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. 2024)

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.	**After completion of the Postgraduate programme the students of St. Mary's College will be able to**
PO 1	acquire expertise knowledge in their respective disciplines and become professionals.
PO 2	develop critical/logical thinking skills, managerial skills and become locally, nationally & globally competent and be a lifelong learner
PO 3	pursue research / higher learning programme & apply their experiment and research skills to analyze and solve complex problems.
PO 4	compete in the job market by applying the knowledge acquired in Arts, Science, Economics, Commerce and Management studies
PO 5	be an empowered and economically independent woman with efficient leadership qualities and develop the themselves as a holistic person

Program Specific Outcome

PSO No	Students of M.Sc., Chemistry will be able to	PO Mapped
PSO 1	To prepare the students who will demonstrate respectful engagement with others' ideas, behaviors, believes and apply diverse frames of reference to decisions and actions.	1
PSO 2	To create effective entrepreneurs by enhancing their critical thinking, problem solving, decision making and leadership skill that will facilitate startups and high potential organizations.	2
PSO 3	Design and implement HR systems and practices grounded in research that comply with employment laws, leading the organization towards growth and development.	3
PSO 4	To produce employable, ethical and innovative professionals to sustain in the dynamic business world.	4
PSO 5	To contribute to the development of the society by collaborating with stakeholders for mutual benefit.	5

ST.MARY'S COLLEGE (AUTONOMOUS), THOOTHUKUDI

Master of Science (Chemistry)

Course structure (w. e. f. 2024)

Semester – I

Course	Course Code	Course Title	Contact Hours / Week	Credits	Max Marks		
					CIA	ESE	Total
Core I	24PCHC11	Inorganic Chemistry - I	5	4	40	60	100
Core II	24PCHC12	Organic Chemistry - I	5	4	40	60	100
Core III	24PCHC13	Physical Chemistry - I	5	4	40	60	100
Core Practical I	24PCHCR1	Inorganic Chemistry Practicals - I	4	2	40	60	100
Core Practical II	24PCHCR2	Organic Chemistry Practicals - I	3	-	-	-	-
Elective I	24PCHE11 / 24PCHE12	**A. Green Chemistry** B. Pharmaceutical Chemistry	4	3	40	60	100
Skill Enhancement Course I	24PCHSE1	Industrial Processes	4	3	40	60	100
MOOC (Compulsory)				+2			
		Total	**30**	**20+2**			

Semester – II

Course	Course Code	Course Title	Contact Hours / Week	Credits	Max Marks		
					CIA	ESE	Total
Core IV	24PCHC21	Inorganic Chemistry-II	5	4	40	60	100
Core V	24PCHC22	Organic Chemistry-II	5	4	40	60	100
Core VI	24PCHC23	Physical Chemistry-II	5	4	40	60	100
Core Practical II	24PCHCR2	Organic Chemistry Practicals - I	3	4	40	60	100
Core Practical III	24PCHCR3	Physical Chemistry Practicals - I	4	2	40	60	100
Elective II	24PCHE21/ 24PCHE22	**A.Nanoscience and Nanotechnology** B. Medicinal Chemistry	4	3	40	60	100
Skill Enhancement Course II	24PCHSE2	Computational Chemistry	4	3	40	60	100
		Total	**30**	**24**			

Note: MOOC should be completed in the I Year. Internship can be completed during the II Semester vacation.

Semester – III

Course	Course Code	Course Title	Contact Hours / Week	Credits	Max Marks		
					CIA	ESE	Total
Core VII	24PCHC31	Inorganic Chemistry – III	5	5	40	60	100
Core VIII	24PCHC32	Organic Chemistry - III	5	4	40	60	100
Core IX	24PCHC33	Physical Chemistry - III	5	4	40	60	100
Core Practical IV	24PCHCR4	Physical Chemistry Practicals - II	4	2	40	60	100
Core Practical V	24PCHCR5	Inorganic Chemistry Practicals - II	3	-	-	-	-
Elective III	24PCHE31 / 24PCHE32	**A. Research Methodology** B. Industrial Chemistry	4	3	40	60	100
Skill Enhancement Course III	24PCHSE3	Mini Project	4	3	40	60	100
Internship / Self Study (Optional)	24PCHI31			+2			
		Total	**30**	**21+2**			

Semester – IV

Course	Course Code	Course Title	Contact Hours / Week	Credits	Max Marks		
					CIA	ESE	Total
Core X	24PCHC41	Inorganic Chemistry – IV	6	5	40	60	100
Core XI	24PCHC42	Organic Chemistry – IV	5	5	40	60	100
Core XII	24PCHC43	Physical Chemistry - IV	5	5	40	60	100
Core Practical V	24PCHCR5	Inorganic Chemistry Practicals – II	4	4	40	60	100
Core Practical VI	24PCHCR6	Physical Chemistry Practicals - III	4	2	40	60	100
Core	24PCHP41	Project	6	4	40	60	100
		Total	**30**	**25**			

Master of Science (Chemistry)

Components	Credit per Semester	No. of Courses	Total Credits
Core	**4/5**	**12**	**52**
Core Practical	**2 (Semester)** **4 (Non-Semester)**	**4 (Semester)** **2 (Non-Semester)**	**16**
Elective	**3**	**3**	**9**
Skill Enhancement Course	**3**	**3**	**9**
Core Project	**4**	**1**	**4**
Total credits			**90**

Semester – I			
Core I	**Inorganic Chemistry - I**		
Course Code : 24PCHC11	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Objectives

- To understand the atomic structure and periodical properties of elements.
- To explain the various concepts of acids and bases.
- To sketch the various crystal structures of the compounds.
- To explain the various electronic theories involved in conducting and semiconducting materials.

Course Outcome

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	discuss about the periodic properties of the elements	K3
CO 2	demonstrate about the theories of VSEPR, Valance bond and Molecular Orbital.	K4
CO 3	demonstrate various theories of acids and bases and compare the chemistry of non-aqueous solvents.	K3, K4
CO 4	understand the various types of ionic crystal systems and analyze their structural features.	K2, K4
CO 5	sketch and figure out the various types of defects in crystals.	K3, K5

Semester – I			
Core I	**Inorganic Chemistry - I**		
Course Code : 24PCHC11	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit – I 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-Lande equation - 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.

Unit – II Molecular Structure

VSEPR theory – Structure of molecules containing lone pairs of electrons (SF_4,OSF_4, $CH_2{=}SF_4$, OCF_2, BrF_3, PX_3, ICl_2^-, ICl_4^-, TeF_5^-, NO_2, NO_2^-, NO_2^+) - Walsh diagram (H_2O) - Effect of lone pair and electronegativity of atoms (Bent's rule) on the geometry of the molecules – Apicophilicity - Valence Bond theory - MO theory of homo and heteronuclear diatomic molecules and poly atomic molecules (O_2, N_2, CO,CO_2, HCl and $BeCl_2$).

Unit – III Acids and Bases

Acid base theories - Arrhenius, Bronsted-Lowry theory, Factors affecting strength of acids and bases - Lewis theory - Solvent system - Lux-Flood concept - Usanovich concept - 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 – IV Solid State I

Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing - Voids in crystal lattice, Radius ratio & Packing efficiency – Crystal Growth methods: Hydrothermal & Sol-Gel methods – Crystal structures of common ionic compounds Rock salt, Zinc blende & Wurtzite, fluorite and anti-fluorite, rutile and anatase, cadmium iodide and nickel arsenide; Spinels -normal and inverse types and Perovskite structures.

Unit – V Solid State II

Band theory- Features and its application of conductors, insulators, semiconductors and superconductors, Intrinsic and Extrinsic semiconductors - Defects in crystals – Point defects :

Schottky, Frenkel defects, metal excess (Colour centre: F-centre) and metal deficient defects – Line defects and its effects due to dislocations – Surface Defects – Dislocations – Grain Boundary and Stacking Fault – Solid electrolytes, superconductors, High-temperature superconductors, BCS theory, Cooper electrons – Meissner effect and levitation.

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 2009.
2. 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.
3. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic Chemistry*. ELBS, Oxford University Press. 1994.
4. West A.R. *Solid State Chemistry and its Application*. Asia: John Wiley & Sons. 2007.

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.
6. Azaroff L.V. *Introduction to solids*. Tata McGraw Hill publishing Ltd. 2000.
7. Kittel C. *Introduction to solid state physics*. Wiley Eastern Ltd. 7th Edition 2006.

E- Learning Resources

1. https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	2	3	2	3	1	3	1	2	2	3
CO-2	1	2	1	3	3	2	3	1	1	3
CO-3	2	2	1	3	3	2	3	1	2	3
CO-4	2	1	3	3	2	1	2	3	2	3
CO-5	1	2	3	2	3	2	3	3	1	2
Ave.	1.6	2	2.2	2.8	2.4	2	2.4	2.2	1.6	2.8

Semester – I			
Core II	**Organic Chemistry - I**		
Course Code : 24PCHC12	**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**	**CL**
CO 1	Understand and predict cyclic organic molecules on the basic of aromaticity	K2, K4
CO 2	understand the various types of aliphatic and aromatic substitution reactions	K2
CO 3	Outline the mechanisms involved in aliphatic and aromatic substitution reactions	K3
CO 4	explain the generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals	K5
CO 5	To predict the reaction mechanism of organic reactions and evaluate stereochemistry of organic compounds.	K3, K5

Semester – I			
Core II	**Organic Chemistry - I**		
Course Code : 24PCHC12	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit – I Aromaticity and Ring System

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

Unit – II Aliphatic and Aromatic Electrophilic Substitution

Aliphatic Electrophilic Substitution: S_E1 and S_E2 and S_Ei - Mechanism and evidences.

Aromatic Electrophilic Substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

Unit – III Aliphatic and Aromatic Nucleophilic Substitution

Aliphatic Nucleophilic Substitution: S_N1, ion pair in S_N1, S_N2, S_Ni and SET mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon – Swain- Scott, Grunwald-Winstein relationships – Ambident nucleophiles: Regioselectivity.

Aromatic Nucleophilic Substitution: Mechanisms - S_NAr, S_N1 and Benzyne mechanisms and Evidences – Reactivity: Effect of substrate structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur nucleophiles, Bucherer reaction, Rosenmund reduction, Von Richter, Sommelet-Hauser and Smiles rearrangements.

Unit – IV 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

Unit – V Stereochemistry

Stereoisomerism - Introduction, classification, Principles of axial and planar chirality - Stereochemistry of allenes, spiranes and analogus - Atroisomerism in biphenyl compounds - Stereochemistry of Ansa Compound, Helicity - Topicity of ligands and faces: Homotopic, Enantiotopic, Diastereotopic (Substitution-addition criterion) - Mechanism of racemisation involving free radicals and carbonium ions - Conformations of cyclic systems: monosubstitued, disubstituted cyclohexanes [(1,2), (1,3), (1,4)], decalin, perhydrophenanthrene.

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. Tewari K.S, Vishnoi N.K. *A Textbook of Organic Chemistry*. Noida: Vikas Publishing House Pvt Ltd. 4th Edition 2019.
6. 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.
5. N. Tewari. *Advanced Organic Stereochemistry (Problems & Solutions)*. Kolkata: Books and Allied (P) Ltd.2010.

E- Learning Resource

1. https://sites.google.com/site/chemistryebookscollection02/home/organic-chemistry/organic
2. https://www.organic-chemistry.org/

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	3	3	3	2	2	3	2	3	3	2
CO-2	2	2	1	2	1	2	1	1	2	2
CO-3	2	1	3	3	2	1	2	3	2	3
CO-4	3	3	2	1	3	3	3	2	3	1
CO-5	3	3	3	3	3	3	3	3	3	3
Ave.	2.6	2.4	2.4	2.2	2.2	2.4	2.2	2.4	2.6	2.2

Semester – I			
Core III	**Physical Chemistry - I**		
Course Code : 24PCHC13	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Objectives

- To recall the fundamentals of thermodynamics and the composition of partial molar quantities.
- To understand the classical and statistical approach of the functions.
- To demonstrate and prepare the polymer molecules by various methods.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	CL
CO 1	To explain the classical and statistical concepts of thermodynamics.	K5
CO 2	apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.	K3
CO 3	analyse Onsager relations and Electro kinetic effect and Justify electrochemical mechanisms of nervous system.	K4, K5
CO 4	prepare the polymer molecules by different methods and determine the molecular weight of polymer.	K3, K4
CO 5	Classify the molecules according to their moment of inertia.	K3

Semester – I			
Core III	**Physical Chemistry - I**		
Course Code : 24PCHC13	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit - I Classical Thermodynamics

Partial molar properties - Chemical Potential - Variation of chemical potential with temperature and pressure – Gibbs-Duhem equation - Binary and ternary systems. Determination of partial molar quantities by direct method and from apparent molar properties - Thermodynamics of real gases - Fugacity - Variation of fugacity with temperature and pressure - Determination of fugacity by graphical method and equation of state method - Gibbs-Duhem-Margulus equation - Thermodynamics of ideal and non-ideal binary mixtures - Activity and activity coefficient – Reference states and standard states – Determination of activity and activity coefficients from vapour pressure.

Unit - II Statistical thermodynamics

Introduction to statistical thermodynamics – Assemblies, 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 Maxwell-Boltzmann statistics – Partition function – Evaluation of Translational, Rotational and Vibrational partition functions – Thermodynamic functions E, H, S, A, G, C_v, C_p and equilibrium constant in terms of partition function – Calculation of entropy of monatomic gases (Sackur-Tetrode equation).

Unit - III Irreversible Thermodynamics

Phenomenological laws – Conservation of mass and energy in closed and open systems – Entropy production due to heat flow – Entropy production and entropy flow in open system – 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 systems.

Unit - IV 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.

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 - Rotational energy levels - Selection rules for rotational spectroscopy - Diatomic molecules as rigid rotors - Effect of isotopic substitution - Diatomic molecules as non-rigid rotors - Rotational transitions - Rotational spectra of linear, symmetric top and asymmetric top polyatomic molecules.

Text books

1. Puri B.R, Sharma L.R, Madan S. Pathania. *Principles of Physical Chemistry*. Jalandhar: Vishal Publishing Co. 48th Edition 2022.
2. Gupta M.C. *Statistical Thermodynamics*. Wiley Easter Ltd. 1990.
3. Gowarikar V.R, Viswanathan N.V, Jayadev Sreedhar. *Polymer Science*, New Delhi: New Age International (P) Limited, Publishers. 1st edition, Reprint, 2005.
4. Banwell C.N. *Fundamentals of Molecular Spectroscopy*. Noida: McGraw Hill Education. 4th edition, 1994.

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. Gupta M.C. *Statistical Thermodynamics*. New Delhi: New Age International Pvt. Ltd. 1995.
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 1984.
9. Misra G.S. *Polymer science*. Wiley Eastern. 1986.
10. Barrow G.M. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill. 1964.

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	2	1	1	2	2	1	2	1	2	2
CO-2	3	3	3	2	2	3	2	3	3	2
CO-3	1	2	3	3	3	2	3	3	1	3
CO-4	3	3	3	3	3	3	3	3	3	3
CO-5	3	3	1	2	1	3	1	1	3	2
Ave.	2.4	2.4	2.2	2.4	2.2	2.4	2.2	2.2	2.4	2.4

Semester – I			
Core Practical I	**Inorganic Chemistry Practicals – I**		
Code :24PCHCR1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 2**

Objectives

- To learn the principles and methods of qualitative analysis of familiar and less familiar cations present in a mixture.
- To identify the methodology to analyze qualitatively a metal ion in the presence of another metal ion.
- To recall the principle and theory in preparing standard solutions.
- To train the students for improving their skill in estimating the amount of ion accurately present in the solution.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	CL
CO 1	separate and analyze the cations present in the given salt mixture.	K3, K4
CO 2	identify the cations present in the mixture of salts.	K4
CO 3	acquire the qualitative analytical skills by selecting suitable confirmatory tests and spot tests.	K2
CO 4	choose the appropriate chemical reagents for the detection of anions and cations.	K2
CO 5	separate and estimate the amount of metal ions present in the given mixture of solutions.	K3, K5

Semester – I			
Core Practical I	**Inorganic Chemistry Practicals – I**		
Code :24PCHCR1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 2**

1. Microscale Analysis of mixture of cations: Analysis of a mixture of four cations containing two less familiar cations and two familiar cations. Cations to be tested

Group-I : W and Pb.

Group IA : Se, Te

Group-II : Mo, Cu, Bi and Cd.

Group-III : Ce, Th, Zr, V, Cr, and Ti.

Group-IV : Zn, Ni, Co and Mn.

Group-V : Ba and Sr.

Group-VI : Li.

2. Complexometric Titration:

Estimation of Cu, Zn and Mg by EDTA titration in presence of either Pb or Ba.

Reference

1. Svehla. G. *Vogel's Qualitative Inorganic Analysis*. London: Pearson Education, 7th edition 2002.
2. V. V. Ramanujam. *Inorganic Semimicro Qualitative Analysis*. Chennai: The National Publishing Company. 3rd Edition 1974.

Semester – I			
Elective I	**A. Green Chemistry**		
Course Code : 24PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

Objectives

- To design the green synthesis
- To propose green solvents for industrial production of Surfactants, Organic and inorganic chemicals.
- To understand theory behind the greener techniques

Course Outcomes

CO No.	Upon completion of this course, students will be able to	CL
CO 1	recall the basic principles of green chemistry	K1
CO 2	understand the role of green solvents used in alteration to toxic organic and inorganic solvents	K2
CO 3	compare the advantages of organic reactions assisted by renewable energy sources and non-renewable energy sources.	K4
CO 4	apply the principles of PTC, ionic liquid, microwave and ultrasonic assisted organic synthesis.	K3
CO 5	design and synthesize new organic compounds by green methods.	K4, K6

Semester – I			
Elective I	**A. Green Chemistry**		
Course Code : 24PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

UNIT-I Basic Principles of Green Chemistry and Designing a Green Synthesis.

Introduction - Need for Green Chemistry. Goals of Green Chemistry. Limitations of Green Chemistry. Chemical accidents, terminologies, International green chemistry organizations and Twelve principles of Green Chemistry with examples. Green chemistry in day today life.

Choice of starting materials, reagents, catalysts and solvents

UNIT-II Green Solvents

Water: Introduction, Properties and Reactions in aqueous medium: Diel's Alder reaction, Claisen rearrangement and Benzoin condensation - Advantages.

Super Critical Water and Near Water Region (NCW): Introduction, Organic reactions in SC-H_2O - Organic reactions in NCW.

Ionic Liquids: Introduction, Properties, Types, Preparation and Applications as solvents for Polymerization process.

Supercritical Carbon Dioxide: Introduction, properties, use as extracting natural products, as dry cleaning - SC-CO_2 as solvents for organic reactions: supercritical polymerization, photochemical reactions, Friedel-Craft's reaction – Synthesis of Silica nanoparticles using SC-CO_2.

UNIT-III Green Catalysis

Green Catalysis - Acid catalysts - Oxidation catalysts - Polymer supported catalysts - Basic catalysts: Biocatalyst, Photocatalyst, Phase transfer catalysis and crown ethers – Poly styrene aluminum chloride, polymeric super acid catalysts, Poly supported photosensitizers.

UNIT-IV Greener Reactions

Microwave Induced Green Synthesis: Introduction – Applications: Stille reaction, Suzuki reaction, Krohnke reaction, Hiyama reaction and Sonogashira reaction.

Ultrasound Assisted Green Synthesis: Introduction – Applications: Homogeneous reaction, Strecker reaction, Heterogeneous liquid-liquid reactions, Hydrolysis and Solvolysis - Heterogeneous solid-liquid reactions - Bouveault reactions, Barbier reaction of carbonyl compounds.

UNIT-V Green Techniques

Micro wave induced green synthesis: Introduction, Instrumentation, Principle and applications.

Sonochemistry: Instrumentation, Cavitation theory - Ultra sound assisted green synthesis and Applications: Preparation of porous carbon powder and Sonochemical treatment of polluted water.

Text Books

1. Ahluwalia V.K. *Green Chemistry - A Text Book.* New Delhi: Narosa Publishing House. 2016.
2. Ahluwalia V.K, Rajender S. Varma. *Green Solvents for Organic synthesis*. Narosa Publishing House Pvt. Ltd. 2009.
3. Ahluwalia V.K, Kidwai, M.R. *New Trends in Green Chemistry*. New Delhi: Anamalaya Publishers. 2nd Edition 2007.

Books for Reference

1. Kumar V. *An Introduction to Green Chemistry*. Jalandhar: Vishal Publishing CO. 1st Edition 2018.
2. Ahluwalia V.K, Aggarwal R. *Organic Synthesis: Special Techniques*. New Delhi: Narosa Publishing House. 2001.
3. Paul T. Anastas. *Text Book on Green Chemistry*. OUP. 2006.
4. Chandrakanta Bandyopadhyay. *An Insight into Green Chemistry*. Books and Allied (P) Ltd. 2019.

E-Learning Resource

1. https://www.organic-chemistry.org/
2. https://www.studyorgo.com/summary.php

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	PO-2	PO-3	PO-4	PO-5	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5
CO-1	2	1	1	2	2	1	2	1	2	2
CO-2	2	1	3	1	2	1	2	3	2	1
CO-3	3	3	2	3	3	3	3	2	3	3
CO-4	3	3	3	3	3	3	3	3	3	3
CO-5	3	3	3	3	1	3	1	3	3	3
Ave.	2.6	2.2	2.4	2.4	2.2	2.2	2.2	2.4	2.6	2.4

Semester – I			
Elective I	**B. Pharmaceutical Chemistry**		
Course Code : 24PCHE12	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

Objectives

- To understand the advanced concepts of pharmaceutical chemistry.
- To recall the principle and biological functions of various drugs.
- To train the students to know the importance as well the consequences of various drugs.
- To have knowledge on the various analysis and techniques.
- To familiarize on the drug dosage and its structural activities.

Course Outcomes

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	identify the suitable drugs for various diseases.	K2
CO 2	apply the principles of various drug action and drug design.	K3
CO 3	acquire the knowledge on product development based on SAR.	K2
CO 4	synthesize new drugs after understanding the concepts SAR.	K4
CO 5	apply the knowledge on applications of computers in chemistry.	K3

Semester – I			
Elective I	**B. Pharmaceutical Chemistry**		
Course Code : 24PCHE12	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

UNIT- I Physical properties in Pharmaceuticals

Physical properties of drug molecule: physical properties. Refractive index- Definition, explanation, formula, importance, determination, specific & molar refraction. Optical activity\rotation- monochromatic & polychromatic light, optical activity, angle of rotation, specific rotation examples, measurement of optical activity. Dielectric constant & Induced Polarization- Dielectric constant explanation & determination. Rheology of pharmaceutical systems: Introduction, Definition, Applications, concept of viscosity, Newton's law of flow, Kinematic, Relative, Specific, Reduced & Intrinsic viscosity. Newtonian system, non-Newtonian system- Plastic flow, Pseudoplastic flow, Dilatent flow. Viscosity measurements- selection of viscometer for Newtonian and non-Newtonian system.

UNIT- II Isotopic Dilution analysis

Neutron activation analysis: Principle, advantages and limitations, Scintillation counters: Body scanning. Introduction to radiopharmaceuticals. Properties of various types of radiopharmaceuticals, Radiopharmaceuticals as diagnostics, as therapeutics, for research and sterilization. Physico Chemical Properties and drug action. Physico chemical properties of drugs (a) Partition coefficient, (b) solubility (c) surface activity, (d) degree of ionization.

UNIT- III Drug dosage and product development

Introduction to drug dosage Forms & Drug Delivery system – Definition of Common terms. Drug Regulation and control, pharmacopoeias formularies, sources of drug, drug nomenclature, routes of administration of drugs products, need for a dosage form, classification of dosage forms. Drug dosage and product development. Introduction to drug dosage Forms & Drug Delivery system – Definition of Common terms. Drug Regulation and control, pharmacopoeias formularies, sources of drug, drug nomenclature, routes of administration of drugs products, need for a dosage form, classification of dosage forms.

UNIT-IV Development of new drugs

Introduction, procedure followed in drug design, the research for lead compounds, molecular modification of lead compounds. Structure-Activity Relationship (SAR): Factors effecting bioactivity, resonance, inductive effect, isoterism, bioisosterism, spatial considerations, biological properties of simple functional groups, theories of drug activity, occupancy theory, rate theory, induced-fit theory,4.3 Quantitative structure activity relationship (QSAR): Development of QSAR, drug receptor interactions, the additivity of group contributions, physico-chemical

parameters, lipophilicity parameters, electronic parameter, ionization constants, steric parameters, chelation parameters, redox potential, indicator-variables

UNIT-V Computers in Pharmaceutical Chemistry

Need of computers for chemistry. Computers for Analytical Chemists-Introduction to computers: Organization of computers, CPU, Computer memory, I/O devices, information storage, software components. Application of computers in chemistry: Programming in high level language (C+) to handle various numerical methods in chemistry – least square fit, solution to simultaneous equations, interpolation, extrapolation, data smoothing, numerical differentiation and integrations.

Text books

1. Bahl and Tuli. *Essentials of Physical Chemistry*. S. Chand
2. C.V.S. Subramanyam. *Text Book of Physical Pharmaceutics*. Vallabh Prakashan. II Edition
3. G.R Chatwal. *Medicinal Chemistry (Organic Pharmaceutical Chemistry).* Himalaya Publishing House.
4. Hubert H. Willard. *Instrumental method of Analysis*. 7th edition.
5. Jayshree Ghosh. *Textbook of Pharmaceutical Chemistry*. S. Chand & Company Ltd.
6. Dr. S. Lakshmi. *Pharmaceutical Chemistry*. Sultan Chand & Sons.

Books for Reference

1. K.V. Raman. *Computers in chemistry* .Tata Mc.Graw-Hill, 1993.
2. S.K Pundir, Anshu Bansal, A Pragate Prakashan. *Computers for Chemists.* New Delhi: New age international (P) limited. 2nd edition.
3. Martins, Patrick J. Sinko, Lippincott. William and Wilkins. *Physical Pharmacy and Pharmaceutical Sciences*
4. S.J. Carter. *Cooper and Gunn's Tutorial Pharmacy*. CBS Publisher Ltd. 6th edition.
5. Allen Popvich and Ansel. *Ansels pharmaceutical Dosage forms and Drug Delivery System*. Indian edition. B.I. Publication Pvt. Ltd.

E-Learning Resource

1. https://www.ncbi.nlm.nih.gov/books/NBK482447/
2. https://training.seer.cancer.gov/treatment/chemotherapy/types.html

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	2	1	3	2	2	1	2	3	2	2
CO-2	3	3	1	2	1	3	2	1	3	2
CO-3	3	2	3	3	3	2	3	3	3	3
CO-4	3	3	3	3	3	3	3	3	3	3
CO-5	3	2	2	3	3	2	1	2	3	3
Ave.	2.8	2.2	2.4	2.6	2.4	2.2	2.2	2.4	2.8	2.6

Semester – I			
Skill Enhancement Course I	**Industrial Processes**		
Course Code : 24PCHSE1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

Objectives

- To learn the basic concepts and various processes in industries.
- To understand the importance of industrial waste management.
- To explain the corrosion control processes.

Course Outcomes

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	compare the uses of renewable and non-renewable energy resources	K4
CO 2	discuss the process of manufacturing different types of fuels	K3
CO 3	Demonstrate the various techniques involved in water treatment process	K4
CO 4	explain the corrosion inhibition by alloying	K5
CO 5	manage the waste emitted from different industries.	K6

Semester – I			
Skill Enhancement Course I Industrial Processes			
Course Code : 24PCHSE1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

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 Water and it's treatment

Water: Sources and impurities, Water quality parameters: Definition and significance of-color, odour, turbidity, pH, hardness, alkalinity, TDS, COD and BOD, flouride and arsenic. Municipal water treatment: primary treatment and disinfection (UV, Ozonation, break-point chlorination). Desalination of brackish water: Reverse Osmosis, Electrodialysis. Boiler troubles: Scale and sludge, Boiler corrosion, Caustic embrittlement, Priming &foaming. Treatment of boiler feed water: Internal treatment (phosphate, colloidal, sodium aluminate and calgon conditioning) and External treatment – Ion exchange demineralization and zeolite process.

UNIT-IV Alloys and Corrosion

Alloys – Introduction - General characteristics of Alloys – manufacture – purpose of alloying - the Iron-Carbon Alloys - Carbon steels - Types of alloys - Heat treatment of alloys (Hardening of steel and Annealing) – Steel - Alloy steel – Stainless steel – Cast iron – Brass – Bronze – Nichrome.

Corrosion – Definition - Rusting of iron - Chemical corrosion - electrochemical corrosion - Factors influencing corrosion - Atmospheric and soil corrosion - Corrosion control - Hot dipping (galvanizing and tanning), Electroplating and Anodizing.

UNIT-V Industrial Waste Management

Definition, Classification, sources and composition of solid, liquid and gaseous wastes, hazardous and non-hazardous wastes, special waste materials, Storage and transport of wastes, Transportation and collection systems, Management of wastes, minimization, reuse and recycling, waste utilization and materials recovery. Treatment of wastes: biological treatment, composting, anaerobic digestion, combustion, incineration and landfills, ultimate disposal – Radiochemical waste.

Text Books

1. P. C. Jain and Monica Jain. *A text book of Engineering Chemistry*. New Delhi: Dhanpat Rai Publishing Co (P) Ltd. 15th Edition.
2. S.S. Dara. *Text book of Engineering Chemistry*. Chand and Co, 2009.
3. Sharma B.K. *Industrial Chemistry*. Goel Publishing House.

Books for Reference

1. E.W.Berg. *Chemical Methods of Separations*. New Delhi: McGraw Hill. 1st Edition 1963., New York.
2. H. A. Strobel. *Chemical Instrumentation: A Systematic approach*. Addition Wesley Reading Mass. 2nd Edition 1973
3. R. L. Pecsok, L.D. Shields, T. Cavins and L. C. Mcwilliam. *Modern methods of chemical analysis.* New York: John Wiley &Sons, Inc. 2nd Edition 1976.

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	PO-2	PO-3	PO-4	PO-5	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5
CO-1	2	3	3	2	3	2	3	3	2	3
CO-2	3	3	2	3	3	3	3	2	3	2
CO-3	3	2	3	2	2	2	2	3	3	2
CO-4	3	2	2	2	3	2	3	2	3	3
CO-5	2	3	3	3	3	3	3	3	2	3
Ave.	2.6	2.6	2.6	2.4	2.8	2.4	2.8	2.6	2.6	2.6

Semester – II			
Core IV	**Inorganic Chemistry –II**		
Course Code : 24PCHC21	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Objectives

- To explain the biological redox systems.
- To discuss the synthesis, properties and structures of inorganic rings, chains, cages and clusters.
- To demonstrate the principle and applications of IR, Raman and Electronic spectroscopies.

Course Outcome

CO No.	Upon completion of this course, students will be able to	CL
CO 1	Understand the mechanisms of oxygen transfer in heme and non-heme protein	K2
CO 2	explain the energy sources of life using photosynthetic and non-photosynthetic processes	K5
CO 3	distinguish between Homocyclic and heterocyclic inorganic ring systems.	K4
CO 4	calculate STYX notation for boranes and carboranes and apply rules to prdict the structure of complexex	K3,K5
CO 5	interpret the charge transfer spectra in electronic spectroscopy	K5

Semester – II			
Core IV	**Inorganic Chemistry –II**		
Course Code : 24PCHC21	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit – I Bioinorganic Chemistry I

Micro and macronutrients - Oxygen carriers -Hemoglobin and myoglobin - Structure and oxygenation Bohr Effect - Cooperative effect - Binding of CO, NO, CN– to Myoglobin and Hemoglobin. Biological redox system: Cytochromes-Classification, cytochrome a, b and c. Cytochrome P-450. Non-heme oxygen carriers-Hemerythrin and hemocyanin. Iron-sulphur proteins - Rubredoxin and Ferredoxin - Blue copper protein - Iron storage and transport proteins: Transferrin, Hemosiderin, Ferritin and Siderophores.

Unit – II Bioinorganic Chemistry II

Enzymes – Zinc enzymes: Carboxypeptidase A, Carbonic anhydrase. Iron enzymes – catalase, peroxidase. Copper enzyme: Superoxide dismutase, Enzyme catalysis - Michelis - Menton equation - Effect of pH, temperature on enzyme reactions. Factors contributing to the efficiency of enzyme. Nitrogen fixation – *Invitro* and *Invivo* conditions. Photosynthesis: PS-I, PS-II– Structure and function of Chlorophyll.

Unit – III Inorganic chains, rings and cages

Chains – Chain catenation – Heterocatenation – Isopoly and heteropoly anions – Silicate minerals – Classification – Aluminosilicates –,Structural and bonding features of B-N, S-N and P-N compounds – Intercalation compounds.

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

Cages – Synthesis, properties and structure of boranes - styx notation - Structural features of closo, nido, arachano and klado boranes, heteroboranes, metalloboranes and carboranes, metallocarboranes, Structure of 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 $[Mo_6Cl_8]Cl_4$ – Chevrel phases – Zintl ions – mno rule.

Unit – V Spectroscopy I (IR, Raman & Mossbauer)

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.

Electronic Spectroscopy – Microstates, Term symbols, selection rules – Orgel (d^1 to d^4 & d^6 to d^9 complexes) and Tanabe-Sugano diagrams (d^6 complex) – Charge transfer spectra – Calculation of Dq, B for octahedral d^2 and d^8 systems ($[V(H_2O)_6]^{3+}$, Ni(II) complexes) – Nephelauxetic ratio

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 2009.
2. Shriver D.F, Atkins P.W, Langford C.H. *Inorganic chemistry*, ELBS, Oxford University Press. 1994.
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.. 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. Drago R.S. *Physical Methods in Inorganic Chemistry*. W.B.Saunders. 1977.
6. Ebsworth David E.A.V, Rankin Stephen Credock W.H. *Structural Methods in Inorganic Chemistry*. ELBS. IV edition 1988.
7. Hemant Kulsherstha, Ajay Taneja, *Upkar's CSIR-UGC NET/JRF/SET for Chemical Science*. Agra: Upkar Prakashan. Revised & Enlarged Edition. 2021.

E-Learning Resource

1. https://www.pdfdrive.com/instant-notes-in-inorganic-chemistry-the-instant-notes-chemistry-series-d162097454.html

2. https://www.pdfdrive.com/shriver-and-atkins-inorganic-chemistry-5th-edition-d161563417.html

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	3	2	2	1	2	2	2	2	3	1
CO-2	3	3	2	3	3	3	3	2	3	3
CO-3	2	2	2	2	2	2	2	2	2	2
CO-4	3	3	3	2	2	3	2	3	3	2
CO-5	3	3	3	3	3	3	3	3	3	3
Ave.	2.8	2.6	2.4	2.2	2.4	2.6	2.4	2.4	2.8	2.2

Semester – II			
Core V	**Organic Chemistry - II**		
Course Code : 24PCHC22	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Objectives

- To understand the mechanism involved in various types of organic reactions with evidences.
- To understand the applications of synthetically important reagents.
- To correlate the reactivity between aliphatic and aromatic compounds.

Course Outcome

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO1	organize the various methods of determination of reaction mechanism	K5
CO2	Discuss various rearrangements involved in organic chemistry	K3
CO 3	understand the mechanism of various types of organic reactions	K2
CO 4	predict the suitable reagents for the conversion of selective organic compounds and design new routes to synthesis organic compounds.	K3, K6
CO 5	isolate and determine the alkaloids and flavonoids	K3, K4

Semester – II			
Core V	**Organic Chemistry - II**		
Course Code :24PCHC22	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit – I Elimination and Free Radical Reactions

Elimination Reactions: E2, E1, and E1CB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination.

Free Radical Reactions: Long lived and short-lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radical reactions and free radical, reactions of radicals; polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent

Unit – II Molecular Rearrangements

Migration to electron deficient carbon – Wagner-Meerwein, Demjanov, Benzil-Benzilic acid and Dienone-Phenol rearrangements.

Migration to electron deficient nitrogen – Hofmann, Beckmann, Curtius and Lossen rearrangements.

Migration to electron deficient oxygen – Baeyer-Villiger oxidation and Dakin rearrangements.

Migration to electron rich carbon – Neber, Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements.

Aromatic rearrangements – Fries rearrangement and Hofmann-Martius rearrangement

Unit – III Methods of Determination of Reaction Mechanism

Reaction intermediates, Transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions: Hammond postulate.

Methods of determining mechanism: Kinetic methods of determination: Rate law – Primary and secondary isotope effect. Non-kinetic methods of determination: Testing and Trapping of intermediates, Isotopic labelling, Cross–over experiment, Product analysis and stereo chemical evidence.

Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, partial rate factor, substituent and reaction constants.

Unit – IV Reagents and Modern Synthetic Reactions

Lithium diisopropylamine (LDA), Azobisisobutyronitrile (AIBN), Sodium cyanoborohydride ($NaBH_3CN$), *meta*-Chloroperbenzoic acid (m-CPBA), Dimethyl aminiopyridine (DMAP), Triethylamine (TEA), Diethylazodicarboxylate (DEAD), *N*-bromosuccinimide (NBS), Trifluoroacetic acid (TFA), Phenyltrimethylammonium tribromide (PTAB), Diazomethane Diethyl maleate (DEM), Copper diacetylacetonate ($Cu(acac)_2$), $TiCl_3$, $NaIO_4$, Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC), Meisenheimer complex**.**

Suzuki coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction.

Unit – V Alkaloids and Flavonoids

Alkaloids: Introduction, occurrence, classification, isolation and functions of alkaloids. Classification, general methods of structural elucidation - Degradation studies - HEM, Emde and Von-Braun - Structural elucidation of Piperine, 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.

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. O.P. Agarwal. *Chemistry of Organic Natural Products Vol I*. Meerut: Krishna Prakashan Media (P) Ltd. 47th Edition 2017

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: Sp
7. inger and Business Media, LLC. Third edition 1994.

E-Learning Resoruce

1. https://sites.google.com/site/chemistryebookscollection02/home/organic-chemistry/organic
2. https://www.organic-chemistry.org/

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
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CO-1	2	3	2	3	3	3	3	2	2	3
CO-2	3	2	2	2	2	2	2	2	3	2
CO-3	3	2	2	2	2	2	2	2	3	2
CO-4	2	3	3	3	3	3	3	3	2	3
CO-5	3	3	3	3	3	3	3	3	3	3
Ave.	2.6	2.6	2.4	2.6	2.6	2.6	2.6	2.4	2.6	2.6

Semester – II			
Core VI	**Physical Chemistry – II**		
Course Code : 24PCHC23	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Objectives

- To understand the essential characteristics of wave functions and need for the quantum mechanics.
- To gain knowledge about the principles of surface chemistry and photochemistry.
- 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**	**CL**
CO 1	discuss the characteristics of wave functions and symmetry functions and the importance of quantum mechanical models of particle in a box and harmonic oscillator.	K3
CO 2	Apply the approximation methods to different atoms and find the dissociation energy and bond order for various molecules by applying Huckel molecular orbital theory.	K3, K4
CO 3	compare the different types of adsorption isotherm and elaborate the theories and concepts of homogeneous and heterogeneous catalysed reactions.	K3, K4
CO 4	develop the idea about the photophysical and photochemical processes and deduce the experimental techniques involved in photochemical processes.	K4, K6
CO 5	evaluate the vibrational spectroscopic techniques to diatomic and polyatomic molecules and differentiate the molecules whether they are IR active or Raman active.	K3, K5

Semester – II			
Core VI	**Physical Chemistry – II**		
Course Code : 24PCHC23	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit – I Quantum Chemistry – I

Wave particle duality, Uncertainty principle – Postulates of quantum mechanics - wave function, properties of wave function – Different types of operators – Position operator, linear momentum operator, angular momentum operator, kinetic energy operator and Hamiltonian operator – their nature and Hermitian operator - Eigen functions and Eigen values - Orthogonality and Normalization Theorems - Schrodinger Wave equation (Time dependent and Time independent) - Setting up and solution of Schrodinger equations and interpretation with regard to particle in a box 1-D and 3-D box - Harmonic Oscillator: wave equation and solution, anharmonicity, force constant.

Unit – II Quantum Chemistry – II

Hydrogen atom and hydrogen like ions, Hamiltonian-wave equation and solutions, radial and angular functions, representation of radial distribution functions - 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 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 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 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.

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. Puri B.R, Sharma L.R, Madan S. Pathania. *Principles of Physical Chemistry*. Jalandhar: Vishal Publishing Co. 48th Edition 2022.
6. 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.
7. Barrow G M. *Introduction to Molecular Spectroscopy*. New York: McGraw Hill. 1964.

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	2	2	2	2	2	2	3	2	2	2
CO-2	3	2	2	3	2	2	2	2	2	3
CO-3	2	3	2	2	2	3	2	2	2	2
CO-4	3	3	3	3	3	3	3	3	3	3
CO-5	3	3	3	3	2	3	3	3	2	3
Ave.	2.6	2.6	2.4	2.6	2.2	2.6	2.6	2.4	2.2	2.6

SEMESTER – I & II			
Core Practical II	**Organic Chemistry Practicals - I**		
Course Code : 24PCHCR2	**Hrs / Week : 3**	**Hrs / Sem : 60**	**Credits : 4**

Objectives

- To understand the concept of preparation of organic compounds.
- To develop analytical skill in the handling of chemical reagents.
- To construct suitable experimental setup for the organic preparations involving two stages.
- To experiment different purification and drying techniques for the compound processing.

Course Outcomes

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	formulate a method of estimation of organic compounds	K3
CO 2	analyze the purity of the organic compounds	K3, K4
CO 3	Understand mechanism involved in estimation and preparation of organic compounds	K2
CO 4	design suitable procedure for organic preparations.	K4, K6
CO 5	develop strategies to prepare organic compounds	K3, K5

SEMESTER – I & II			
Core Practical II	**Organic Chemistry Practicals - I**		
Course Code : 24PCHCR2	**Hrs / Week : 3**	**Hrs / Sem : 60**	**Credits : 4**

1. Quantitative Analysis

i) Estimation of ethyl methyl ketone (Iodimetry)

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 (Bromination)

viii) Estimation of aniline. (Bromination)

ix) Estimation of Glycine (Acidimetry)

x) Estimation of Formalin (Iodimetry)

xi) Estimation of Acetyl group in ester (Alkalimetry)

xii) Analysis of purity of Glucose

xiii) 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 phthalimide from Phthalic acid

3. Course work

i) Estimation of Ascorbic acid (Iodimetry)

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.5th 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.

Semester – II			
Core Practical III	**Physical Chemistry Practicals - I**		
Code : 24PCHCR3	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Objectives

- To scientifically plan and perform all the experiments.
- To understand the principle of conductivity experiments through conductometric titrations.
- To determine saturation point diagram of two component system forming congruent melting solid and find its eutectic temperatures and compositions.

Course Outcomes

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	recall the principles associated with various physical chemistry experiments	K1
CO 2	determine the solubility product and dissociation constant using conductometry	K3
CO 3	observe and record systematically the readings in all the experiments.	K1, K2
CO 4	calculate and process the experimentally measured values and compare with graphical data.	K3
CO 5	interpret the experimental data scientifically to improve students' efficiency for societal developments.	K4, K5

Semester – II			
Core Practical III	**Physical Chemistry Practicals - I**		
Code : 24PCHCR3	**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

1. Distribution of Benzoic acid between Toluene and Water.

III Thermometry

Determination of solution enthalpy

- i) Ammonium oxalate – Water
- ii) Naphthalene – Toluene

Books for Reference

1. Viswanathan.B, Raghavan.P.S. *Practical Physical Chemistry*. Viva Books Pvt. Ltd. 2005.
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.
4. Peter Mathews.G. *Experimental Physical Chemistry*. Clarendan Press Oxford, 1985.

Semester – II			
Elective II	**A. Nanoscience and Nanotechnology**		
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.
- To assimilate existing and new concepts, methodology and researches and apply them in their academic research environment

Course Outcomes

CO No.	Upon completion of this course, students will be able to	CL
CO 1	recall a thorough knowledge of basic underline disciplines of nanoscience and nanotechnology	K1
CO 2	synthesize the nanomaterials by physical, chemical and biological methods and determine the properties of nanomaterials	K3, K4
CO 3	Characterize and examine the synthesized nanomaterials by various techniques.	K4, K5
CO 4	analyze the types and properties of carbon nanotubes	K4
CO 5	apply the nanomaterials in energy storage, food and in day-to-day life.	K3

Semester – II			
Elective II	**A. Nanoscience and Nanotechnology**		
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 of Nanoparticles

Synthesis of nanomaterials - Top down and Bottom up approach - Physical methods: Arc discharge method, Laser Ablation, Evaporation, Sputtering and Inert gas condensation, Microwave assisted synthesis - Chemical methods: Thermolysis (solvothermal and hydrothermal), Sonochemical approach, Sol-gel and electrochemical syntheses – Biosynthesis of nanomaterials.

Unit - III Characterization and Techniques

Structural characterization of nanomaterials - X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM), Transition Electron Microscopy (TEM), X-ray Photo Electron Spectroscopy (XPES) and Atomic force microscopy (AFM): Principle, instrumentation and applications.

Unit - IV Carbon nanotubes

Carbon nanotubes - Carbon allotropes (Diamond, Graphite, Carbon nanotubes) - Types of Carbon nanotubes - Synthesis of carbon nanotubes, metal and metal oxides - 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 - V Nanocomposites and Applications of Nanotechnology

Nanocomposites: Metal-, ceramic- and polymer-matrix composites - Applications.

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).

Text Book

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.

Books for Reference

1. Bandyopadhyay A.K. *Nano Materials*. New Age International Publishers, 2nd Edition 2012.
2. Viswanathan B. Nano Materials. *New Delhi:* Narosa Publishing House. 2013.
3. Khanna O.P. *A Text Book of Nanochemistry*. New Delhi: Astha Publishers & Distributors. 2014.
4. Guozhong Cao. *Nanostructures & Nanomaterials: Synthesis, Properties & Applications*. Imperial College Press. 2004.

E-Learning Resource

1. http://xrayweb.chem.ou.edu/notes/symmetry.html.
2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf.

Relation matrix – specimen table

Course Outcomes	Programme Outcomes (PO)					Programme Specific Outcomes (PSO)				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	2	2	2	1	1	2	1	2	2	1
CO-2	3	3	3	3	3	3	3	3	3	3
CO-3	3	3	3	3	3	3	3	3	3	3
CO-4	2	3	2	2	2	3	2	2	2	2
CO-5	3	3	3	3	3	3	3	3	3	3
Ave.	2.6	2.8	2.6	2.4	2.4	2.8	2.4	2.6	2.6	2.4

Semester – II			
Elective II	**B. Medicinal Chemistry**		
Course Code : 21PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Objectives

- To study the chemistry behind the development of pharmaceutical materials.
- To gain knowledge on mechanism and action of drugs.
- To understand the need of antibiotics and usage of drugs.
- To familiarize with the mode of action of diabetic agents and treatment of diabetes.
- To identify and apply the action of various antibiotics.

Course Outcomes

CO No.	Upon completion of this course, students will be able to	CL
CO 1	predict the drug properties based on its structure.	K3
CO 2	describe the factors that affect its absorption, distribution, metabolism and excretion, and hence the considerations to be made in drug design.	K3, K4
CO 3	explain the relationship between drug's chemical structure and its therapeutic properties.	K5
CO 4	design to give the knowledge of different theories of drug actions at molecular level.	K6
CO 5	identify the different targets for the development of new drugs for the treatment of infection us and GIT.	K4

Semester – II			
Elective II	**B. Medicinal Chemistry**		
Course Code : 21PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

UNIT-I Introduction to receptors

Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action.

UNIT-II Antibiotics

Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicllins and tetracyclins, clinical application of penicillins, cephalosporin. Current trends in antibiotic therapy.

UNIT-III Antihypertensive agents and diuretics

Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol.

Classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

UNIT-IV Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer - Introduction of carcinolytic antibiotics and mitotic inhibitors - Synthesis of mechlorethamine, cyclophosphamide, melphalan, and uracil - Recent development in cancer chemotherapy.

UNIT-V Analgesics, Anti-inflammatoryand Anti-inflammatory Drugs

Introduction, Mechanism of inflammation, classification and mechanism of action and paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine. Medicinal Chemistry of Antidiabetic Agents Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, Mechanism of action, Treatment of diabetic mellitus. Chemistry of insulin, sulfonyl urea.

Text Books

1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry,
2. Wilson, Charles Owens: Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011.

3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5th edition, Oxford University Press, 2013. Jayashree Ghosh, A text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, 1999,1999 edition.
4. O. LeRoy, Natural and synthetic organic medicinal compounds, Ealemi, 1976.
5. S. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993, New edition.

Books for Reference

1. ,Lipincott Williams. *Foye's Princles of Medicinal Chemistry*. 7th Edition, 2012
2. Donald J. Abraham, David P. Rotella, Alfred Burger. *Burger's Medicinal Chemistry, Drug Discovery and Development*. Academic press, 2010.
3. John M. Beale Jr and John M. Block, Wolters Kluwer. *Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry*. , 12th Edition, 2011.
4. P. Parimoo, *A Textbook of Medical Chemistry,* New Delhi: CBS Publishers.1995.
5. Ramakrishnan, K. G. Prasannan and R. Rajan, *Textbook of Medical Biochemistry,* Hyderabad: Orient Longman. 3rd edition, 2001.

E-Learning Resource

1. https://www.ncbi.nlm.nih.gov/books/NBK482447/
2. https://training.seer.cancer.gov/treatment/chemotherapy/types.html
3. https://www.classcentral.com/course/swayam-medicinal-chemistry-12908

Relation matrix – specimen table

Course Outcomes	**Programme Outcomes (PO)**					**Programme Specific Outcomes (PSO)**				
	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PSO-1**	**PSO-2**	**PSO-3**	**PSO-4**	**PSO-5**
CO-1	3	3	3	3	3	3	3	3	3	3
CO-2	2	2	1	2	2	2	2	1	2	2
CO-3	3	2	2	2	2	2	2	2	3	2
CO-4	2	3	3	3	3	3	3	3	2	3
CO-5	3	3	3	3	3	3	3	3	3	3
Ave.	2.6	2.6	2.4	2.6	2.6	2.6	2.6	2.4	2.6	2.6

Semester – II			
Skill Enhancement Course II	**Computational Chemistry**		
Course Code : 24PCHSE2	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

Objectives

- To impart skills on use of various chemistry tools that are essential for any student with chemistry as a major.
- To learn the techniques of molecular simulations which will enhance the students' employability in academia and industry.

Course Outcomes

CO No.	**Upon completion of this course, students will be able to**	**CL**
CO 1	recall the basics of computational methods and molecular docking.	K1
CO 2	sketch the complicated structures using Chemsketch and Chemdraw	K3
CO 3	determine the physical parameters using softwares	K4
CO 4	calculate and process the experimentally measured values and compare with theoretical data.	K3
CO 5	interpret the experimental data scientifically to improve students' efficiency for societal developments.	K4, K5

Semester – II			
Skill Enhancement Course II	**Computational Chemistry**		
Course Code : 24PCHSE2	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 3**

Drawing of organic compounds and determination of physical parameters

Basic idea of Molecular Docking – A brief introduction about computational methods and their applications chemistry - Basic terminologies used in computational methods (relevant to the exercises given in UNIT II). Computing software - introduction and stepwise approach to **Chemdraw**, **ACD/Chemsketch**, **Argus Lab**, **AVOGADRO**, **Molinspiration**, **preADMET**, **SwissADME**, **SwissDock**, **1-Click online server**, **Autodock** and **Crystal Explorer**.

Lectures include entire process of downloading and installation of the software.

The experiments are related to the topics covered in B.Sc. – M.Sc. Chemistry courses. The students must do the following exercises depending on the availability of time and suitable computational chemistry software.

A. Drawing the structures of organic molecules and reaction schemes using **Chemdraw** or **ACD/Chemsketch**.

B. For the following experiments, **Argus Lab** or **ACD/Chemsketch** or **Avogadro Molecular Editor** or **Gaussian software** can be used. Minimum of six experiments is required to be carried out in this section.

1. Geometry optimization and single point energy calculations of simple organic molecules.
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualisation of molecular orbitals.
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis.
5. Calculation of Resonance energy of aromatic compounds.
6. Prediction of the stability of *ortho, meta* and *para* products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in of organic molecules.
8. Calculation of dimerization energy of carboxylic acids.
9. Perform the conformational analysis of butane using potential energy scan.
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.

14. Calculation of pK_a of simple organic molecules and compare it with experimental values.

15. Calculation of electrophilicity index in hard-soft acids and bases.

C. Prediction of molecular properties, bioactivity and molecular docking of drug molecules.

1. Calculation of molecular properties and bioactivity of the simple drug molecules like aspirin, paracetamol and the drugs of your choice using the online server **Molinspiration.**

2. Prediction of drug likeliness, ADME and Toxicity of the drug classes like antibiotics, antihistamines, anesthetics and drug molecules of your choice using the online servers **preADMET** or **SwissADME** or **SwissDock.**

3. Perform molecular docking of your choice using **1-Click online server** tool at mcule.com. Website: **https://mcule.com/**. First register at the site and perform molecular docking. Similarly, Autodock tools or Autodock Vina or Argus Lab can be used for molecular docking.

D. Learn to generate Hirshfeld surfaces, study the interaction energies and draw the electrostatic potential map using **Crystal Explore** software.

Links for Downloading Softwares

ACD/Chemsketch: https://www.acdlabs.com/resources/ freeware/chemsketch /index.php

Molinspiration: https://www.molinspiration.com/

PreADMET: https://preadmet.bmdrc.kr/

SwissADME: https://www.swissadme.ch/index.php

Crystal Explorer: https://crystalexplorer.scb.uwa.edu.au/

1-Click docking online server: https://mcule.com/

Autodock Tools: https://mgltools.scripps.edu/downloads

Autodock Vina: https://vina.scripps.edu/

Discovery Studio Visualizer: https://www.3dsbiovia.com/product/co.

Avogadro Molecular Editor: https://avogadro.cc/

Argus Lab: https://www.arguslab.com/ArgusLab.html

Text Books

1. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edition, Springer, New York, 2011.

2. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.

Books for Reference

1. Jan H. Jensen, Molecular Modelling Basics, CRC Press, 2010

2. Waren J. Hehre, Alen J.Shurterman, Janet E. Nelson, The Molecular Modelling Workbook for Organic Chemistry, Wavefunction Inc., 1998.

3. James B. Foresman, Eleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., Third Edition, 2015.

4. Donald W. Rogers, Heats of Hydrogenations: Experimental and Computational Hydrogen Thermochemistry of Organic Compounds, World Scientific Publishing Co., 2006.