion of this course, students will be able to	PSOs addressed	CL
CO 1	detect the use of chemical kinetics in understanding the reaction mechanisms.	2	Ev
CO 2	apply the theories and concepts of chemical kinetics for homogeneous and heterogeneous catalysed reactions.	4	Ap
CO 3	sketch the phase diagram for one, two and three component systems	5	An
CO 4	apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.	4	Ap
CO 5	formulate dosimetry and dosimeters in radiation chemistry	6	Cr
CO 6	interpret electron spin resonance and Mössbauer spectroscopies.	3	Ev
CO 7	examine the spin labeling studies of biomolecules using ESR spectroscopy.	7	An
CO 8	judge the structure of molecules by applying various spectroscopic techniques.	5	Ev

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

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 hard sphere 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 Equlibria

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, microcanonical 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 monoatomic 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, Turcottee D.L. *Statistical Thermodynamics*. 1972.
2. Donald McQuarrie. *Stastistical 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 McGraw Hill Co. Third edition 1984.
6. SpinksJ.W.T, WoodsR.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 Jersy: 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.

Semester – III & IV			
Core Practical IV	**Inorganic Chemistry Practicals – II**		
Course Code : 21PCHCR4	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Preparation of inorganic complexes (a minimum of 6 complexes)

    1. cis potassiumdiaquadioxalatochromate(II) dihydrate
    2. trans potassiumdiaquadioxalatochromate(II) dihydrate
    3. tristhioureacopper(I)chloride dihydrate
    4. hexathiourealead(II)nitrate
    5. aquapentamminecobalt(III)chloride
    6. pentakisthioureadicopper(I) nitrate trihydrate
    7. Potassium triooxalatoferrate(III)nonahydrate
    8. pentaamminechlorocobalt(III) chloride
    9. tristhioureacopper(I)sulphate dihydrate

2. Quantitative estimation of a mixture containing two metal ions (Volumetric and Gravimetric estimations).
    1. Estimation of Cu^{2+} and Ni^{2+} ions.
    2. Estimation of Cu^{2+} and Zn^{2+} ions.
    3. Estimation of Fe^{2+} and Cu^{2+} ions.
    4. Estimation of Fe^{2+} and Ni^{2+} ions.
    5. Estimation of Ca^{2+} and Ba^{2+} ions.
    6. Estimation of Cu^{2+} (V), Ba^{2+} (G) and Zn^{2+} (G) ions in a mixture
    7. Estimation of Fe^{2+} (V), Cu^{2+} (G) and Ni^{2+} (G) ions in a mixture

3. Analysis of ores and alloys (Course work only).

Note: For examination, a mixture may be given from which one cation is to be estimated volumetrically and the other gravimetrically.

References

1. Arthur I. Vogel. *A Text book of Quantitative Chemical Analysis*.

2. Mendtam J et. al. *Vogel's Text book of Quantitative Chemical Analysis.* Pearson Education.

6^{th} edition.

SEMESTER – III & IV			
Core Practical V	**Organic Chemistry Practicals - II**		
Course Code : 21PCHCR5	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Quantitative Analysis

i) Estimation of ethyl methyl ketone

ii) Estimation of glucose - Lane Eynon method

iii) Estimation of glucose - Bertrand's method

iv) Determination of saponification value of oil.

v) Estimation of iodine value of oil.

vi) Estimation of Acetone by Messinger's method.

vii) Estimation of phenol

viii) Estimation of aniline.

ix) Analysis of purity of Glucose

x) Determination of Percentage purity in an unsaturated acid.

2. Preparation of Organic compounds (Double stage)

i) Preparation of p-bromoaniline from acetanilide

ii) Preparation of m-nitrobenzoic acid from ethyl benzoate

iii) Preparation of p-nitro aniline from acetanilide

iv) Preparation of 1, 3, 5-tribromobenzene from aniline

v) Preparation of benzpinacolone from benzophenone

vi) Preparation of benzilic acid from Benzoin

vi Preparation ofphthalimide from Phthalic acid

3. Course work

i) Estimation of Ascorbic acid

References

1. Furniss B.S, Hannaford A.J, Smith P.W.G, Tatchell A.R. *Vogel's Textbook of Practical Organic Chemistry*. Pearson Education Ltd.V Edition.
2. Ganapragasm, Ramamurthy. *Organic Chemistry Lab Manual*. Chennai: Second Edition, S.Vishwanathan Printers and Publishers (P) Ltd.
3. Ragupathi Mukhopadhyay, Pratul Chatterjee. *Advanced Practical Chemistry.* Books and Allied (P) Ltd. Third edition 2007.
4. Bidhan Chandra Ray, Satyanarayan Das. A textbook on Chemistry Practical.London: New Central Book Agency Ltd. 2014.

Semester – III & IV			
Core Practical VI	**Physical Chemistry Practicals - II**		
Course Code : 21PCHCR6	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Potentiometry

1. Determination of solubility product of sparingly soluble salts.
2. Determination of dissociation constant of a weak acid.

2. Potentiometric titrations

Determination of pH of buffer Potentiometrically

a) Redox titrations	**b) Precipitation titrations**
i) Fe^{2+} Vs $Cr_2O_7^{2-}$	i) Cl^- Vs $AgNO_3$
ii) Fe^{2+} Vs Ce^{2+}	ii) I- Vs $AgNO_3$
iii) Fe^{2+} vs MnO_4^-	iii) Mixture of Cl^- and I- Vs $AgNO_3$
iv) I^- Vs MnO_4^-	

3. Adsorption

Adsorption of acetic acid / oxalic acid on activated charcoal – Verification of Freundlich isotherm – Determination of unknown concentration.

4. Conductivity method

Study of kinetics of ester hydrolysis and comparison of acid strength by conductivity method.

5. Spectroscopy

Verification of Beer-Lambert's law. Determination of $[Mn^{2+}]$ and $[Cr^{3+}]$ by using UV-Visible spectrophotometer.

References

1. Viswanathan B, Raghavan P.S. *Practical Physical Chemistry*. Viva Books. 2017.
2. Michell J. Sienko, Robert A, Plane, Stanley T. Martu. *Experimental Chemistry*. International student edition. 1984.
3. David P. Shoemaker, Carl W. Garland, Joseph W. Nibler. *Experiments in Physical Chemistry.* McGraw Hill International edition. 1988.
4. Levitt B.P. *Findlay's Practical Physical Chemistry*. Edition IX.
5. Yadav J.P. *Advanced Practical Physical Chemistry Practicals*. Krishna Prakashan Media. 2015.
6. Peter Mathews G. *Experimental Physical Chemistry*. Oxford University Press. 1986.

Semester – IV			
Project			
Course Code : 21PCHP41	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 6**

Format for preparation of project report

1. Identification of the problem

Students are given the freedom of choosing the topic of the project. It may be theoretical or practical.

2. Arrangement of contents

The sequence in which the project report material should be arranged and bound should be as follows:

- Cover page and Title page
- Bonafide Certificate
- Abstract
- Table of contents
- List of Tables
- List of Figures
- List of Symbols, Abbreviations & Nomenclature
- Chapters
- Appendices
- References

3. Page dimension and binding specifications

- The dimension of the project report should be in A4 size. The project report should be bound using flexible cover of the thick white art paper. The cover should be printed in black letters and the text for printing should be identical.
- Total number of pages should not exceed 70.

4. Typing instructions

- The impression on the typed copies should be black in colour.
- One and a half spacing should be used for typing the general text. The general text shall be typed in the Font style “Times New Roman” & Font size 12.