PG DEPARTMENT OF CHEMISTRY

M.Sc., Chemistry

CHOICE BASED CREDIT SYSTEM (CBCS)

&

LEARNING OUTCOMES BASED CURRICULUM FRAMEWORK (LOCF)

Batch 2023-2025

PROGRAMME OUTCOMES (PO)

After completion of the programme, the student will be able to

PO1	To identify and analyze the complex problem searching substantiated conclusions domain knowledge
PO2	To apply investigative research , specialize in problem identification , formulate research design , utilize analytical tools , draw valid inferences and provide suggestions leading to nation building initiatives .
PO3	To strengthen professional ethics and career planning with systematic building of intrapersonal and interpersonal skills to participate in the intellectual diasporas .
PO4	To establish oneself as a self - reliant, empowered individual for an inclusive , healthy and compassionate understanding towards life and society .
PO5	To equip with technical / managerial expertise to innovate and critically analyze various attributes which constitute pivotal issues in a multidisciplinary scenario .
PO6	To emerge as innovators and pioneers to create new avenues of employment catering to the global trends as well as demands

PROGRAMME SPECIFIC OUTCOMES (PSO)

The students at the time of graduation will

PSO1	Build up a broad knowledge, understanding of advanced concepts and execute critical thinking in different areas of Chemistry and also in interdisciplinary fields.
PSO2	Enhance skills in handling scientific instruments, and interpret analytical data for structure elucidation using characterization techniques.
PSO3	Execute professional skills as chemists, entrepreneurs or in higher education with the available opportunities in the field of research and Industries.

SEM	PART	COURSE TYPE	COURSE CODE	COURSE TITLE	CREDITS	HRS	CIA	ESE	TOTAL
I	I	Core Theory I	22PCHCT1001	Basic Principles of Organic Chemistry	4	90	40	60	100
		Core Theory II	22PCHCT1002	Structural Inorganic Chemistry and Photochemistry	4	90	40	60	100
		Core Theory III	22PCHCT1003	Chemical Kinetics and Thermodynamics	4	90	40	60	100
		Elective Theory I	22PCHET1001	Analytical Techniques in Chemistry	3	75	40	60	100
		Core Practical I	22PCHCP1001	Inorganic Chemistry Practical I	4	90	40	60	100
	II	Skill Based Elective	22PSSCS1001	Cyber Security	3		50	---	100
				Total	**22**				**600**
II	I	Core Theory IV	22PCHCT2004	Organic Reaction Intermediates and its Mechanism	4	90	40	60	100
		Core Theory V	22PCHCT2005	Co-ordination Chemistry: Bonding, Reaction and Spectra	4	90	40	60	100
		Core Theory VI	22PCHCT2006	Group Theory and Quantum Chemistry	4	90	40	60	100
		Core Practical II	22PCHCP2002	Organic Chemistry-Practical	4	90	40	60	100
		Elective Theory II	22PCHET2002	Heterocyclics and Natural Products	3	75	40	60	100
	II	Soft skill	18MOOC2002	SWAYAM (MOOC)	4		50	---	100
				Total	**23**				**600**
III	I	Core Theory VII	22PCHCT3007	Retro synthetic Analysis and Pericyclic Reactions	4	90	40	60	100
		Core Theory VIII	22PCHCT3008	Molecular Spectroscopy and its Applications	4	90	40	60	100
		Core Theory IX	22PCHCT3009	Electro and Computational Chemistry	4	90	40	60	100
		Core Practical III	22PCHCP3003	Physical Chemistry Practical	4	90	40	60	100
		Elective Theory III classroom/Coursera	24PCHET3A03/ 24PCHET3B03	Green Chemistry and Sustainable Development/ Drug Chemistry	3	75	40	60	100
	II	Skill Based Elective	18PSSRS3003	Research Skills	3		50	---	100
	II	Internship	17PCSIP3001	Internship	2		40	60	100
				Total	**24**				**700**

IV	I	Core Theory X	22PCHCT4010	Advanced Inorganic Chemistry	4	90	40	60	100
		Elective Theory IV	24PCHET4A04/ 24PCHET4B04	Research Methodology/ Introduction to Sustainability	3	75	40	60	100
		Elective Theory V	24PCHET4A05/ 24PCHET4B05	Introduction to material science/ Nanotechnology: A Maker's Course	3	75	40	60	100
		Core Practical IV	23PCHCP4004	Inorganic Chemistry Practical II	4	90	40	60	100
		Core Project I	20PCHPR4001	Project	4		40	60	100
		Soft Skill	23PSECR4004	Skill Enhancement –Course era	4		50		100
				Total	**22**				**600**
				Grand Total	**91**				**2500**

SEMESTER I

Basic Principles of Organic Chemistry

Course code: 22PCHCT1001 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Describe the concepts of aromaticity and various types of aromaticity.
2. Explain basic concepts in stereochemistry and conformational analysis of organic molecules.
3. In addition, mechanisms of some of the important rearrangements in organic chemistry will be discussed.

Syllabus

UNIT – I **Aromaticity** **18 Hrs**

Concept of aromaticity,Types – Huckel and Craig's rule, Benzenoid, non-benzenoid, homo (Five, Six, seven and eight, membered rings), hetero(furan, thiophene and pyrrole), annulenes, ferrocene, cyclic carbocations and carbanions and anti- aromatic systems. Frost circle diagram for cyclobutadiene, benzene and cyclooctatetraene.

UNIT – II **Methods of determining Reaction mechanism** **18 Hrs**

Kinetic and non-kinetic methods of determining reaction mechanisms. .. Thermodynamic and kinetic aspects-spectroscopic studies- Hammond's postulate- Effect of structure on reactivity, resonance and field effect, steric effect quantitative treatment, isotope effects- linear free

energy relationship-Hammett equation .– energy profile diagrams – intermediate vs transition state – product analysis and its importance – crossover experiments and Taft equation.

UNIT – III: Stereochemistry 18 Hrs

Chirality, conditions for optical activity, optical purity. Absolute configuration-D/L and R/S notation in acyclic chiral molecules, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature. Dissymmetry of allenes, biphenyls and trans-cyclooctene, ansa and cyclophanic compounds, and spiranes. Stereospecific and Stereoselective reactions.Inter conversion of Sawhorse, Newman and Fischer projections. Topicity of ligands and faces .Cram's rule. Identification of enantiotopic, homotopic, diastereotopic hydrogen and prochiral carbon in compounds- prochiral carbon (up to 10 carbons only) - pro R and pro S & Re and Si face.

Geometrical isomerism: E, Z nomenclature of olefins. Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutene and cyclopentanes.

UNIT – IV Conformational analysis 18 Hrs

Conformation of some simple, 1, 2-disubstituted ethane derivatives. Conformational analysis of disubstitutedcyclohexanes and their stereo chemical features [cis, trans and optical isomerism (if shown) by these derivatives]. Conformation and reactivity of substituted cyclohexanols (oxidation), cyclohexanones (reduction involving selectrides) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis).Conformational analysis of cyclohexenes. Conformation and stereochemistry of cis and trans decalin and 9-methyl decalin.

UNIT – V Molecular rearrangements 18 Hrs

A detailed study of the mechanism of the following rearrangements with suitable examples Pinacol-Pinacolone (examples other than tetramethylethylene glycol) - Wagner- Meerwein, Demjanov, dienone-phenol, Favorski,Baeyer-Villiger, Cope, Claisen, Stevens, Sommelet-Hauser (in cyclic systems also) and Von Richter rearrangements.

Text Books:

1. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3rdEdition, New age International publisher, 2018.
2. P.S. Kalsi, Organic Reactions Stereochemistry and Mechanism Through Solved problems, 5thEdition,New Age International publisher, 2006.
3. N.Tewari, Advanced Organic stereochemistry, 2ndEdition, Books & Allied Ltd, 2017.
4. V.K. Ahluwalia & Rakesh K. Parashar, Organic Reaction Mechanism, 5thEdition,Narosa Publishing House,2024.
5. F. A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part-B, 5thEdition, Plenum Press., New York, 2008.

Book for References

1. Jagdamba Singh, L.D.S. Yadav,Jaya Singh,Santosh Singh, Stereochemistry with Applications to Organic Reactions, 2ndEdition, New Age International Publisher, 2023.
2. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 8thEdition, 2021.
3. Paula Yurkanis Bruice, Organic Chemistry, 8thEdition,Pearson, 2020.
4. Basic Stereochemistry of Organic Molecules, Subrata Sen Gupta, Oxford University Press; 2ndEdition, 2018.
5. J. Clayden, N. Geeves and S. Warren,Organic Chemistry, 2ndEdition,Oxford University Press, 2021.

E-Learning Resources

1. https://courses.lumenlearning.com/suny-potsdam-organicchemistry2/chapter/13-4-aromaticity/
2. http://epgp.inflibnet.ac.in/epgpdata/uploads/epgp_content/chemistry/05.organic_chemistry-i/05._methods_of_determining_mechanisms_and_isotope_effects_/et/7422_et_et.pdf
3. https://personal.utdallas.edu/~scortes/ochem/OChem1_Lecture/Class_Materials/09_stereo_notes.pdf
4. https://personal.utdallas.edu/~biewerm/8-conformational.pdf

5. https://nptel.ac.in/content/storage2/courses/104101005/downloads/LectureNotes/chapter%2011.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Recognize and distinguish Aromatic, Anti-aromatic and non-aromatic compounds.	**K1–K3 (Understand and Apply)**
CO2	Analyze the various methods of determining reaction mechanism.	**K1 - K4 (Understand, Apply and Analyze)**
CO3	**U**nderstand the details of various aspects of Stereo Chemistry and identify stereochemical notations.	**K1 - K5 (Understand, Apply, Analyze and evaluate)**
CO4	Acquire knowledge on conformations and reactivity.	**K1 - K5 (Understand, Apply, Analyze and evaluate))**
CO5	Understand **t**he chemistry of various types of Molecular rearrangement reactions.	**K1 - K4 (Understand, Apply and Analyze)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	1	2	1	2	2	2	3
CO2	3	3	3	3	3	2	3	1	3
CO3	3	3	3	3	3	3	3	2	3
CO4	3	3	2	3	2	3	3	1	3
CO5	3	3	2	3	2	3	3	1	2
Avg.	2.8	2.8	2.2	2.8	2.2	2.6	2.8	1.4	2.8

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk, LCD/SMART Boards, Student Assignments, Student Seminars/Webinars, MCQ, Quizzes, NPTEL/Others - Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER I

Structural Inorganic Chemistry and Photochemistry

Course code: 22PCHCT1002 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Principles concerning solid-state structures, bonding in solids and various synthesis methods and properties of solids.
2. Chemistry of main group elements, structure and properties of few main group compounds.
3. Basics of photochemical reactions of various inorganic compounds.

Syllabus

UNIT – I **Solid state Chemistry** **18 Hrs**

Preparation Methods: Ceramic method – Sol-gel method – Hydrothermal synthesis –chemical vapour deposition: Structure of solids - Imperfections in solids-point defects, line defects and plane defects, non-stoichometric compounds. Structure of compounds of AX (Zinc blende, Wurtzite), AX2 (Rutile,), AmX2 (Nickel Arsenide), ABX3 (Perosvskite). Spinels. Inverse spinel structures.

Reactions in solid state and phase transitions, diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, formation of spinels. Solid solutions: Order-disorder transformations and super structure.

UNIT – II **Properties of Solids** **18 Hrs**

Band Theory, semiconductor and conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Types of Magnetic Behaviour - Dia, Para, Ferro, Antiferro and Ferrimagnetism, Hysterisis, Mobility of charge carriers. Magnetic properties of Ferrites and garnets.

Super conductivity-Type I and Type II superconductors, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates – YBaCu oxide system, Meisner effect, high temperature superconductors.

UNIT – III **Inorganic Chains and Rings** **18 Hrs**

Chains – Silicate minerals. Structure of silicates-common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Zeolites-synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W.

Rings-topological approach to boron hydrides, Styx numbers. Structure and bonding in borazines and ring silicates, phosphorous-nitrogen compounds, phosphazenes.

UNIT – IV **Inorganic Cages and Metal Clusters** **18 Hrs**

Cages: synthesis, structure and bonding of Boron cage compounds-Wade’s rule, boranes, carboranes, metallacarboranes.

Metal clusters**:** dinuclear compounds of Re, metal-metal multiple bonding in (Re2X8)2-, trinuclear clusters, tetranuclear clusters, hexanuclear clusters.

UNIT – V **Inorganic Photochemistry** **18 Hrs**

Principles of Inorganic Photochemistry – Photoredox reactions and photosubstitution reactions in coordination complexes with particular reference to Co (III), Cr (III) and Pt (II) complexes. Photosensitisation reactions of [Ru(bpy)3]2+ complex and its applications in solar energy conversions and DSSC's (Dye Sensitized Solar Cells).

Text Books

1. A.R. West, Solid-State Chemistry and its Applications, 2nd Edition,John Wiley and Sons,2022.
2. F.A.Cotton, G.Wilkinson and P.Gaus – Basic Inorganic Chemistry, 3rd Edition, John Wiley and Sons, 2021.
3. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, 5th Edition, Pearson Education, 2022.
4. B.Sivasankar, Inorganic Chemistry, 1st Edition, Pearson Education India, 2015.
5. Nicholas J. Turro V. Ramamurthy J. C. Scaiano, Principles of Molecular Photochemistry, Viva Books, 2019.

Book for References

1. Catherine E. Housecroft & Alan G. Sharpe, Inorganic Chemistry, 5th Edition, Pearson, 2018.
2. Mark Weller, Tina Overton, Jonathan Rourke and Fraser Armstrong, Inorganic Chemistry, 7th Edition, Oxford University Press, 2019.
3. Gary L. Miessler, Paul J. Fischer and Donald A. Tarr, Inorganic Chemistry, 5th Edition, Pearson, 2019.
4. Elaine A. Moore and Lesley E. Smart, Solid state Chemistry: An Introduction, 5th Edition, CRC Press, 2020.
5. Carol Ramsey, Photochemistry: A Conceptual Approach, 1st Edition, Wilford Press, 2022.

E-Learning Resources

1. https://www.sciencedirect.com/topics/chemistry/solid-state-chemistry
2. https://www.nature.com/subjects/organometallic-chemistry
3. https://onlinelibrary.wiley.com/doi/10.1002/0471718769.ch12

4. https://www.sciencedirect.com/bookseries/advances-in-inorganic-chemistry/vol/63/suppl/C
5. https://chemed.chem.purdue.edu/genchem/topicreview/bp/ch23/history.php

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Predict the structure, bonding and discuss the reaction of solids with emphasis on some of the most important classes of inorganic materials and also describe the importance and properties of defects in solids.	**K1–K3 (Understand and Apply)**
CO2	Analyze the physical-chemical, electrical and magnetic properties of solids.	**K1-K3 (Understand and Apply)**
CO3	Explain the chemistry of main group elements, and synthesis and properties of few main group compounds.	**K1-K4 (Understand, Apply, Analyze and Evaluate)**
CO4	Describe the various aspects of industrially relevant silicates, boranes, aluminosilicates and zeolites including their classification, structural understanding and able to elaborate their reactions.	**K1-K5 (Understand, Apply, Analyze and Evaluate)**
CO5	Explain what happens when inorganic compounds are excited by irradiation.	**K1-K4 (Understand and Apply)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3

CO1	3	2	2	2	3	2	3	2	2
CO2	3	3	2	2	2	3	3	2	3
CO3	3	2	2	3	2	3	3	3	3
CO4	3	3	2	2	3	3	3	3	2
CO5	3	2	3	3	3	3	3	2	3
Avg.	3	2.4	2.2	2.4	2.6	2.8	3	2.4	2.6

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Lecture, Group discussion, Power point presentation, Seminar, Context based learning

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER I

Chemical Kinetics and Thermodynamics

Course code: 22PCHCT1003 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Describe the reaction rates in the solution as well as in the catalytic surface
2. Examine the behaviour of ideal and real gases in solutions.
3. Attain the knowledge of statistical thermodynamics.

Syllabus

UNIT – I **Chemical Kinetics I** **18 Hrs**

Effect of Temperature on Reaction Rates: Collision Theory – Molecular Beams – Collision Cross section – Effectiveness of Collision – Probability Factor – Potential energy Surface – Transition State Theory –Activated Complex. Eyring Equation – Estimation of Free Energy, Enthalpy and Entropy of Activation and their Significance.

Kinetics of complex reaction: Reversible, Consecutive and Parallel Reactions.

Reactions in Solutions: Effect of Pressure, Dielectric Constant, Ironic Strength and Salt Effect- Kinetic Isotopic Effects – Linear free Energy Relationships – Hammett and Taft Equations.

Study of Fast Reactions: Relaxation Methods – Temperature and Pressure Jump – Stopped Flow and Flash Photolysis Methods.

UNIT – II **Chemical Kinetics II** **18 Hrs**

Catalysis by Enzymes: Rate of Enzyme Catalysed Reactions, Michael's – Menten Equation – Effect of Substrate concentration, PH & Temperature – Inhibition of Enzyme catalysed Reactions – Three Types with Mechanism.

Homogeneous and Heterogeneous catalysis: Acid Base Catalysis – Mechanisms and Bronsted catalysis Law. Heterogeneous Catalysis – Langmuir and BET Adsorption Isotherm – Kinetics of Heterogeneous catalysis – unimolecular reaction Lindemann Theory-Hinshelwood Theory.

Chain Reaction: General Treatment - Rice Herzfeld Mechanism – Decomposition of Acetaldehyde and Hydrobromination. Comparison of HCl & HBr formation and Explosion Limit.

UNIT – III **Thermodynamics of Ideal and Real Gases** **18 Hrs**

Thermodynamics of ideal gases: Partial Molar Properties –physical quantities – chemical potential – Gibbs Duhem equation - variation of chemical potential with temperature and pressure – Chemical Potential in a mixture of ideal gases – application of chemical potential- Nernst distribution law and Henry law- Partial molar volume and partial molar heat content – its significance.

Thermodynamics of real gases: Fugacity – definition –determination of fugacity (graphical method, approximate calculation method) – variation with pressure and temperature – mixture of gases – Duhem Margules equation. Concepts of activity and activity coefficient – variation of gas with temperature and pressure –Activity coefficient of solution-choice of standard free energies.

UNIT – IV **Irreversible Thermodynamics and Heat Capacity of Solids** **18 Hrs**

Irreversible Thermodynamics: Non-equilibrium processes – entropy production in irreversible processes – microscopic reversibility – linear flux and force and its relations – Onsager law – phenomenological equation.

Heat Capacity of Solids: Dulong and petit's law- quantum theory of specific heat (Einstein Theory) – Debye Theory – Ortho and para hydrogen.

UNIT – V Statistical Thermodynamics and partition Function 18 Hrs

Statistical Thermodynamics: Probability theorems in statistical thermodynamics – microstate and macrostate in phase space – concept of thermodynamic probability – distribution law – Maxwell Boltzmann, Fermi – Dirac and Bose – Einstein Statistics – Comparsion.

Partition Function: Parition function – physical significance – translational, rotational, vibrational partition function for ideal gases. Partition functions and thermodynamic functions – internal energy, entropy (Boltzmann Planck equation), work function – application of partition function to mono and diatomic gases molecule – internal energy and entropy – Sackur Tetrode equation.

Text Books

1. Peter Atkins, Physical Chemistry, 12thEdition, Oxford, 2022.
2. K L Kapoor, A Textbook of Physical Chemistry - Dynamics of Chemical Reactions, Statistical Thermodynamics, Macromolecules and Irreversible Processes| Volume 5, 4thEdition, McGraw Hill, 2020.
3. Andrew Cooksy, Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics, 1stEdition, Pearson Education,2018.
4. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Chemistry, 2ndEdition, New Age International Publishers, 2017.
5. Gurudeep Raj, Advanced Physical Chemistry, 4thEdition, Krishna Prakashan Media P. Ltd., 2016.

Books for References

1. Puri and Sharma, Principles of Physical Chemistry, 48thEdition, Vishal Publishing Co., 2023.

2. Katja Lindenberg, Ralf Metzler and Gleb Oshanin, Chemical Kinetics: Beyond The Textbook (import), 1st Edition, World Scientific, 2019.
3. M.Scott Shell, Thermodynamics and statistical Mechanics: Anintegrated Approach, 1stEdition, Cambridge University Press, 2015.
4. Stanley I Sandler, Chemical, Biochemical, and Engineering Thermodynamics, 5th Edition, Wiley, 2020.
5. Arun Bahl, Essential of Physical Chemistry, 28thEdition, S.Chand Publishers, 2022.

E-Learning Resources

1. https://www.mobt3ath.com/uplode/book/book-36973.pdf
2. http://www.colby.edu/chemistry/PChem/notes/ChainMech.pdf
3. http://www.colby.edu/chemistry/PChem/Lecture1.html
4. https://www3.nd.edu/~powers/ame.20231/notes.pdf
5. https://nptel.ac.in/courses/104103112/

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Familiarize with the theories of reaction rate and their utilization.	**K1 – K3 (Understand, Apply, Analyze)**
CO2	Implement the concept of kinetics in the homogeneous and heterogeneous catalysis.Relate the thermodynamic properties of the system and chemical composition	**K2 – K3(Apply, Analyze)**
CO3	Relate the thermodynamic properties of the system and chemical composition	**K1 – K3 (Understand, Apply, Analyze)**
CO4	Understand the interrelationship between the properties of equilibrium and non-equilibrium process in thermodynamics	**K2 – K3(Apply, Analyze)**
CO5	Apply statistics to understand the thermodynamic properties of macroscopic systems	**K3(Analyze)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	1	1	2	2	1	1	3	2	1
CO2	1	2	2	2	3	2	3	3	2
CO3	2	2	3	1	3	2	3	3	3
CO4	2	1	2	3	1	1	2	1	1
CO5	3	2	2	2	1	2	1	2	2
Avg.	1.8	1.6	2.2	2.0	1.8	1.6	2.4	2.2	1.8

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, ICT Tools, Student Seminar, Group activity, Presentation skills, NPTEL/ Mooc's courses

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER I

Analytical Techniques in Chemistry

Course code: 22PCHET1001 **Total Hours: 75**

Credits: 3 **L – T – P: 4-1-0**

Course Objectives

1. Achieve proficiency in applying a wide range of analytical methods and instrumentation to accurately analyze chemical samples and interpret experimental data.
2. Develop the ability to critically evaluate experimental procedures, troubleshoot analytical challenges, and propose effective solutions based on a comprehensive understanding of chemical principles.
3. Foster professionalism through effective communication, collaborative teamwork, and adherence to ethical standards and safety protocols in chemical analysis and research.

Syllabus

UNIT – I **Errors & Data Handling in Chemical Analysis** **15 Hrs**

Terms and definitions – Precision and Accuracy, Types of errors, Measures of central tendency, mean, standard deviation, and measures of variability. Normal Distribution curve, confidence

limit, systematic errors. Confidence intervals, statistical aids to hypothesis testing -t-test and F-test. Correlation coefficient, Rejection of data.

UNIT – II Electroanalytical Techniques 15 Hrs

Polarography- Principle - Theory,Instrumentation,equation for polarographic waves, types of currents, half-wave potential. dropping mercury electrode (advantages and limitations), polarographic diffusion current, the ilkovic equation. Qualitative and Quantitative applications to analysis of inorganic and organic compounds.

Conductometry and high frequency titrations - potentiometry, pH-metry and ion-selective electrodes - coulometry – voltammetry - amperometric titrations and Cyclic voltammetry - principle ,practice and applications.

UNIT – III Thermal and Radio Methods of analysis 15 Hrs

Principles - Instrumentation - factors affecting - applications of Thermo gravimetric and differential thermal analysis, thermometric titrations, and differential scanning colorimetry. Isotope dilution analysis, Neutron activation analysis, Radio immune assay-principle and applications.

UNIT – IV Spectral Methods of Analysis 15 Hrs

Atomic absorption spectroscopy: Theory, atomizers, flame, and electrothermal. radiation sources, instrumentation, spectral and chemical interferences, and application.

Photoelectron spectroscopy (UV and X-Ray)-photoelectron spectra-Koopman's theorem, fine structure in PES, chemical shift, and correlation with electronic charges.

Fluorimetry and Phosphometry - Introduction, theory, instrumentation, applications and comparison of fluorimetry & phosphorimetry (with and without Absorption methods).

Nephelometric and Turbidimetric methods - Introduction, Principles, Instrumentation and applications.

UNIT – V Separation Techniques 15 Hrs

Chromatography – classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. paper, column, TLC, GC, HPLC and

GPC techniques – ion exchange techniques – Capillary electrophoresis – principle, instrumentation and applications.

Text Books

1. Skoog D.A., West D.M., Holler F.J. and Crouch S.R., Fundamentals of Analytical Chemistry, 10thEdition, Cengage Learning India Pvt. Ltd., 2022.
2. Christian G.D., Analytical Chemistry, 10thEdition, John Wiley, 2020.
3. Willard H.H., Merritt L.L., Dean J.A. and Settle F.A., Instrumental Methods of Analysis, 7th Edition, CBS Publication, New Delhi Reprint, 2020
4. B.K.Sharma, Spectroscopy, 5thEdition, Goel publishing house,2015.
5. A.K. Srivastava, P.C.Jain, Instrumental approach to chemical analysis, S. Chand Company,2015.

Book for References

1. Kim Seng Chan, Jeanne Tan, Understanding Advanced Organic and Analytical Chemistry: The Learner's Approach (Revised Edition), 2ndEdition, World Scientific education, 2020.
2. F Rouessac, Chemical Analysis: Modern Instrumentation Methods and Techniques, 3rdEdition, Wiley, 2022.
3. R.Braun, Instrumental Analysis, 1stEdition, McGraw Hill, 2017.
4. Divya Sanganabhatla, Hand Book on Modern Analytical Techniques, 1stEdition, AkiNik Publications, 2024.
5. K. Pranusha, Lagu Surendra Babu and Nammi Usha Rani, Textbook Of Instrumental Methods Of Analysis: Principles And Techniques, 1stEdition, Notion Press, 2024.

E-Learning Resources

1. https://www.calstatela.edu/sites/default/files/dept/chem/06winter/201/pdf/lecture-3.pdf
2. https://www2.chemistry.msu.edu/courses/cem434/Granger%20Ch%2022.pdf
3. https://crimsonpublishers.com/mapp/pdf/MAPP.000509.pdf.
4. https://nptel.ac.in/content/storage2/courses/102103044/pdf/mod5.pdf.
5. https://sites.chem.colostate.edu/diverdi/C431/experiments/atomic%20absorption%20spectroscopy/references/Agilent%20-%20analytic%20methods.pdf.

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Apply statistical methods to ensure precision and accuracy in chemical analysis	**K1 – K4 (Remember, Understand, Apply, Analyze)**
CO2	Master electroanalytical techniques for critical analysis of chemical compounds	**K2 – K3 (Apply, Analyze)**
CO3	Integrate thermal and radio analytical methods to contribute to research and industry	**K1 – K3 (Understand, Apply, Analyze)**
CO4	Utilize spectral methods for structure elucidation, fostering professional skills and ethical practices	**K2 – K3 (Apply, Analyze)**
CO5	Innovate in chemical analysis through separation techniques, supporting career planning and entrepreneurship.	**K1 – K4 (Remember, Understand, Apply, Analyze)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	2	3	2	3	3	2
CO2	2	2	3	2	3	3	3	3	3
CO3	3	3	2	2	3	2	2	2	3
CO4	2	2	3	3	2	2	3	3	3
CO5	2	3	2	2	2	3	2	2	3
Avg.	2.4	2.4	2.4	2.2	2.6	2.4	2.6	2.6	2.8

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, ICT Tools, Student Seminar, Group activity, Presentation skills, NPTEL/ Mooc's courses

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER I

Inorganic Chemistry Practical-I

Course code: 22PCHCP1001 **Total Hours: 90**

Credits: 4 **L – T – P: 1-1-4**

Course Objectives

1. The course provides training and experimental practices in qualitative and quantitative analysis.
2. Develop skills to understand microscale analysis methods in inorganic analysis and their advantages.
3. To determine the concentration of a chemical element in a solution with the aid of a color reagent.

Syllabus

UNIT – I **18*3=54 Hrs**

Semi micro qualitative analysis of mixtures containing two common and two rare cations. The following rare cations are included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.

UNIT – II **Colorimetric analysis** **18*2=36 Hrs**

Spectrophotometric method: Estimation of iron, nickel, manganese and copper.

Reference Books:

1. Amita Dua, Navneet Manav, Practical Inorganic Chemistry, Manakin Press, 2017.
2. Jeyavathana Samuel, Chemistry Practical Book, G.G.Printers, Chennai, 2012.
3. Vickie. M .Williamson, M.Larry Peck, Lab manual for General Chemistry, Cengage Learning India Private Limited, New Delhi, 2009.
4. S. Mumtazuddin, Shailendra Kumar Sinha, Inorganic Lab Manual, Atlantic, 2009.
5. Vogel's "Textbook of Quantitative chemical Analysis", Pearson Education Ltd. Sixth Edition, 2008.
6. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.
7. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Publishing Company, Chennai, third edition,1974.

E-Learning resources:

- http://ncert.nic.in/ncerts/l/lelm107.pdf
- https://www.scribd.com/doc/8397989/Salt-Analysis-Chart
- https://study.com/academy/lesson/qualitative-analysis-of-inorganic-salts.html
- http://www.docbrown.info/page07/appendixtrans09.htm
- http://www.jbc.org/content/114/1/147.full.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Explain the qualitative analysis of a given salt mixture by semi micro method and know how to estimate the Inorganic cations.	**K1–K5 (Understand, Apply, Analyse and Evaluate)**
CO2	Apply the principles of common ion effect and solubility product in Semi micro qualitative analysis.	**K1– K4 (Understand,**

		Apply and Analyze)
CO3	Explain the quantitative determination and know how to estimate the metal Cations using the colorimetric method.	**K1– K3 (Understanding and Apply)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	3	2	2	1	3	3	2	3
CO2	2	3	2	2	2	3	3	1	2
CO3	3	3	2	2	2	3	3	3	3
Avg.	2.6	3	2	2	1.6	3	3	2	2.6

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, Student assignments, Viva MCQs, NPTEL/ Other add-on courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER II

Organic Reaction Intermediates and its Mechanism

Course code: 22PCHCT2004 **Total Hours: 90**

Credits: 4 **L – T – P: 5-1-0**

Course Objectives

1. To understand the importance of reaction intermediates.
2. To suggest mechanisms for a given reaction.
3. To understand the application of oxidation and reduction reactions**.**

Syllabus

UNIT – I **Reactive Intermediates** **18 Hrs**

Generation, Stability, Reactions and applications of Carbocations, Carbanions, Carbenes, Free radicals, Nitrenes, benzynes, ylides, Carbon Radicals, Arynes (Dimerisation Reactions) and enamines. Neighbouring Group Participation - Non-classical Carbonium ion.

UNIT – II Nucleophilic Substitution reactions 18 Hrs

Aliphatic Nucleophilic substitution-SN1, SN2 and SNi mechanism - Nucleophile and leaving groups Stereochemistry and Ion pairs. Reactivity, structural, solvent and steric effects. Substitution in the norbornyl system and at bridgehead carbon. Substitutions by ambident nucleophiles such as CN, NO2, phenoxide and dianion (EAA).Nucleophilic substitution - alkylation and acylation of amines, halogen exchange, Von-Braun reaction. Claisen and Dieckmann condensations.Vicarious Nucleophilic Substitution (VNS), Magic acids, George A-Olah reactions.Aromatic nucleophilic substitution Nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halides. Ziegler alkylation., Chichibabin reaction.

UNIT – III Electrophilic substitution reactions 18 Hrs

Arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups) of nitration, halogenation, alkylation, acylation and diazonium coupling. Formylation reactions - Gatterman, Gatterman-Koch, Vilsmeyer-Hack & Reimer-Tieman Reaction. Synthesis of di & tri substituted benzenes (symmetrical tribromobenzene, 2-amino5- methylphenol, 3-nitro-4-bromobenzoicacid, 3, 4-dibromonitrobenzene, 1, 2, 3 - trimethylbenzene) starting from benzene or any mono substituted benzene.

UNIT – IV Elimination and Addition Reactions 18 Hrs

Mechanisms: E2, E1, and E1cB mechanisms. Sterochemistry of E2 eliminations Syn eliminations - E1-E2-E1cB spectrum. Orientation of the double bond: Hoffmann and Saytzeff rules Reactivity: Effect of substrate, attacking bases, leaving group and medium. Mechanisms and orientation in Pyrolytic eliminations. Elimination reactions: Stereochemistry of eliminations in acyclic and cyclic systems. Examples- Chugaev reactions and Cope elimination, Hofmann degradation, pyrolysis of esters.

Nucleophilic addition to carbonyls and StereoChemical aspects -Crams rule- Prevost rule on addition reaction. Addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylene , hydroboration, Michael reactions. Witting, Peterson Olification. Alkylation and Acylation using Lithium enolates, hydrogenation of ethylene and acetylene Partial reduction.

Addition to double bonds-Simmon Smith reaction, Mannich, Knoevengal, Stobbe, Acyloin condensation. Julia olefination, Sharpio Darzen and Benzoin reactions.

UNIT – V Oxidation and reduction reactions 18 Hrs

Oxidation: Mechanism - study of the following oxidation reactions - oxidation with LTA, SeO2, DDQ, Oxalyl chloride, Dess-martin reagent DMSO in combination with DCC –Swern Oxidation with NCS, Hydroxylations with – OsO4, KMnO4, Woodward prevost, epoxidation (per oxides/per acids). Sharpless asymmetric epoxidation, asymmetry dihydroxylations, AD mix α and β, Reduction and Selectrides and Alanes.

Reductions: Synthetic importance of Clemensen and Wolf-Kishner reductions and its Modifications, Birch reduction, MPV reduction.

Text Books

1. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 8thEdition, 2021.
2. Organic Chemistry, J. Clayden, N. Geeves and S. Warren, Oxford University Press, 2ndEdition, 2021.
3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5thed., Kluwer Academic/Plenum Publishers, 2008
4. Kalsi P S, Organic reaction and their Mechanisms, 5thEdition, New Age International Publishers, 2020.
5. Ahluwalia V K, organic Reaction Mechanism, 5thEdition, Narosa, 2024.

Book of References

1. Nimai Tiwari, Advanced Organic reaction mechanism (Problems and Solutions), 5thEdition, Books and Allied Private Ltd.,2019.
2. William C Groutas and Athri D. Rathnayake, Organic Reaction Mechanisms, selected Problems and Solutions, 2ndEdition, CRC Press, 2023.
3. Maya Shankar Singh, Advanced Organic Chemistry – Reactions & Mechanism, 2ndEdition, Pearson, 2021.

4. Joshi G, Organic Synthesis (Reaction Mechanism and Reagents), MedTech Science Press, 2022.
5. Kalsi P S, Organic Reactions stereochemistry and Mechanism through Solved Problems, 6thEdition, New Age International Publishers, 2018.

E-Learning Resources

1. http :// www.liv.ac.uk/chemistry/links /reactions.html
2. http ://orgchem.chem..uconn.edu/namereact/named.html
3. www.gcocities.com/ chempen softwar4ee/reactions.html
4. www.virtlab.com
5. http://nptel.ac.in

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the preparation, structure, reactions and stereochemical aspects of reactive intermediates	K1–K5 (Understand and Apply)
CO2	Analyze the various types of aliphatic, aromatic, nucleophilic substitution reactions and its mechanism	K1 – K4 (Understand and Apply)
CO3	Learn the name reactions through electrophilic substitution and their reaction mechanisms	K1 - K4 (Understand, Apply and Analyze)
CO4	Know the mechanism and stereochemistry of addition and elimination reactions.	K1 - K5 (Understand, Apply, Analyze and evaluate)
CO5	Adequately learn the catalysts involved in oxidation and reduction reactions with their commercial applications.	K1 - K4 (Understand, Apply and Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	3	2	3	2	3	3	3
CO2	2	3	2	3	2	2	3	2	2
CO3	3	2	2	2	2	2	2	3	2
CO4	3	2	3	3	2	2	2	2	2
CO5	3	3	2	3	2	2	2	2	1
Avg.	2.6	2.4	2.4	2.6	2.2	2.0	2.4	2.4	2.0

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, LCD/SMART Boards, Student Assignments, Student Seminars/Webinars, MCQ, Quizzes, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER II

Co-ordination Chemistry: Bonding, Reaction and Spectra

Course code: 22PCHCT2005 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Learn the d- orbital degeneracy of the complexes in various theories.
2. Explore the reaction and kinetics of the complexes.
3. Understand and study the electronic aspects of the complexes and the IR stretching of different molecules.

Syllabus

UNIT – I **Bonding & Properties** **18 Hrs**

Werner Theory - Valence bond Theory (VBT) - Crystal field theory (CFT) – Crystal field splitting in octahedral, tetrahedral and square planar complexes - Crystal field stabilization energy and its applications magnetic properties- Weak and strong fields - Pairing energy -

Factors affecting the magnitude of crystal field splitting-Jahn-Teller theorem – Limitations of CFT. Comparsion of VBT and CFT for complexes.

Spectrochemical series - metal orbital overlap, Nephlelauxetic effect - Molecular orbital (MO) theory for octahedral complexes – theories of sigma and pi bonding – MO diagram of [Cr(CO)6], [Co(NH3)6] and [CoF6] . Types of pi-bonds-Effect of pi-bonding on crystal field splitting – Evidences for pi-bonding.

UNIT – II Kinetics and Reaction Mechanism I 18 Hrs

Stability of complexes: Thermodynamic stability – stepwise and overall stability constants – relationship – factors affecting the stability - Stability constants of complexes and their determination methods (job's method and spectrometric method).

Substitution reactions: General mechanism - Schemes of octahedral, tetrahedral and square planar complexes – Dissociative– Associative - Interchange and dissociation types - Linear free energy relationships- Acid and base hydrolysis reactions-Substitution reaction without M-L bond breaking - Racemisation and isomerisation.

UNIT – III Reaction Mechanism II 18 Hrs

Stereoisomerism of inorganic complexes – geometrical and optical isomerism.

Trans-effect: Theories of trans-effect, pi-bonding theory and polarization theory-Application of Trans effect-cis effect.

Redox reactions: Inner sphere mechanism - The role of bridging ligand - Outer sphere mechanism - Theoretical treatment of electron transfer – spinels and inverse spinels. Simple applications to bioinorganic chemistry.

UNIT – IV Electronic spectra of Complexes 18 Hrs

Quantum numbers of multi-electron atoms - Russell-Sanders coupling - L-S coupling and micro states – Ground state terms for d1 – d10 ions-Derivation of terms for p2, p3, d1 and d2 configurations - Hund's rules in the determination of lowest energy states - Selection rules for electronic transitions – Charge transfer transitions. Splitting of free ion terms in octahedral field

-correlation diagram - Orgel diagrams for d1 to d9 ions and Tanabe-Sugano diagrams for d2 and d3 ions.

UNIT – V Electronic Spectra of Complexes 18 Hrs

Selection rules for IR and Raman – structural elucidation of simple molecules like H2O, NO2, N2F2, ClF3, No -, ClO - - Group vibration-effect of coordination on ligand vibration – uses of group vibrations in the structural eludication of metal complexes of urea, cyanide, nitrate, sulphate, thiourea, thiocyanato- effect of isotopic substitution on the vibrational spectra of molecule – vibrational spectra of metal carbonyl.

Text Books

1. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, 5thEdition, Pearson Education, 2022.
2. J.D.Lee, *Concise Inorganic Chemistry*, 5thEdition, Oxford University Press, 2018.
3. Gary L. Miessler, Paul J. Fischer and Donald A. Tarr, Inorganic Chemistry, 5thEdition, Pearson, 2019.
4. F.A.Cotton, Geoffrey Wilkinson, C.A. Murillo and Manfred Bochmann, *Advanced Inorganic Chemistry*, *(*An Indian Adaptation), 1stEdition, Wiley, 2021.
5. Asim K. Das, Fundamental Concepts of Inorganic Chemistry, Volume 4, Including Coordination Chemistry, 2ndEdition,CBS Publishers and Distributors Pvt. Ltd.,2023.

Reference Books

1. Puri, Sharma and Kalia, Principles of Inorganic Chemistry, 34rdEdition, Vishal Publishing Co, 2024.
2. Birgit Weber, Coordination Chemistry: Basics and Current Trends, (import), 1st Edition, Springer Spektrum, 2023.
3. Russell Drago, Physical Methods for Chemists, 2ndEdition, Affiliated East West Press Pvt. Ltd., 2016.
4. Catherine E. Housecroft & Alan G. Sharpe, Inorganic Chemistry, 5thEdition, Pearson, 2018.
5. Ajai Kumar, Coordination Chemistry, 7th Edition, Aaryush Education, 2020.

E-Learning **Resources:**

1. https://www.nrcresearchpress.com/doi/pdfplus/10.1139/v92-089
2. http://webcache.googleusercontent.com/search?q=cache:http://chem.yonsei.ac.kr/chem/upl o ad/CHE3103-01/119265830654522.pdf
3. https://opentextbc.ca/chemistry/chapter/19-3-spectroscopic-and-magnetic-properties-of-coordination-compounds/
4. https://nptel.ac.in/courses/104105033/
5. https://www.adichemistry.com/inorganic/cochem/reactionmechanism/transeffect/trans-effect-1.html

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Apply Werner Theory, VBT, and CFT to analyze bonding in complexes	**K1 – K4 (Remember, Understand, Apply, Analyze)**
CO2	Evaluate stability and kinetics of complexes, understand substitution reactions	**K2 – K3 (Apply, Analyze)**
CO3	Analyze stereochemistry and reaction mechanisms in inorganic complexes	**K1 – K3 (Understand, Apply, Analyze)**
CO4	Interpret electronic spectra and quantum numbers of multi-electron atoms	**K2 – K3 (Apply, Analyze)**
CO5	Apply selection rules for IR and Raman spectroscopy in structural elucidation	**K1 – K4 (Remember, Understand, Apply, Analyze)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	2	2	3	2	3	3	2
CO2	2	3	2	2	3	3	2	3	3
CO3	3	2	3	2	2	2	3	2	3

CO4	2	3	3	3	2	2	3	3	2
CO5	2	2	2	2	3	3	2	3	3
Avg.	2.2	2.4	2.4	2.2	2.6	2.4	2.6	2.8	2.6

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, ICT Tools, Student Seminar, Group activity, Presentation skills, NPTEL/ Mooc's courses

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER II

GROUP THEORY AND QUANTUM CHEMISTRY

Course code: 22PCHCT2006 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. To learn the symmetrical orientation of molecules and its point groups
2. To understand the importance of group theory in spectroscopy
3. To identify the roots of quantum mechanics from classical mechanics.
4. To know the different aspects of quantum mechanics

Syllabus

UNIT – I **Basics Principles of Group Theory** **18 Hrs**

Molecular Symmetry: Symmetry elements and operations – rotation, reflection, inversion, proper and improper axes of rotations - Products of symmetry operations.

Symmetry Groups: Groups – concepts of groups, subgroups, classes, order, abelian and non-abliean groups and group multiplication table. Point groups – identification and determination – representation of groups (reducible and irreducible representations) – the direct product representation – the Great Orthogonality Theorem and its consequences – construction of Character table for C2v and C3v.

UNIT – II Applications of Group Theory 18 Hrs

Hybridisation: Symmetry of hybridisation of various non-linear molecules (CH4, XeF4, BF3, SF6, H2O and NH3).

Symmetry of Vibrational mode and electronic transistion: Determination of symmetry of vibrational modes in non – linear molecules (CH4, XeF4, BF3, SF6 and NH3). Symmetry selection rules for infrared, Raman and Electronic spectra – mutual exclusion principle. Electronic spectra of Ethylene and Formaldehyde.

UNIT – III Classical and Mathematical Formalism of Quantum Chemistry 18 Hrs

Inadequacy of classical theory: Black body radiation, Planck quantum hypothesis , photoelectric effect - the Compton effect - Bohr's Quantum theory and subsequent developments -wave particle duality- de Broglie equation, Heisenberg uncertainty principle.

Introductory concepts: Orthogonal functions – definition of expansion interval, inner product, normalization – odd and even function – expansion in terms of orthonormal functions.

Mathematical Formalism: Operators – algebra of Operators, Commutative property, linear operator, commutative operator, Hamiltonian, Eigenvalues and Eigenfunctions. Basic postulates of quantum Chemistry - The time-dependent Schrodinger wave equation.

UNIT – IV Simple Applications of Quantum Chemistry 18 Hrs

Translational motion of a particle: Schrodinger equation for a particle in a box (one, two and three dimensional cases).

Vibrational Motion of a particle: The harmonic oscillator – classical and quantum treatment – solution – wave function – energy – physical significance.

Rotational motion of a particle: Particle in a Ring - the rigid rotor- the hydrogen atom- the Schrodinger equation for hydrogen atom- angular momentum -the solution- the origin of quantum numbers and its significances.

UNIT – V Atomic structure and Theory of Chemical Bonding 18 Hrs

Approximation methods: perturbation and variation method – application to hydrogen and helium atoms – Slater orbital and HF –SCF methods.

Treatment of monatomic molecules: Born Oppenheimer Approximation – MOT and VBT – LCAO approximation, application for hydrogen molecule ion.

Chemical bonding in polyatomic molecules: Hybridisation – concept, wave equation (derive only for sp and sp2 hybridisation). Empirical Method: Huckel Molecular Orbital (HMO) Theory Huckel for conjugated molecules (ethylene and butadiene). Semi Empirical Methods – Valence electrons, Zero Differential Overlap (basic concept only).

Text Book

1. R.K.Prasad, Quantum Chemistry, 6th Revised Edition, New Age International Publishers, 2024.
2. K.Veera Reddy, Symmetry and Spectroscopy of Molecules, 2ndEdition, New Age International Publishers, 2020.
3. F. Albert Cotton, Chemical Applications of Group Theory, An Indian Adaptation, 1stEdition, Wiley, 2020.
4. Donald A. Mcquarrie, Quantum Chemistry, 5thEdition, viva Books, 2016.
5. Jay Martin Anderson, Mathematics for Quantum Chemistry,1st Revised Edition, Dover Publication, 2015.

Book for References

1. Lowe J.P, Quantum Chemistry, 3rdEdition, Elseiver Science, 2012.
2. Swarnalakshmi, Saroja and Ezhilarasi, A Simple Approach to Group Theory in Chemistry, 1stEdition, Universities Press, 2008.
3. Ira N. Levine, Quantum Chemistry, 7thEdition, Pearson Publications,2016.
4. Robert L.Carter, Molecular Symmetry and Group Theory, Wiley, student Edition, 2021.
5. ROY R K, Application of Group Theory in Chemistry, 1stEdition, CBS Publisher, 2020.

E-Learning Resources

1. https://nptel.ac.in/courses/104104080/
2. https://www.mat.univie.ac.at/~gerald/ftp/book-schroe/schroe.pdf
3. http://nanowires.berkeley.edu/teaching/104a/201405.pdf
4. http://vergil.chemistry.gatech.edu/notes
5. https://www.southampton.ac.uk/assets/centresresearch/documents/compchem/perturbation_theory.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Construct the character table as well as identify the irreducible representation for different point groups.	K1–K3(Understand and Apply)
CO2	Predict the hybridization and vibration modes of different molecules using a character table.	K1-K3 (Understand, Apply, Analyze and Evaluate)
CO3	Get the overview of the fundamental mathematical formalism of quantum Chemistry.	K1-K4 (Understand, Apply and Analyze)
CO4	Solve the wave function expression for hydrogen and hydrogen – like atoms.	K1-K5(Understand, Apply and Analyze)
CO5	Outline the chemical bonding of polyatomic molecules based on empirical methods.	K1-K4 (Understand, Apply and Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	3	3	3	3	3	3
CO2	3	3	3	2	3	3	3	3	3
CO3	3	3	2	3	3	2	3	3	3
CO4	3	2	2	2	2	2	2	2	3

CO5	3	2	2	2	2	3	2	3	3
Avg.	3	2.4	2.2	2.4	2.6	2.6	2.6	2.8	3

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Lecture, Power point presentation, Quiz, Problem based Learning, Seminar

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER II

HETEROCYCLICS AND NATURAL PRODUCTS

Course code: 22PCHET2002 **Total Hours: 75**

Credits: 3 **L – T – P: 4-1-0**

Course Objectives

1. To study the structure, properties and synthesis of natural products like alkaloids, proteins, flavonoids, steroids, and terpenoids.
2. To study the structure and role of nucleic acids
3. To introduce the basics of supramolecular Chemistry
4. To study the synthesis and properties of heterocyclic compounds like Pyrazole, Oxazole and Thiazole and its derivatives.
5. To study the Biosynthesis of Nucleotides.

Syllabus

UNIT – I **Heterocyclic Compounds** **15 Hrs**

Nomenclature, synthesis and properties of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, benzimidazole, benzoxazole, benzthiazole, indole, isoindole pyridines, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid, xanthiones and flavonoids.

UNIT – II **Alkaloids and Proteins** **15 Hrs**

Total synthesis of quinine, morphine reserpine. (No Structural elucidation). Peptides and their synthesis-(Synthesis of any tripeptide using glycine, alanine, lysine, cystine, glutamic acid and argenine). Solid Phase Peptide synthesis- Merrifield synthesis, Determination of primary structure of a protein, secondary tertiary and quaternary structure of proteins.

UNIT – III **Anthocyanins** **15 Hrs**

General nature of anthocyanins – structure of the anthocyanidins. General methods of synthesizing anthocyanidins. Structural elucidation of cyanidin chloride, pelargolidin chloride, Histidinium chloride. Flavones – flavonols – isoflavones. Biosynthesis of flavonoids – depsides – tannins.

UNIT – IV **Terpenoids and Steroids** **15 Hrs**

Synthesis of Vitamin A (Reformatsky and Wittig reaction . methods only) Abietic acid, Camphor, Terpeneol, Licopenes and carotenes-biological functions. Steroids- Elucidation of structure of Cholesterol and Oestrone. Conversions of Cholesterol to Progesterone, Testosterone and Oestrone, androgens cortisone.

UNIT – V **Nucleic acids** **15 Hrs**

Pyrimidine and purine bases (synthesis not required) – structure and role of nucleic acid – nucleotide, nucleoside and poly nucleotides – DNA and RNA – structure, types – biological functions – genetic code. Replication and protein synthesis. Nucleotide monophosphate (NMP), diphosphate (NDP) and triphosphate (NTP). ATP as currency of energy. Supramolecules-General methods of synthesis and application of supramolecules.

Text Books

1. O.P.Agarwal, Organic Chemistry Natural Products- Volume I, 1st Edition,Visionias, 2021.
2. Raj K Bansal, Heterocyclic Chemistry, 7th Edition, New Age International Publishers, 2022.
3. Goutam Brahmachari, Total Synthesis of Bioactive Natural Products, 1st Edition, Manohar Publisher & Distributors, 2019.
4. Dieter Sicker, Klaus-Peter Zeller, Natural Products: Isolation, Structure elucidation, History, 1st Edition, Wiley, 2019.
5. Kar A, Chemistry of Natural Products (Volume 3), 1st Edition, CBS Publishers, 2020.

Book for References

1. Lura Faucit, Steroids: Chemistry and Applications in Drug Design and Delivery, 1st Edition, American Medical Publishers, 2023.
2. Subhash C. Mandal, Vivekananda Mandal, Natural products and Drug Discovery: An Integrated Approach, 1st Edition, Elsevier,2018.
3. Nigel Stokes, Protein Chemistry, 1st Edition, Syrawood Publishing house, 2018.
4. Anees Ahmad Siddiqui, Chemistry of selected Natural Products and heterocyclic Compounds, 2nd Edition, 2024.
5. John A.Joule, Keith Mills, Heterocyclic Chemistry, 5th Edition, Wiley, 2015.

E-Learning Resources

1. https://archive.nptel.ac.in/courses/104/105/104105034/
2. https://www.uou.ac.in/lecturenotes/science/MSCCH-17/CHEMISTRY%20LN.%203%20HETEROCYCLIC%20COMPOUNDS-converted%20(1).pdf
3. https://chemistry.ucr.edu/sites/default/files/2019-10/Chapter23.pdf
4. https://microbenotes.com/cholesterol-synthesis/
5. https://www.imperial.ac.uk/media/imperial-college/research-centres-and-groups/spivey-group/teaching/org4biosynthesis/lecture341415.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the nomenclature, synthesis and properties of the heterocyclic compounds	K1–K3 (Understand and Apply)
CO2	Elucidate the structure of alkaloids, apply the principles of peptide synthesis to Synthesize a tripetide and understand the different levels of structure of proteins and its properties.	K1-K4 (Understand, Apply and Analyze)
CO3	Learn the preparation, properties of flavonoids, anthocyanins	K1-K3 (Understand and Apply)
CO4	Study the structure and synthesis of vitamin A, carotenes & cholesterol and methods of inter conversion of cholesterol to hormones.	K1-K4 (Understand, Apply and Analyze)
CO5	Recognize the structure of DNA & RNA, its properties, synthesis and applications of supramolecules.	K1-K4 (Understand, Apply and Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	1	2	1	1	2	2	2
CO2	3	2	2	3	3	2	2	2	3
CO3	3	2	3	3	2	3	2	2	3
CO4	2	2	3	3	2	3	3	2	3
CO5	3	2	2	3	3	2	2	2	3

Avg.	2.6	2	2.2	2.8	2.2	2.2	2.2	2	2.8

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk, Power Point presentation, Student Assignments, Student Seminars/Webinars, MCQ, Quizzes, NPTEL/Others-Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER II

ORGANIC CHEMISTRY PRACTICAL

Course code: 22PCHCP2002 **Total Hours: 90**

Credits: 4 **L – T – P: 1-1-4**

Course Objectives

1. To separate and analyze organic mixtures by micro methods.
2. To synthesis and purify an organic compound.
3. To estimate the organic compound in titration methods.

Syllabus

UNIT – I **Analysis of the organic mixture** **30 Hrs**

1. Solvent separation of the binary mixture by Pilot & Bulk Analysis
2. Systematic semi micro spot analysis and functional group identification
3. Derivatization of organic compounds

UNIT – II **Preparation of the following (Any five)** **30 Hrs**

1. Sym-Tribromobenzene from aniline.
2. p-nitro aniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. Methyl orange from sulphanilic acid.
5. m-Nitro benzoic acid from benzaldehyde
6. p-bromoaniline from acetanilide
7. p-Nitrobenzoic acid from p-Nitrotoluene
8. m-Nitroaniline from m-dinitrobenzene
9. Anthroquinone from anthracene

UNIT – III **Quantitative estimation of organic compounds (Any Three)** **30 Hrs**

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose (Bertrands Methods)4. Estimation of Ascorbic acid
5. Estimation of Aromatic nitro groups
6. Estimation of Glycine

Text Books

1. Syed Mumtazuddin, Advanced Practical Chemistry,2nd Edition,,Pragati Prakashan, Meerut, 2015
2. V K Ahluwalia & Sunita Dhingra, Advanced Experimental Organic Chemistry, 4th Edition, University Press, 2020.
3. James F. Norris, Experimental Organic Chemistry, 1st Edition, Sarup Book, 2019.
4. Hans Thacher Clarke, A Handbook Organic Analysis: Qualitative & Quantitative, 4th Edition, CBS Publishers, 2021.

5. Venkateswarlu Peesapati, Comprehensive Approach to Practical Organic Chemistry, 1st Edition, 2023.

Book For References

1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry,5th Edition, Pearson Education Dorling Kinderslay, 2019 .
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry,3rd Edition, Wiley Eastern Limited, 2019.
3. Julius Berend Cohen, Practical Organic Chemistry, 1st Edition, Forgotten Books, 2018.
4. Mahadik and Bhosale, Practical Chemistry (Inorganic & Organic), 14th Edition, Nirali Prakashan, 2018 .
5. John Leonard, Advanced Practical Organic Chemistry, 3rd Edition, Taylor and Francis Books India Pvt. Ltd., 2018.

E-Learning Resources

1. https://youtu.be/WkawbF-yHME
2. https://youtu.be/N96JaRnE7n0
3. http://rushim.ru/books/praktikum/Mann.pdf
4. https://youtu.be/V8lKqD3UjFk
5. http://wwwchem.uwimona.edu.jm/lab_manuals/c1901exp8.html

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Plan and perform an organic synthesis and produce the maximum yield of an organic compound	K1 – K4 (Remember, Understand, Apply, Analyze)
CO2	Understand the nature of solvents used in the organic synthesis.	K1 – K4 (Remember, Understand, Apply, Analyze)
CO3	Choose the right solvent for the separation of a binary mixture of organic compounds	K1 – K4 (Remember, Understand, Apply, Analyze)
CO4	Analyze and identify the functional groups in the	K1 – K4 (Remember,

	given components.	Understand, Apply, Analyze)
CO5	Develop their ability to handle the organic compounds in the protective manner	K1 – K4 (Remember, Understand, Apply, Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	2	2	2	3	3	2
CO2	2	3	2	2	2	2	2	3	2
CO3	2	2	3	2	2	2	2	2	3
CO4	2	2	2	3	2	2	2	2	2
CO5	2	2	2	2	3	2	2	2	2
Avg.	2.2	2.2	2.2	2.2	2.0	2.2	2.4	2	2.2

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Demonstration Activity, PPT, Group Activity, Quiz, Interactive session, Assignment

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER III

RETROSYNTHETIC ANALYSIS AND PERICYCLIC REACTIONS

Course code: 22PCHCT3007 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. To understand the basics of retro analysis .
2. To learn the carbon - carbon formation in organometallic compounds.
3. To study the pericyclic and photochemistry concepts.

Syllabus

UNIT – I **Retro Analysis - I** **18 Hrs**

Introduction to retrosynthesis: Synthon, synthetic equivalent, target molecule, functional group interconversion, disconnection approach, importance of the order of events in organic synthesis.

One group C-C and C-X disconnections: Chemoselectivity, (disconnection of alcohols, alkenes, and carbonyl compounds).

Two group C-C & C-X disconnections: 1,3 and 1,5 diffunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensation.

UNIT – II **Retro Analysis - II** **18 Hrs**

Ring Synthesis: Synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-Alder reaction, connection in retro synthesis.

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, amino groups. Umpolung reagents, definition of umpolung, acyl anion equivalent, protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

UNIT – III Formation of Carbon - Carbon bonds via Organometallic reagents 18 Hrs

Synthesis and applications of Organolithium, Organomagnesium, Organoboron, Organozinc, Organocopper - Gilman reagents.

Organopalladium: metal mediated C-C coupling reactions - Mechanism and synthetic applications of Heck, Stille, Suzuki, Negishi, Sonogashira, McMurray, Metathesis and Carbonylation reactions.

UNIT – IV **Pericyclic Reactions** **18 Hrs**

Pericyclic reactions-classification, electrocyclic, cycloaddition reactions and sigmatropic reactions. Woodword Hoffman rules, FMO-Analysis of electrocyclic, cycloaddition and sigmatropic reactions-correlation diagram for cycloaddition reaction(2+2) and (4+2), butadiene – cyclobutene system and Inter conversion of hexatriene to cyclohexadiene. Claisen, cope and aza cope rearrangements. Diels-Alder and 1,3-dipolar cycloaddition. Cheletropic reactions.

UNIT – V **Photochemistry** **18 Hrs**

Frank-Condon principle-Non-radiative process and radiative process-stern volmer equation. Photo chemistry of ketones, photo oxygenation, photo reduction, photocycloaddition, Paterno - Buchi reaction, Di –pi- methane rearrangement. cis- trans isomerisation, Barton reaction, photo- Fries reaction, photochemistry of cyclohexadienones ,Photochemistry of Santonine.

Text Books

1. Kalsi P S, Organic Synthesis Through Disconnection Approach, 3rdEdition, MedTech Science Press, 2022.
2. Jagdamba Singh and Jaya singh., Photochemistry and Pericyclic Reactions, 5thEdition, New Age International Publishers, 2022.
3. Kalsi P S, Organic reaction and their Mechanisms, 5thEdition, New Age International Publishers, 2020.
4. Carruthers W., and Coldham I., Modern methods of Organic Synthesis, 4thEdition, South Asian Edition, Cambridge University Press, 2024.
5. George S Zweifel, Modern Organic Synthesis: An introduction, 2ndEdition, Wiley, 2017.

Book for References

1. Tiwari N K, Aromaticity and Pericyclic Reactions, 1stEdition, Ayushman Publication House, 2018.
2. Michael Smith, Organic Synthesis, 5thEdition, Academic Press Inc., 2024.
3. Stuart Warren, Organic Synthesis: The disconnection Approach, 2ndEdition, Wiley, 2008.
4. Ian Fleming, Pericyclic Reactions, 2ndEdition, Oxford University Press, 2015.
5. J. Clayden, N. Geeves and S. Warren,Organic Chemistry, 2ndEdition,Oxford University Press, 2021.

E-Learning Resources

1. https://www.asu.edu/courses/chm332/PericyclicReactions.pdf
2. https://www.researchgate.net/publication/303044457_Disconnection_Approach_Retrosynthetic_Principles_and_Synthetic_Applications

3. https://www-oc.chemie.uni-regensburg.de/OCP/ch/chb/oc5/Strategy_in_Synthesis-08.pdf
4. https://nptel.ac.in/content/storage2/courses/104103023/download/module3.pdf
5. www.nptelvideos.in/2012/11/organic-photochemistry-and-pericyclic.html

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the introduction of retro synthesis as well as role on disconnection approach**.**	K1–K3 (Understand and apply)
CO2	To apply the techniques of retro-synthetic analysis to plan synthesis of a given target molecule**.**	K1 – K4 (Remember, Understand, Apply, Analyze)
CO3	Acquire knowledge on the role of modern synthetic reagents in organic transformations.	K1 – K3 (Understand and Apply)
CO4	Interpret the symmetry orbital overlapping with the thermal/photochemical condition.	K1 – K4 (Remember, Understand, Apply, Analyze)
CO5	Understand the fundamentals of organic photochemistry and photochemical reactions	K1 – K3 (Understandand Apply)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	3	3	3	3	2	3	2	3
CO2	3	3	2	2	3	3	2	1	3
CO3	3	3	2	2	1	3	3	2	2
CO4	2	3	2	1	2	2	3	2	1

CO5	3	3	3	3	2	3	3	1	3
Avg.	2.8	3	2.4	2.2	2.6	2.6	2.8	1.6	2.4

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk&Talk, Group Disussions, Student Assignments, Student Seminars/Webinars, MCQ, NPTEL/Others-Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER III

MOLECULAR SPECTROSCOPY AND ITS APPLICATIONS

Course code: 22PCHCT3008 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Understand the basics of electromagnetic spectrum
2. Study the electronic spectra of different simple molecules
3. Interpretation of various molecules using spectral techniques

Syllabus

UNIT – I **Electromagnetic radiation** **18 Hrs**

Quantization of energy- rotational, vibrational and electronic energy levels and transitions in molecules- regions and representation of spectra. Resolution and intensity of spectral transition: signal to noise ratio- width of spectral lines- collision broadening – Doppler broadening – Heisenberg uncertainty principle – intensity of spectral lines- selection rules and transition probability- transition moment integral- Einstein absorption coefficient.

UNIT – II **Electronic Spectroscopy** **18 Hrs**

Rotational spectroscopy- Rotational spectroscopy of a rigid rotor – non-rigid rotor-diatomic and polyatomic molecules.

UV Spectroscopy: Types of transitions – Woodward Fieser rules – differentiate geometrical isomers and position isomers (disubstituted benzene derivatives), Conjugated cyclic ketones, acetophenones, esters – the study of steric effect in aromatic compounds – steric inhibition of resonance.

IR Spectroscopy: Introduction – principle – selection rules – fundamental vibrations – normal modes of vibration- overtones, combination and difference bands- Fermi resonance. Fingerprints regions – characteristics of vibrational frequencies of alkenes, alkanes, alkynes, aromatic compounds, alcohols, ethers, amines, and carbonyl compounds(ketones, aldehyde, esters, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds) – effect of hydrogen bonding and solvent effect on vibrational frequencies.

UNIT – III **Nuclear Spin Resonance Spectroscopy** **18 Hrs**

Proton NMR: Introduction – Larmor frequency - Chemical Shift – factors affecting chemical shift – equivalent and non-equivalent protons in the magnetic and non-magnetic environment – correlation to protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) – protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acid, amines, amides) – chemical exchange – spin-spin interaction between two, three and four interacting nuclei – coupling constant – Nuclear Magnetic Double Resonance (NMDR) – simplification of complex spectra using shift reagents. FT and two-dimensional NMR spectroscopy: the principle of FT NMR-FIDs.

Carbon -13 Nuclear Magnetic Resonance: Chemical shift – proton-coupled and decoupled spectra – Nuclear Overhauser Effect (NOE) – off-resonance decoupling – DEPT.

NMR Spectra of 11B, 19F, and 31P in different simple molecules.

UNIT – IV Mass and Mossbauer Spectroscopy 18 Hrs

Mass Spectroscopy: Mass spectral fragmentation of organic compounds – common functional groups – molecular ion peaks – metastable peak – McLafferty rearrangements – general rules for the interpretation of the spectrum – molecular weight, isotope effect, nitrogen rule, ring rule – examples of mass spectral fragmentation of organic compounds with respect to their structure determination – applications – molecular weight and molecular formula determination.

Mossbauer Spectroscopy: Condition for MB spectroscopy – isomer shift for Fe and Sn system – application of MB in Iron metal complexes like Fe[Fe(CN)6], Fe(CO)5, Fe2(CO)9, Fe3(CO)12, sodium nitroprusside, Prussian Blue and Turnbull's Blue.

UNIT – V ESR and NQR Spectroscopy 18 Hrs

Electron Spin Resonance Spectroscopy: Introduction – Zeeman effect – spin-orbit coupling, presentation of the spectrum. g value – Nuclear hyperfine splitting – interpretation of ESR spectrum of simple carbon-centered free radicals. Anisotropy in g value and hyperfine splitting constant – McConnel's equation Kramer's Theorem – ESR of a transition metal of Copper, Manganese, and Vanadyl Complexes**.**

Nuclear Quadrupole Resonance Spectroscopy: Introduction – Principles - nuclear charge distribution and quadrupole moment, quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, quadrupole energy levels.

Text Books

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, J.A. Vyvyan, Introduction to spectroscopy, 5th Edn., Brooks Cole, 2015.
2. R.M.Silverstein, F.X.Webster and D.Kiemel, Spectroscopic Identification of Organic Compounds (An Indian Adaptation), 8thEdition., John Wiley & sons, 2022.
3. W.Kemp, Organic Spectroscopy,5th Edn., McMillan Ltd., 2019.
4. D. N. Sathyanarayana,Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, 2ndEdition, I K International Publishing House Pvt. Ltd, 2021.

5. D.N. Sathyanarayana, Handbook of Molecular Spectroscopy: From Radio Waves to gamma Rays, 2nd Edition, Wiley, 2020.

Book for References:

1. Kalsi P S, Spectroscopy of Organic Compounds, 10th Edition, New Age international Publishers, 2024.
2. Banwell, Fundamentals of Molecular Spectroscopy, 4th Edition, McGraw Hill, 2017.
3. Jagdamba Singh, Organic Spectroscopy Principles, Problems and Their Solution, 1st Edition, A Pragati Edition, 2019.
4. Jagdamba Singh, Spectroscopy of Inorganic Compounds: Principles, Problems and their Solutions, 2nd Edition, New Age International Publishers, 2023.
5. Anita Salunkhe, Fundamental of 1H NMR and 13C NMR Spectroscopy, Orange Books Publication, 1st Edition, 2025.

E-Learning Resources

1. https://nptel.ac.in/content/storage2/courses/115101003/downloads/module2/lecture23.pdf
2. https://www.vanderbilt.edu/AnS/Chemistry/Rizzo/chem220a/Ch13slides.pdf
3. https://nptel.ac.in/content/storage2/courses/115101003/downloads/module2/lecture24.pdf
4. https://en.wikipedia.org/wiki/Fluorine-19_nuclear_magnetic_resonance_spectroscopy
5. http://www.chem.ucla.edu/~harding/notes/notes_14C_solvspec.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Explain principles of quantized energy levels and spectral transitions, and analyze factors affecting spectral line characteristics.	K1 – K4 (Remember, Understand, Apply, Analyze)
CO2	Interpret UV and IR spectra, apply Woodward-Fieser rules,	K2 – K3 (Apply,

	and distinguish between isomers.	Analyze)
CO3	Analyze NMR spectra, interpret chemical shifts and spin-spin coupling, and utilize advanced NMR techniques for structural elucidation.	K1 – K3 (Understand, Apply, Analyze)
CO4	Interpret mass spectra for molecular weight and structure, and apply Mössbauer spectroscopy principles to iron and tin complexes.	K2 – K3 (Apply, Analyze)
CO5	Explain ESR and NQR spectroscopy principles, interpret spectra of free radicals and transition metal complexes, and understand quadrupole interactions.	K1 – K4 (Remember, Understand, Apply, Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	2	2	2	3	2	2
CO2	3	3	2	3	2	2	3	3	2
CO3	3	2	2	2	3	2	3	3	2
CO4	3	2	2	2	3	2	3	3	2
CO5	3	2	2	3	3	2	3	3	2
Avg.	3	2.2	2.0	2.4	2.6	2.0	3	2.8	2.0

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk and Talk, ICT Tools, Student Seminar, Group activity, Presentation skills, NPTEL/ Mooc's courses

Rubrics for Continuous Assessment

Assignment	✓

Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER III

ELECTRO AND COMPUTATIONAL CHEMISTRY

Course code: 22PCHCT3009 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. To understand the concepts, principles and theories of ionic and electronic interactions in solutions.
2. To explore thermodynamic models of electrode-electrolyte interface.
3. To study the working and applications of electrochemical systems – Cells and Batteries
4. To derive the kinetics and the parameters affecting them.
5. To understand first principles atomic structure using computational methods.

Syllabus

UNIT – I **Electrochemistry I** **18 Hrs**

Ionics: Ions in solutions, Born model of ion-solvent interaction ion – solvent , ion –ion interactions, ionic strength- concept and calculations, Debye Huckel theory of strong electrolytes , Poisson equation, Poisson- Boltzman equation, activity co- efficient and mean ionic activity efficient of electrolytes, Debye Huckel limiting law – Derivation, verification and its extensions, Debye Huckel Onsager equation derivation and verification.

UNIT – II **Electrochemistry II** **18 Hrs**

Electrodics: Electode-electrolyte interface, adsorption at electrified interface-electrical double layer, Structure of double layer-Helmholtz-Perrin, Guoy Chapmann and Stern models of electrical double layers. Thermodynamic derivation of electrified interfacescapillary equation-electro capillary phenomenon, Polarizable and Non Polarizable electrodes. Electrokinetic phenomenon- explanation of these phenomenon with the concept of forces and flux-Onsager reciprocity.

UNIT – III **Electrochemistry III** **18 Hrs**

Electrodics- Butler Volmer equation for one electron transfer reactions. Limiting cases- Tafel and Nernst equation. Significance of equilibrium exchange current density and symmetry factor, transfer co-efficient. Electrochemical reactions and its examples. Mechanism of electrode reactions-polarizations and over potential.

UNIT – IV **Electrochemistry IV** **18 Hrs**

Corrosion and passivation of metals- Pourbaix (Iron and Lead systems only) and Evans diagrams, Theories of corrosion. Prevention from corrosion–anodic and cathodic protection, corrosion inhibitors. Electrochemical energy systems - primary and secondary batteries- dry cells, lead acid storage batteries, silver zinc cell, nickel cadmium battery, mercury cell, fuel cells. Electrodeposition - principles and applications.

UNIT – V Computational Chemistry 18 Hrs

A brief outline of molecular mechanics, semiempirical approximations, *ab initio* methods, basis sets and Z-matrix; Gaussian, Slater type. Density Function Theory- overview- Kohn Hohenberg and Kohn Sham equation (no derivation) Hartree -Fock calculations for determining electronic energies. Basic concepts of molecular dynamics and simulations.

TEXT BOOKS:

1. Samuel Glasstone, An Introduction to Electrochemistry (Import),1st Edition, Legare Street Press, 2022.
2. Saman Alavi, Molecular Simulations:Fundamentals and Practice, 1st Edition, wiley, 2020.
3. Gulliver Altman, Computational Pharmaceutics: Application of Molecular modeling in Drug Delivery, 1stEdition, 2023.
4. Sananda Chatterjee, Advanced Electrochemistry, 1stEdition, Discovery Publishing House Pvt Ltd., 2020.
5. Jeremy Harvey, Computational Chemistry: A Mediterranean History, 1st Edition, Oxford University Press, 2018.

Book for References

1. Svante Arrhenius, Text-Book of electrochemistry, 1st Edition, MJP Publisher, 2021.
2. Browne Wesley R, Electrochemistry, 1st Edition, Oxford University Press, 2018.
3. Ashutosh Tripathi, Computational Chemistry, 1st Edition, Sarup Book, 2019.
4. Andrew R. Leach, Molecular modelling Principles and Applications, 2nd Edition, Pearson, 2013.
5. Puri, Sharma, Pathania, Solution, Phase Equilibrium, Conductance and Electrochemistry, 1st Edition, Vishal Publishing Co., 2021.

E-Learning Resources

1. http://nptel.ac.in
2. http://search.ebscohost.com
3. http://www.chem.swin.esu.au/chem_ref.html
4. http://www.colby.edu/chemistry/PChem/Lecture1.html
5. http://hyperphysics.phy-astr.gsu.edu/hbase/chemical/electrode.html#c3

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Acquaint the concepts of ion-ion interactions, ion solvent interactions, calculations of ionic activity and ionic strength	K1–K3 (Understand, Apply and Analyze)
CO2	Analyze and compare various thermodynamic models of electrode electrolyte interface and derive mathematical equations	K1-K3 (Understand, Apply and Analyze)
CO3	Derive mathematical expressions for electrocapillary, single and multi-step electrodics and exchange current density.	K1-K4 (Understand, Apply and Analyze)
CO4	Compare the causes and control of corrosion using Pourbaix and Evans diagrams and to design primary and secondary batteries, dry cells with maximum energy efficiency	K1-K5 (Understand, Apply and Analyze)
CO5	Apply the tools of computational Chemistry, calculate atomic and molecular energy levels using software tools and molecular modelling techniques.	K1-K4 (Understand, Apply, Analyze and Evaluate)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3

CO1	3	2	2	3	2	2	3	3	2
CO2	3	3	3	2	2	2	3	3	2
CO3	3	3	3	2	2	2	3	3	2
CO4	3	3	3	2	3	3	3	3	3
CO5	3	2	2	2	2	2	3	3	2
Avg.	3	2.4	2.6	2.4	2.2	2.2	3	3	2.2

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Lecture (Chalk& Talk), Power point presentation

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER III

GREEN CHEMISTRY AND SUSTAINABLE DEVELOPMENT

Course code: 24PCHET3A03 **Total Hours: 75**

Credits: 3 **L – T – P: 4-1-0**

Course Objectives

1. Principles and advantages of green chemistry. ·
2. Applications of ionic liquids and phase transfer catalyst.
3. Principles and uses of microwave as a green technology.
4. Organic green synthesis in aqueous and solid phase.
5. Green chemistry in sustainable development

Syllabus

UNIT – I **Introduction of Green Chemistry** **15 Hrs**

Introduction - need and goals of green chemistry - Twelve principles of Green chemistry - concept of atom economy and selectivity in organic reactions

Designing a green synthesis: choice of starting materials, reagents, catalyst and solvents with suitable examples.

Green reagents - dimethyl carbonate and polymer supported reagents - peracids, chromic acid, thioanisolyl resins, N-bromosuccinimide, polystrener carbodiimide, polystyrene anhydride, sulfonazide polymer.

UNIT – II **Catalysis and Ionic Liquid** **15 Hrs**

Catalyst - acid, basic , oxidation and polymer supported catalyst.

Phase Transfer Catalyst (PTC): introduction - applications of PTC in organic synthesis - generation of carbenes (dihalocarbenes and vinylidene carbenes), C, N, S- alkylation and crown ethers in saphonification, esterification, anhydride formation, displacement reaction and superoxide anion reaction. (in preliminary level)

Biocatalyst: Introduction - Biochemical oxidations and reductions (Microbial) and Enzymes Catalyzed hydrolytic Processes.

Ionic liquids: Introduction - green solvents, Reactions in Acidic and neutral ionic liquids - application of ionic liquids in synthesis of pharmaceutical compounds.

UNIT – III Microwave assisted and ultrasound assisted green reaction 15 Hrs

Microwave assisted reactions in water, organic solvents and solvent- free reactions. Neat reaction of microwave Technology for the synthesis of Heterocyclic Compounds - synthesis of 1,2 - dihydrotriazine Derivatives, Benzimidazoles and 2,3-dihydro imidazo[1,2-c]pyrimidine derivatives.

Ultrasound assisted reactions and their applications in hydroboration, Coupling reactions, Bouveault reaction, Strecker reaction and synthesis of chromenes.

Some Organic Synthesis involving Green Chemistry: Introduction - Synthesis of styrene, catechol, 3-dehydroshikimic acid, Urethane, methyl methacrylate,Ibuprofen, Furfural, Paracetamol and Citral.

UNIT – IV Organic synthesis in aqueous and solid phase 15 Hrs

Aqueous Phase Reaction - Introduction - electrochemical synthesis of Adiponitrile, sebacic acid and miscellaneous reaction in isomerisation of alkenes, carbonylation, hydroformylation of olefins, homologation of 1,3 - dihydroxyacetone, Weiss-Cook reaction and synthesis of Octadienols.

Solid Supported Organic Synthesis: Synthesis of Aziridines, Coumarins, Quinoline, Oxadiazepines and Thiadiazepines.

UNIT – V Green chemistry in sustainable development 15 Hrs

Introduction - industrial interest in green chemistry- energy conservation - green chemistry in education.

Sustainable Chemistry: Green Chemistry in Sustainable Development - starting points and prospects - current status: bio-based renewables, Green Engineering Education for Sustainability for developing countries and Compressed CO2: An environmental friendly solvent.

Future Trends in Chemistry: Introduction - biomimetic, Multifunctional Reagents - Proliferation of Solventless reactions - Combinatorial Green Chemistry.

Text Books

1. Rakesh K Sharma and Anju Srivastava, Green Chemistry for Beginners with a foreword by Paul Anastas, 1st Edition, Jenny Stanford Publishing Pte.Ltd., 2021.
2. Sujata Sengupta, Green Chemistry: An Introduction, 1st Edition, Prestige Publishers, 2019.
3. Sankar P Dey and Nayim Sepay, A Textbook of Green Chemistry, 1st Edition, Techno World, 2024.
4. Shefali Shukla, A textbook of Green Chemistry Benign by Design, 1st Edition, Shree Kala Prakashan, 2023.
5. Mark Anthony Benvenuto, Green Chemistry in Government and Industry, 1st Edition, De Gruyter, Stevenson University, 2020.

Books for References

1. Bela Torok and Timothy Dransfield, Green Chemistry, An Inclusive Approach, 1st Edition, Elseiver, 2017.
2. Felicia A Etzkorn, Green Chemistry, Principles and Case Studies, Royal Society of Chemistry, 2019.
3. Anil Kumar, A Textbook of Green Chemistry, 1st Edition, AG Publishing House, 2024.
4. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, 3rd Edition, Ane Books Pvt. Ltd., 2021.
5. Vera M Kolb, Green Organic Chemistry and its interdisciplinary Applications, CRC Press, Taylor and Francis Group, 2020.

E- Learning Resources

1. https://www.asdlib.org/onlineArticles/ecourseware/Manahan/GreenChem-2.pdf
2. http://ngc.digitallibrary.co.in/bitstream/123456789/2320/1/Green%20Chemistry%20and%20Engineering%20by%20Mukesh%20Doble.pdf
3. https://tech.chemistrydocs.com/Books/Environmental/Environmental-Chemistry-by-Stanley-E.-Manahan.pdf
4. https://youtu.be/GI8g6x179t0?si=RT0eO96pPbPI1plo
5. https://www.msuniv.ac.in/images/distance%20education/learning%20materials/ug%20pg%202023/pg%202021/Msc%20chemistry%202023/SCHE21_II_Sem_Green_Chemistry.pdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the applications and advantages of Green Chemistry	K1–K4 (Understand and Apply)
CO2	Application of supported catalysts and bio-catalysts for green synthesis to various alternative reagents and chemicals for green synthesis.	K1 – K4 (Understand and Apply)
CO3	Synthesis of Organic material using microwave and ultrasound methods.	K1 - K4 (Understand, Apply and Analyze)
CO4	Different phases (aqueous and solid) study by green route synthesis method	K1 - K54(Understand, Apply, Analyze and evaluate)
CO5	Green chemistry used for future goals through sustainable energy and environment development studies.	K1 - K4 (Understand, Apply and Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	3	2	3	2	3	3	2
CO2	2	3	2	3	3	2	3	2	3
CO3	3	2	2	2	3	2	2	3	3
CO4	3	2	3	3	3	2	2	2	2
CO5	2	3	3	3	3	2	2	2	2
Avg.	2.4	2.4	2.6	2.6	3	2.0	2.4	2.4	2.4

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk**,** LCD/SMART Boards, Student Assignments, Student Seminars/Webinars**,** MCQ, Quizzes, NPTEL/Others - Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER III

PHYSICAL CHEMISTRY PRACTICAL

Course code: 22PCHCP3003 **Total Hours: 90**

Credits: 4 **L – T – P: 1-1-4**

Course Objectives

1. To understand and verify the principles and theory of physical chemistry experiments.
2. To carry out conductometric and potentiometric experiments in order to acquire skill in the determination of strength of acids.

Syllabus

UNIT – I **Electrical and Non - Electrical experiments** **72 Hrs**

1. Study of the kinetics and determination of the Arrhenius parameters, activation energy Ea and frequency A factor graphically for the acid catalysed hydrolysis of methyl acetate.
2. Comparison of acid strengths of hydrochloric acid for hydrolysis of methyl acetate catalysed by acid.
3. Kinetic study of the reaction between acetone and iodine in acidic medium and determination of rate constant with respect to iodine and acetone.
4. Determination of the rate constant and order of reaction for the reaction between potassium persulfate and potassium iodide.
5. Standardisation of sodium hydroxide using standard hydrochloric acid and determination of strengths of hydrochloric acid and acetic acid in a mixture.
6. Determination of the strength of HCl and CH3COOH in the given mixture by titration against NaOH using a quinhydrone electrode by potentiometric method
7. Determination of the strength of the given solution of Fe2+ by potentiometric titration against standard potassium dichromate by potentiometric method
8. Determination of the strength of the given solution of KI by potentiometric titration against standard potassium permanganate by potentiometric method

UNIT – II **Phase study** **18 Hrs**

Construction of a phase diagram for a binary system.

Simple Eutectic

a) Naphthalene – Biphenyl

b) Naphthalene – diphenylamine

Text Books

1. Venkateswaran V, Veeraswamy R., Kulandaivelu A.R., Basic Principles of Practical Chemistry, 2nd Ed., New Delhi, Sultan Chand & sons, 1997.
2. Daniels et al., Experimental Physical Chemistry, 7th Ed., New York, McGraw Hill, 1970.
3. Findlay A, Practical Physical Chemistry, 7th Ed., London, Longman, 1959.
4. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.
5. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.
6. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
7. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
8. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Explain the principle of conductivity, potentiometry, kinetics and phase rule experiments.	**K1-K3**
CO2	Determine the strength of unknown solutions by potentiometric and Conductometric methods.	**K1-K5**
CO3	Determine the kinetics, thermodynamics and other factors influencing reactions	**K1-K5**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	2	2	3	2	3	3	3	3	2
CO2	2	3	2	3	2	2	2	2	2
CO3	3	2	2	2	2	3	2	3	2
Avg.	2.3	2.3	2.3	2.3	2.3	2.6	2.2	2.4	2.2

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Lecture, Powerpoint, Presentation/Seminar, Exercises and discussions, Viva-voce

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER IV

ADVANCED INORGANIC CHEMISTRY

Course code: 22PCHCT4010 **Total Hours: 90**

Credits: 4 **L – T – P: 4-1-1**

Course Objectives

1. Bonding concepts, mechanistic aspects and stability of organometallic compounds and their applications as industrial catalysts.
2. Structure and biological functions of proteins and the role of metals in biology.
3. Basics of nuclear chemistry and its application.

Syllabus

UNIT – I **Organometallic Chemistry** **18 Hrs**

Carbon donors: Alkyls and aryls, metalation, bonding in carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene, and allyl systems. Metallocenes: synthesis, structure and bonding. Reactions: Association, substitution, addition, elimination, ligand protonation, electrophilic and nucleophilic attack on ligands, carbonylation, decarboxylation and oxidative addition.

UNIT – II **Industrial applications of Organo Metallic compounds** **18 Hrs**

Catalysis – Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalyst(Oxo process), oxidation of olefins to aldehydes and ketones(Wacker process):polymerisation(Ziegler-Natta catalyst); Cyclo oligomerisation of acetylene using nickel catalyst(Reppe's catalyst), polymer bound catalysts.

UNIT – III **Bio-Inorganic Chemistry I (Transport of metal ions)** **18 Hrs**

Uptake, transport and storage of metal ions by organisms - structure and functions of biological membranes - the generation of concentration gradients (the Na+ -K + pump) - mechanisms of ion-transport across cell membranes – bleomycin - siderophores (e.g. enterobactin and desferrioxamine) - transport of iron by transferring - storage of iron by ferritin - bio chemistry of calcium as hormonal messenger.

UNIT – IV Bio-Inorganic Chemistry II (Metalloporphyrins/Metalloenzymes) 18 Hrs

Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemeythrin and hemocyanine - synthetic oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe)- cytrochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, vitamin B12 and B12 coenzymes, photosynthesis - photosystem-I & II, nitrogen fixation, cisplatin.

UNIT – V Nuclear Chemistry 18 Hrs

Nuclear properties-nuclear spin and moments, origin of nuclear forces. Types of radioactive decay: Orbital electron capture, nuclear isomerism, internal conversion, detection and determination of activity by bubble chamber, G.M., Scintillation and Cherenkov counters; Accelerators- Linear and Cyclotron. Photonuclear and thermo nuclear reactions.

Radioactive tracers: Preparations - principles of tracer technique - application of tracers in the study of reaction mechanism and in analytical chemistry - neutron activation analysis, isotope dilution analysis - radio chemical determination of age of geological specimen. Tracers as applied to industry and agriculture - radioactive tracer in the diagnosis and treatment in the field of medicine.

Text Books

1. R.H. Crabtree, The Organometallic Chemistry of Transition Metals, 7th Edition, Wiley, 2019.
2. Mehrotra, Organometallic Chemistry: A Unified Approach, 2nd Revised Edition, New Age International Publishers, 2020.
3. Ajai Kumar, Organometallic Chemistry& Bioinorganic Chemistry, 4th Edition, Visionias, 2023.
4. Kalsi P S, Bioorganic, Bioinorganic and Supramolecular Chemistry, 5th Edition, New Age International Publishers, 2024.
5. Hari Jeevan Arnikar, Essential of Nuclear Chemistry, 5th Edition, New Age International Publishers, 2022.

Book for References

1. Michael Gonzalez, Bioinorganic Chemistry, 1st Edition, Oxford Book Company, 2022.
2. Ankita Das, Asim K Das and Mahua Das, Bioinorganic Chemistry, 1st Edition, Books and Allied Pvt. Ltd., 2017.
3. Hussain Reddy, Bioinorganic Chemistry, 2nd Edition, New Age International Publishers, 2020.
4. G.O. Spessard and G. L. Miessler, Organometallic Chemistry, 3rd Edition, Oxford University Press,2015.
5. Peter A C Mcpherson, Principles of Nuclear Chemistry, 1st Edition (Reprint), World Scientific Europe Ltd., 2017.

E-Learning Resources

1. https://www.nature.com/subjects/organometallic-chemistry
2. https://nptel.ac.in/courses/104108062/
3. https://nptel.ac.in/content/syllabus_pdf/104104109.pdf
4. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Book%3A_Inorganic_Chemistry_(Saito)/8%3A_Reaction_and_Physical_Properties/8.2%3A_Bioinorganic_chemistry

https://www.visionlearning.com/en/library/Chemistry/1/Nuclear-Chemistry/59

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Explain the synthetic route, structure and bonding involved in organometallic compounds.	**K1 - K3 (Understand and apply)**
CO2	Understand the reactivity of organometallic compounds including the industrial application in synthesis.	**K1 – K4 (Understand, Apply and analyze))**
CO3	Explain how metal ions interact with biological environments and how these interactions influence the properties of metal centers	**K1 - K3 (Understand and apply)**

CO4	Understand the role of metal ions in photosynthesis, cobalamine B12 and in basic functions of living organisms	**K1 - K3 (Understand and apply)**
CO5	Learn about the importance of nuclear chemistry and its applications.	**K1 – K3 (Understand and Apply)**

CO – PO – PSO Mapping

COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**
CO1	3	3	2	2	2	2	3	2	2
CO2	2	3	2	3	2	3	3	2	2
CO3	2	2	2	2	3	3	3	2	2
CO4	3	3	3	3	3	3	3	2	2
CO5	2	3	3	3	3	3	3	2	3
Avg.	2.4	2.8	2.6	2.8	2.6	2.6	3	2.0	2.2

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk, Group Discussion, Student Assignments, Student Seminars/Webinars, MCQ, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER IV

RESEARCH METHODOLOGY

Course code: 24PCHET4A04 **Total Hours: 75**

Credits: 3 **L – T – P: 4-1-0**

Course Objectives

1. To provide an awareness about the developing avenues in Chemistry.
2. To give training in seminars, group work, communication and thesis writing .
3. To equip the students in using computing techniques in solving problems, to visualize and draw molecules

Syllabus

UNIT – I **Research Problem and Source of Literature** **15 Hrs**

Objectives of research, types of research – basic, applied, and other types. Problem selection – project proposal - funding agencies, Chemistry literature survey –primary, secondary and tertiary sources.

Journals published by the ACS and RSC – Indian Journals – reviews, monographs, data books and indexes. Methods of searching, compilation,preservation and retrieval of collected literature. Impact factor and citation index.

UNIT – II **Research planning, methods and materials** **15 Hrs**

Planning and conducting experiments. Methods of collecting data – primary and secondary – sources of secondary data.

Classification and tabulation of data – types of classification –general rules for tabulation–types of tables. Simple sampling techniques and size of the sample.

UNIT – III **The Chemical abstract services** **15 Hrs**

The Chemical Abstracts: Current awareness searching: CA weekly issues, CA issue indexes. Retrospective and forward searching. CA Collective indexes: Collective index (CI), decennial index (DI).

Access points for searching CA indexes: index guide, general subject terms, chemical substance names, molecular formula, ring systems, author names, patent numbers. Locating the

reference: finding the abstract, finding the original document, chemical abstract service source index.

UNIT – IV **Report writing** **15 Hrs**

The Art of Scientific Writing – Forms of Scientific Writing, Research Reports, Theses, Journal Articles and Books. Format of Research Report - Abbreviations, symbols, SI units**.** ChemicalNomenclature, Project report writing – general, chapter and page format. Procedure for presenting tables, graphs and figures, foot-notes, bibliography and appendices. Abbreviations, symbols and SI units. Plagiarism, copy right and patent laws. Publication of research paper.

UNIT – V **Computational Techniques in Chemistry** **15 Hrs**

Components of Origin- Plotting and Customizing Graphs, Batch Plotting graphs, Merging Graphs. Chemdraw-Writing Chemical Equation Schemes using Software, Editing, Transporting a Picture to a Word Document. Building Molecules, Measurement of Bond Angles, Bond Energy and Bond Length using softwares. Introduction to Cheminformatics in Drug Discovery – 2D database and database searching.

Text Books

1. J Anderson, B.H. Dursten and M. Poole, Thesis and Assignment Writing, 4th Edition, Wiley Eastern, 2019.
2. Kothari C.R. and Gaurav Garg. Research Methodology: Methods and Techniques, 5th Edition, New Age International, 2023.
3. Upendra Pratap Singh, Research and Publication Ethics, 1st Edition, Sultan Chand & Sons, 2023.
4. Rajdeep Banerjee and joyeeta Banerjee, Patent Law, 1st Edition, Notion Press, 2020.
5. Ranjit Kumar, Research Methodology: A Step-by-Step Guide for Beginners, 4th Edition, Sage Publication, 2024.

Book for References

1. Sansanwal, Research Methodology and Applied Statistics, 1st Edition, Shipra Publications, 2020.

2. Siva prasad Bose and Joy Bose, Introduction to Patents and Patent Law in India, 1st Edition, Joy Bose Publishers, 2022.
3. John W.Creswell and David Creswell, Research Design: Qualitative, Quantitative and Mixed Methods Approaches, 6th Edition, Sage Publication, 2022.
4. Margaret Cargil, Writing Scientific Research Articles: Strategy and Steps, 3rd Edition, Wiley Blackwell, 2021.
5. Kishor and Ajay and Gitanjali, Research and Publication Ethics, 2nd Edition, Das Ganu Prakashan, 2023.

E-Learning Resources

1. https://www.researchgate.net/publication/2174858_Research_Methodology
2. https://mfs.mkcl.org/images/ebook/Fundamental%20of%20Research%20Methodology%20and%20Statistics%20by%20Yogesh%20Kumar%20Singh.pdf
3. http://www.sciencedirect.com/
4. http://ww42.scifinder.com/
5. https://www.southwestern.edu/live/files/4169-guide-for-writing-in-chemistrypdf

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the basics, types and interpret current chemical research.	K1–K3 (Understand and Apply)
CO2	Employ the online tools to survey chemical literature and related Journals	K1-K3 (Understand and Apply)
CO3	Learn the concept of formatting, statistical data analysis and ethical guidelines for research.	K1-K4 (Understand, Apply and Analyze)
CO4	Identify the accurate format of writing scientific report and thesis	K1-K5 (Understand, Apply and Analyze)
CO5	Acquire the skill of presenting the research work to	K1-K4

	public forums using modern software tools.	(Understand, Apply, Analyze and Evaluate)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	2	2	2	3	3	3
CO2	3	3	2	2	2	2	3	3	2
CO3	3	2	2	3	3	2	3	2	2
CO4	3	3	2	2	3	3	3	3	2
CO5	3	2	2	3	3	3	3	3	2
Avg.	3	2.4	2	2.4	2.6	2.4	3	2.8	2.2

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Lecture (Chalk & Talk), Power point presentation

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER IV

INTRODUCTION TO MATERIAL SCIENCE

Course code: 24PCHET4A05 **Total Hours: 75**

Credits: 3 **L – T – P: 4-1-0**

Course Objectives

1. Explore the students in the new avenues of material science.
2. Introduce the various fields of material synthesis.
3. Extended the concept of morphology of materials in solid state Chemistry

Syllabus

UNIT – I **Overview of polymers** **15 Hrs**

Basic concepts of polymer chemistry: Repeating unit, degree of polymerisation, classification, stereochemistry of polymers and nomenclature of stereoregular polymers.

Free radical chain polymerization- kinetics, cationic and anionic polymerisation. Molecular weight and size: Number and weight average molecular weights. Polydispersity and molecular weight distribution in polymers. Polymerisation techniques: Bulk, solution, suspension and emulsion polymerisation. Melt, solution and interfacial polycondensation. Solid and gas phase polymerisation. Factors affecting Crystallinity and glass transition temperature.

UNIT – II **Synthetic resins, plastics and fibers** **15 Hrs**

Synthetic fibers: Rayon, nylons, polyesters, acrylics, modacrylics and spinning techniques. Synthetic rubber: SBR, butyl rubber, nitrile rubber, neoprene, silicone rubber and polysulphides. Synthetic resins and plastics: Manufacturing and applications of polyethylene, PVC, teflon, polystyrene, polymethylmethacrylate, polyurethane, phenol – formaldehyde resins, urea – formaldehyde and melamine – formaldehyde resins and epoxy polymers.

UNIT – III **Nanomaterials** **15 Hrs**

Basics -Nano revolution -Basic idea of nano materials-Structure-Nucleation and grain growth-Grain boundaries-Properties at Nanoscale: Strength and Hardness, optical, electrical, magnetic, mechanical and chemical properties.

Synthesis - Chemical Vapour Deposition (CVD), sol-gel processing. Nano tubes, Nano rods, Buckyballs-fullerenes, Nanofibers, Nanoshells. Semiconductor Nanoparticles- Energy band structure of Semiconductors Quantum dots-Quantization effect.

UNIT – IV Characterisation and Applications of nanomaterials 15 Hrs

Theories and Techniques used for characterization-UV-Visible and PL spectroscopy-XRD-Electron microscopes-SEM, TEM, HR-TEM (SAED), AFM.

Solar energy conversion and catalysis - Uses of Nano composites, Nanoelectronics, chemical and biosensors. Nanoparticles in Pollution control. Nano materials in bone substitutes and dentistry, Food and cosmetic applications, textiles, paints, drug delivery and its application-nanoparticles in cancer targeting and treatment. Nanotechnology in agriculture, fertilizer and pesticides.

UNIT – V Crystallography 15 Hrs

Introduction - Crystal planes and directions – Unit cells, Miller indices, Two and three dimensional space lattices, crystal systems, reciprocal lattices, symmetry elements (2D &3D), matrix representation of symmetry operations, point groups (2D & 3D) operators - proper and improper axis, mirror planes, Glide planes, screw axis, derivation of space groups (2D and 3D).

Crystal structure – Analysis by powder X-ray diffraction and single crystal analysis, single crystal analysis and its applications. Electron charge density maps, neutron diffraction – method and applications.

Growth methods - Kinds of nucleation - equilibrium stability and metastable state-classical theory of nucleation. Single crystal growth – Low and high temperature, solution growth technique. Melt growth - Bridgeman-Stockbarger method, Czochralski method.

TEXT BOOKS

1. V. R. Gowarikar, N.V. Viswanathan and JayadevSreedhar, Polymer Science, 4thEdition, New Age international (P) ltd., Publishers New Delhi, 2021.
2. N B Singh, Introduction to Polymer Science and Technology, 2ndEdition, New Age International Publishers, 2017.
3. Pradeep T., “Nano: the Essentials”, Tata McGraw Hill, New Delhi, 2017.

4. Nandi, Nanomaterials Theory Problems and Solutions, 2nd Edition, Techno World, 2020.
5. Asim K Das, An Introduction to Nanomaterials and Nanoscience, 2nd Edition, CBS Publishers & Distributors Pvt. Ltd., 2024.

REFERENCE BOOKS

1. Anushu Srivastava and Shakun Srivastava, Fundamental of Polymer Science and Technology, 12th Edition, S.K.Kataria & Sons,2016.
2. Prashant D Ashtaputrey, Polymer Chemistry: Synthesis and Characterization techniques, 1st Edition, Prints Publications Pvt Ltd., 2018.
3. Rupali Ajesh, Fundamentals of Nano Chemistry, 1st Edition, AG Publishing House, 2023.
4. Sulalit Bandyopadhyay, Fabrication and Application of Nanomaterials, 1st Indian Edition, McGraw Hill, 2022.
5. Jehova Jire L Hmar, Synthesis, Characterisation and Multi-functional Applications of Nanomaterials, 1st Edition, EvincePub Publishing, 2024.

WEB RESOURCES

1. https://www.element.com/nucleus/2017/08/15/18/45/considerations-for-measuring-glass-transition-temperature
2. https://omnexus.specialchem.com/selection-guide/epoxy-resins-a-to-z-technical-review-of-thermosetting-polymer
3. https://www.understandingnano.com/nanomaterials.html
4. https://www.nano.gov/you/nanotechnology-benefits
5. http://www.essentialchemicalindustry.org/materials-and-applications/nanomaterials.html

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Familiar with the basic concepts and types of polymerization techniques and molecular weight and size, Glass Transition Temperature and crystallinity in polymers.	K1–K3 (Understand and Apply)
CO2	Elucidate the synthesis and applications of various synthetic	K1 – K3 (Understand

	resins and plastics.	and Apply)
CO3	Describe basics nanomaterials, properties and also familiarize the classification ofnanostructures, Size Dependency in nanostructures and quantum size effects in nanostructures.	K1 - K4 (Understand, Apply and Analyze)
CO4	Interpret the experimental data using the characterization technique of nanomaterials for the research work.	K1 – K3 (Understand, Apply, Analyze and evaluate)
CO5	To introduce and give an insight into the fascinating area of solid state physics, solid state chemistry and material science.	K1 - K4 (Understand, Apply and Analyze)

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	2	2	2	3	2	3	2	2
CO2	3	2	2	2	3	3	3	3	3
CO3	2	3	3	1	2	2	2	3	2
CO4	3	3	1	2	3	3	2	2	2
CO5	2	2	1	3	2	3	2	2	3
Avg.	2.6	2.4	1.8	2.0	2.0	2.6	2.4	2.4	2.4

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk**,** LCD/SMART Boards, Student Assignments, Student Seminars/Webinars**,** MCQ**,** Quizzes, NPTEL/Others - Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓

SEMESTER IV

INORGANIC CHEMISTRY PRACTICAL -II

Course code: 23PCHCP4004 **Total Hours: 90**

Credits: 4 **L – T – P: 1-1-4**

Course Objectives

1. Quantitative analysis of mixtures of metal ions by volumetric and gravimetric analysis.
2. Preparation of various metal complexes.

Syllabus

UNIT – I **Preparation of the following** **18 Hrs**

1. Sodium bis(thiosulphato)cuprate (I)
2. Sodium hexanitrocobaltate (III)
3. Hexammine nickel (II) chloride
4. Tris (thiourea) copper (I) chloride
5. Potassium tris (oxalato) chromate (III) trihydrate
6. Tris (thiourea) copper (I) sulphate
7. Preparation of Chloropentammine Cobalt(III) Chloride
8. Preparation of Bis(Acetyl Acetanato) Copper(II)
9. Preparation of Potassium Tris(Oxalato) Aluminato(III) Trihydrate

UNIT – II **18*4=72 Hrs**

Quantitative analysis:Mixture of metal ions(gravimetrically and volumetrically)

1) Magnesium and Iron in the mixture of Iron and Magnesium
2) Nickel and Copper in the mixture of Copper and Nickel
3) Zinc and Copper in the mixture of Copper and Zinc.
4) Nickel and Iron in the mixture of Iron and Nickel.

Reference Books:

1. Vogel's "Textbook of Quantitative chemical Analysis", Pearson Education Ltd. Sixth Edition, 2008.

2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.
3. J. Mendham, R.C. Denney, J. Basset and G.H. Jeffery, Vogel's Text book of quantitative Inorganic Analysis, fourth edition ELBS, Longmann, 1978.
4. G. Brauer (Ed.), Handbook of Preparative Inorganic Chemistry, Vols. I and II, Academic Press, 1963.

Web Resources:

1. http://egyankosh.ac.in/bitstream/123456789/15906/1/Experiment-17.pdf
2. https://www.slideshare.net/mjkwezi/synthesis-of-tris-thiourea-copper-i-sulphate-by-kwezi-mwaka-julius
3. https://thosci.com/synthesis-of-hexaamminenickelii-chloride/.

Course Outcomes (CO): On completion of the course the students will be able to

COs	CO Statement	Knowledge Level
CO1	Understand the reaction involved in formation metal complexes and analyze it	**K1–K4 (Understand, Apply and Analyze)**
CO2	Estimate the amount of metal ions in the given solutions.	**K1– K5 (Understand, Apply, Analyze and Evaluate)**
CO3	Acqiure skills on Re-Crystallization, Separation, Digestion and Co-Precipitation methods.	**K1-K3 (Understand and Apply)**

CO – PO – PSO Mapping

COs	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3
CO1	3	3	3	2	2	3	3	2	2
CO2	3	3	2	3	1	3	3	3	3
CO3	3	2	2	3	3	1	3	1	2
Avg.	3	2.7	2.3	2.7	2	2.3	3	2	2.3

Strong - 3 Moderate -2 Week -1 No Correlation-0

Pedagogy (Teaching Methodology) :

Chalk & Talk, Student Assignments, Viva-MCQ, NPTEL/Others-Add-on-courses, Web Resources

Rubrics for Continuous Assessment

Assignment	✓
Seminar	✓
Field visit	---
Participatory Learning	✓
Group Discussion	✓
Flipped/Blended Learning	✓