NEP and Learning Outcome-based Curriculum Framework (LOCF)
For
M.Sc. (Chemistry) Programme
Academic Session (w.e.f. 2024-2025)

I & II Semesters

DEPARTMENT OF CHEMISTRY
MAHARAJA SURAJMAL BRIJ UNIVERSITY
BHARATPUR

Dr. Farbat Singh
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Acad.I

(Dr. Nisha Chauhan) (Dr. Rakhee Choudhary) (Dr. Anshu Dandia)

Scheme of Examination

The examination pattern comprises 30% internal assessment and 70% external assessment.

Internal Assessment

The internal assessment is divided as follows:

1. 10% from two sessional exams
2. 20% from attendance, assignments, demonstrations, and presentations

External Assessment

Theory Papers:

1. Each theory paper in the end-of-semester examination (EoSE) carries 70% marks.
2. The EoSE will be of 3 hours duration.
3. The questions will be designed in alignment with Bloom's Taxonomy.

Part A of the question paper shall contain 10 very short answer type questions covering the entire syllabus. Each question carries equal marks.

Part B of the question paper shall contain 04 descriptive type questions one from each unit with internal choice. Each question carries equal marks.

Value-Added Papers

1. Each theory paper in the end-of-semester examination (EoSE) carries 70% marks.
2. The EoSE will be of 2 hours duration.
3. Question paper shall contain 40 multiple choice questions covering the entire syllabus. Students have to attempt any 35 questions. Each question carries 1 mark.
4. If a student attempts more than 35 questions, only the first 35 attempted questions will be considered.

Practical:

Internal: continuous evaluation (30%).

External: end term practical /written exam (40%) and viva-voce (30%).

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About the Department

The Department of Chemistry at Maharaja Surajmal Brij University, Bharatpur, India, was established in 2020. The department introduced the postgraduate program **M.Sc. in Chemistry** in the academic session 2020–2021.

Vision:

To establish the department as a leader in world-class teaching and research, contributing to civilisation through innovative, creative, and scholarly endeavours.

Mission:

- To provide high-quality education in chemical sciences that integrates theoretical knowledge, practical training, and ethical values to enhance personal and professional growth.
- To develop skilled scientists, educators, entrepreneurs, and innovative researchers who contribute to societal advancement.
- To promote interdisciplinary research and collaboration to address national and global challenges.
- To drive progress and sustainable development for the betterment of individuals and the nation
- The department aims to encourage critical thinking and develop research skills among students.

Program Highlights:

- The initial intake for the **M.Sc. Chemistry** program during the 2021–2022 sessions was 20 students.
- The intake was increased to 25 students for the 2022–2024 sessions.
- In the 2023–2024 sessions, the intake rose to 30 students, and a new program, **B.Sc. (Hons.) in Chemistry**, was introduced.
- The department also started offering a **Ph.D. in Chemistry** and provides chemistry classes for:
    - **B.Sc. Physical Sciences** (Physics, Chemistry, and Mathematics)
    - **B.Sc. Life Sciences** (Chemistry, Botany, and Zoology)

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Scheme of Programme

Semester 1

Course Code	Course ID	Course Title	L	T	P	L	T	P	Total Credits	MARKS				
			(Hrs)			Credits				TI	TE	PI	PE	Total
Core Course(s)														
PCSC-01	Inorganic Chemistry-I	Group Theory, Bonding and Metal-Ligand Equilibria	4			4			4	30	70	-	-	100
PCSC-02	Physical Chemistry-I	Fundamentals and Applications of Quantum Mechanics	4			4			4	30	70	-	-	100
PCSC-03	Organic Chemistry-I	Reaction Mechanisms -I Organic Chemistry	4			4			4	30	70	-	-	100
PCLAB-01	Chemistry Lab-I				12			6	6	-	-	45	105	150
Discipline Specific Elective Courses: Students have to choose Any One														
PCDSE- 01A		Chemistry of Life Science	2			2			2	15	35	-	-	50
PCDSE-01B		Mathematics for Chemist	2			2			2	15	35			50
Multidisciplinary Course(s)														
PCMDC-01		Chemistry of Materials	2			2			2	15	35	-	-	50
Value-added Course(s)														
PCVAC-01		Green Chemistry	2			2			2	15	35	-	-	50
Total Credits									24					

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Semester 2

Course Code	Course ID	Course Title	L	T	P	L	T	P	Total Credits	MARKS				
			(Hrs)			Credits				TI	TE	PI	PE	Total
Core Course(s)														
PCSC-05	Inorganic Chemistry-II	Transition and Organometallic complexes	4			4			4	30	70	-	-	100
PCSC-06	Physical Chemistry-II	Thermodynamics, Kinetics and Polymerization	4			4			4	30	70	-	-	100
PCSC-07	Organic Chemistry-II	Reaction Mechanism-II and Stereochemistry	4			4			4	30	70	-	-	100
PCLAB-02	Chemistry Lab-II				12			6	6	-	-	45	105	150
Discipline Specific Elective Course														
PCDSE- 02		Spectroscopic Methods in Chemistry-I	2			2			2	15	35			50
Skill Enhancement Course(s)														
PCSEC- 01		Analytical Chemistry	2			2			2	15	35	-	-	50
Multidisciplinary Course(s)														
PCMDC-02		Drug Design and Discovery	2			2			2	15	35	-	-	50
Total Credits									24					

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PCSC-01: INORGANIC CHEMISTRY - I
(Group Theory, Bonding and Metal-Ligand Equilibria)

Course Outcomes:

By the end of the course, the students will be able to:

1. Use group theory and character tables to describe molecular symmetry and predict optical activity.
2. Calculate and interpret metal-ligand formation constants and the chelate effect.
3. Predict molecular shapes and bonding using VSEPR theory and Walsh diagrams.
4. Explain bonding in metal-ligand complexes using crystal field and molecular orbital theories.
5. Describe and predict mechanisms of substitution reactions and the trans effect in metal complexes.

UNIT-1 SYMMETRY AND GROUP THEORY IN CHEMISTRY

Definitions of group, subgroup, relation between orders of finite groups and its subgroups. Conjugacy relation and classes. Symmetry elements and symmetry operations, Point symmetry group. Schönflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out explicitly). Character of a representation, reducible and irreducible representations. The great orthogonality theorem (without proof) and its importance, Derivation of character tables of C_2v, C_3v and D_2h Character tables and their use. Molecular asymmetry, dissymmetry, and optical activity.

UNIT-2 BONDING MODELS

Stereochemistry and Bonding in Main Group Compounds

VSEPR Theory, Walsh diagrams (tri-atomic molecules), dπ-pπ bonds, Bent rule and energetics of hybridization

Metal-Ligand Bonding

Valence bond theory, electroneutrality principle and its limitations, Crystal field theory and its limitation, Crystal field effects, John Teller distortion, nephelauxetic series, spin-orbital coupling, molecular orbital theory of octahedral, tetrahedral and square planar complexes (with and without π-bonding).

UNIT-3 METAL-LIGAND EQUILIBRIA IN SOLUTION-I

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and

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ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

UNIT-4 METAL-LIGAND EQUILIBRIA IN SOLUTION-II

Substitution reactions in octahedral complexes-acid hydrolysis, Base hydrolysis, racemization of tris chelate complexes, theories of trans effect with respect to Pt(II) complexes. Brief account of electron transfer reactions, inert and labile complexes.

References:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, Harper & Row.
3. Chemical Applications of Group Theory; F.A. Cotton, Wiley, New York.
4. Inorganic Chemistry: Principles of Structure and Reactivity; J.E. Huheey, E.A. Keiter, and R.L. Keiter (Indian Edition)
5. Modern Aspects of Inorganic Chemistry; H.J. Emeleus and Sharpe.
6. Concepts and Models of Inorganic Chemistry; B. Douglas, D.H. McDaniel and J.J. Alexander; John Wiley and Sons.
7. Inorganic Chemistry, A Modern Introduction; T. Moeller, John Wiley and Sons.

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PCSC-02: PHYSICAL CHEMISTRY - I
(Fundamentals and Applications of Quantum Mechanics)

Learning Outcomes:

After the completion of this course, the students will be able to:

1. Explain foundational concepts of quantum mechanics, including wave-particle duality, uncertainty principle, and the Schrödinger equation.
2. Solve quantum mechanical problems for simple systems like the particle in a box, harmonic oscillator, rigid rotor, and hydrogen atom.
3. Apply perturbation theory to solve problems involving simple quantum systems.
4. Utilize the variational principle to approximate solutions for complex systems.

UNIT-I BASIC PRINCIPLES OF QUANTUM MECHANICS

Introduction to Quantum Mechanics, Historical background of quantum mechanics, Blackbody radiation and Planck's hypothesis, Photoelectric effect and Einstein's explanation, Compton effect, De Broglie hypothesis and matter waves, Heisenberg uncertainty principle, Wave-particle duality, Introduction to wave functions, Schrödinger equation: Time-dependent and time-independent forms, Interpretation of wave functions: Probability density and Normalization.

UNIT-II QUANTUM MECHANICS OF SIMPLE SYSTEMS

Particle in a one-dimensional box: Derivation and interpretation, Particle in a three dimensional box, Harmonic oscillator: Schrödinger equation and solutions, Quantum mechanical treatment of the rigid rotor,

UNIT-III APPLICATIONS OF QUANTUM MECHANICS

Hydrogen atom: Schrodinger equation and solution, Quantum numbers and their significance, Shapes of atomic orbitals, Spin angular momentum, Quantum mechanical tunnelling. Quantum Mechanics of Atoms: Application to multi-electron atoms, Introduction to the Pauli exclusion principle, Electronic configuration of atoms.

UNIT-IV APPROXIMATE METHODS OF QUANTUM MECHANICS

Perturbation theory: Time-independent perturbation theory (first and second order), Applications of perturbation theory to simple systems, Quantum mechanical treatment of the helium atom. Time-dependent perturbation theory, Stark effect, Zeeman effect, Advanced

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perturbation techniques, Applications in molecular systems, Variational principle: Concept and applications

References:

1. Introduction to Quantum Mechanics by David J. Griffiths, 2nd Edition, Pearson
2. Principles of Quantum Mechanics by R. Shankar, 2nd Edition, Springer.
3. Quantum Chemistry by Ira N. Levine, 7th Edition, Pearson.
4. Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman, 5th Edition, Oxford University Press.
5. Quantum Chemistry by Donald A. McQuarrie, 1st Edition, University Science Books.
6. Quantum Chemistry by R.K. Prasad, 4th Edition, New Age International Publishers.

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PCSC-03: ORGANIC CHEMISTRY - I
(Reaction Mechanisms-I in Organic Chemistry)

Learning Outcomes:

After the completion of this course, the students will be able to:

1. Analyze organic reaction mechanisms by evaluating structure–reactivity relationships using concepts such as resonance, steric effects, and linear free energy correlations.
2. Explain and compare mechanisms of nucleophilic substitution and aromatic substitution reactions, including their stereochemical outcomes and energy profiles.
3. Differentiate between E1, E2, and E1cB elimination mechanisms and predict product formation using stereoelectronic and regioselectivity principles.
4. Describe the mechanisms of electrophilic and nucleophilic addition reactions to C=C and C≡C bonds, including hydroboration and organoborane chemistry.

UNIT-1 REACTION MECHANISM: STRUCTURE AND REACTIVITY

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatment-The Hammett equation and linear free energy relationship, substituent and reaction constants and Taft equation. Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining reaction mechanisms. Generation, structure, stability and reactivity of carbocations, carbanions, carbenes and nitrenes.

UNIT-2 MECHANISM OF NUCLEOPHILIC SUBSTITUTION

The limiting cases SN^1 and SN^2, detailed mechanistic description and borderline mechanisms, nucleophilicity and solvent effects, competition between nucleophilicity and basicity, ambident nucleophiles, hard and soft nucleophiles and electrophiles, leaving group effects, steric and other substituent effects on substitution and ionization rates, stereochemistry of nucleophilic substitution. SN^i, $SN^{1'}$, $SN^{2'}$ and $SN^{i'}$ mechanisms.

Aromatic Electrophilic Substitution

Basic concept of aromaticity, Theoretical treatment of aromatic substitution reactions, structure-reactivity relationship in mono substituted benzene ring, orientation in other ring system, energy profile diagram, Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Bischler-Napieralski reaction, Pechmann reaction, Houben-Hoesch reaction, Fries rearrangement

Aromatic Nucleophilic Substitution

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Mechanism of Nucleophilic substitution in aromatic systems via diazonium ions, by addition-elimination and elimination-addition mechanism (involving arynes); von-Richter rearrangement, Sommelet-Hauser and Stevens rearrangements.

UNIT-3 MECHANISM OF ELIMINATION

The El, ElcB and E2 mechanisms, Orientation Effects in Elimination Reactions, Saytzeff and Hoffman rules, Stereochemistry of E2 Elimination Reaction and Eclipsing Effects in E2 Eliminations. Dehydration of Alcohols, Elimination not involving C-H Bonds, Pyrolytic eliminations.

UNIT-4 ADDITION REACTIONS TO C-C MULTIPLE BOND

General mechanistic considerations, Mechanism of addition of hydrogen halide, H_2O, halogens, HOX and mercuric salt to alkenes and alkynes. Hydroboration, formation of C-C bonds via organoboranes, hydroboration of acetylenes, and nucleophilic addition to alkenes.

Reference:

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, New York, 5th Edition, 2007.
2. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, Springer, New York, 5th Edition, 2008.
3. M.B. Smith and J. March, March's Advanced Organic Chemistry, John Wiley & Sons, Inc., Hoboken, New Jersey, 6th Edition, 2007.
4. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper & Row Publishers, New York, 2nd Edition, 1981.
5. M.S. Singh, Reactive Intermediates in Organic Chemistry, Structure, Mechanism, and Reactions: Wiley-VCH, 2014.
6. N.S. Isaacs, Physical Organic Chemistry, Longman Scientific & Technical, Wiley & Sons Longman, UK, 2nd Edition, 1995.
7. P.S. Kalsi, Organic Reactions and their Mechanisms (Multi Colour Edition), New Age International Private Limited, 5th Edition, 2020.
8. P. Sykes, A Guide Book to Mechanism in Organic chemistry, Orient-Longman, John Wiley & Sons Inc. New York, 6th Edition, 1996.

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PCLAB-01: CHEMISTRY LAB-I

Course Outcomes:

After the completion of this course, the students will be able to:

- Perform qualitative analysis and synthesize inorganic compounds for spectroscopic analysis.
- Perform practical experiments on viscosity, conductometry, and adsorption.
- Proficiently perform crystallization, distillation, solvent extraction, and chromatography, demonstrating accurate execution and understanding.
- Successfully synthesize, purify, and characterize organic compounds, submitting recrystallized products along with their melting points for all stages of preparation.

"Students assigned to inorganic, physical, and organic laboratory work will perform at least nine experiments—three from each section."

A. INORGANIC PRACTICALS:

Qualitative Analysis
Separation of the metal ions and determination of any one of them are using volumetric/gravimetric methods.
Cu-Ni, Cu-Zn, Cu-Al, Ca-Ba, Fe-Mg, Fe-Ni etc.

1. Preparations:
Preparation of the following inorganic compounds and their spectroscopic studies.
I. $Hg[Co(SCN)_4]$
II. $[Cu(NH_3)_4]SO_4.H_2O$
III. Prussian Blue and Turnbull's Blue
IV. $Na[Cr(NH_3)_2(SCN)_4]$
V. $Mn(acac)_3$
VI. $[Ni(NH_3)_6]Cl_2$
VII. $VO(acac)_2$

All the students must submit the recrystallized product along with m.p. for all the stages of preparation.

B. PHYSICAL PRACTICALS:

Viscosity

[1] Study the variation of viscosity with concentration for a glycerol solution using Ostwald viscometer and thereafter determine the concentration of unknown solution of glycerol.

[2] Determination of molar mass of a polymer.

Conductometry

[3] Determine the strength of strong acid by conductometric titration with strong base.

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[4] Determine the strength of weak acid by conductometric titration with strong base.

[5] Determine the strength of strong acid and weak acid in a mixture by conductometric titration with strong base.

[6] Study precipitation titration between KCl and $AgNO_3$ conductometrically. Determine the strength of given solution of $AgNO_3$.

[7] Determine solubility and solubility product of sparingly soluble salts like $PbSO_4$, $BaSO_4$.

[8] Determine the relative strength of chloroacetic acid and acetic acid by conductivity measurements.

Adsorption and others

[9] Verify the Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid/oxalic acid on activated charcoal.

[10] Determination of critical solution temperature of phenol-water system.

C. ORGANIC PRACTICALS:

ISOLATION AND PURIFICATION TECHNIQUES

1. Laboratory Safety
2. Crystallization, recrystallization and sublimation
3. Distillation: Simple, Steam and Vacuum
4. Solvent Extraction
5. Drying of ethanol/ acetone/ diethylether/THF
6. Paper Chromatography
7. Thin Layer Chromatography

TWO-STEP PREPARATION OF SOME IMPORTANT ORGANIC COMPOUNDS INVOLVING THE REACTIONS OUT OF THE FOLLOWINGS REPRESENTATIVE REACTIONS)

1. Acetylation (Synthesis of Aspirin, Paracetamol)
2. Esterification and saponification
3. Oxidation
4. Reduction or Hydrogenation
5. Partial Reduction
6. Nucleophilic substitution
7. Aromatic electrophilic substitution reaction
8. Condensation reactions
9. Hoffman's Bromamide reaction
10. Heterocyclic synthesis

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11. Any other reaction as per requirement

All the students must submit the recrystallized product along with m.p. for all the stages of preparation.

Note: Any experiment can be introduced or deleted in the practical class on the basis of availability of instruments/chemicals.

References:

1. A Text Book of Macro and Semi-micro quantitative Analysis, A. I. Vogel, Orient Longman.
2. A Vogel's Text Book of Quantitative Inorganic Analysis, J. Bassett, R. C. Denney, G. B. Jaffery and J. Menaham, Longman, London.
3. Advanced Practical Physical Chemistry by J.B. Yadav, 20th Edition, Goel Publishing House.
4. Experiments in Physical Chemistry by Carl W. Garland, Joseph W. Nibler, and David P. Shoemaker, 8th Edition, McGraw-Hill Education
5. Experimental Physical Chemistry by Farrington Daniels and J.H. Mathews, 7th Edition, McGraw-Hill Education
6. Practical Physical Chemistry by Alexander Findlay, 9th Edition, Longmans, Green and Co.
7. Vogel's Textbook of Quantitative Chemical Analysis by G.H. Jeffery, J. Bassett, J. Mendham, and R.C. Denney, 6th Edition, Pearson
8. Experimental Physical Chemistry by Arthur M. Halpern and George C. McBane, 3rd Edition, W.H. Freeman and Company.
9. A Hand book of Organic Analysis-Qualitative and Quantitative by H.T. Clarke, and revised by B.Haynee, Edward Arnold, London 1975.
10. Vogel's Text Book of Practical Organic Chemistry by B.S. Furhenet. al., Longman-Group Ltd.
11. Systematic Qualitative Organic Analysis by H. Middleton, Edward Arnold (Publishers) Limited, London 1959.
12. Elementary Practical Organic Chemistry by Arthur I. Vogel, EX CBS Publishers and Distributors.
13. Experiments in Organic Chemistry by Louis, F.Fieser, D.C. Heath and Company Boston, 1955.
14. College Practical Chemistry by V. K. Ahluwalia, S. Dhingra and A. Gulati.

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PCDSE-01A: CHEMISTRY OF LIFE SCIENCE

Learning Outcomes

After the completion of this course, the students will be able to:

1. Describe the structures and functions of important carbohydrates and glycoconjugates and explain their significance in biological systems and cellular recognition.
2. Demonstrate knowledge of cell structures and their functions, as well as an understanding of metabolic pathways and lipid biochemistry, including carbohydrate metabolism and lipid aggregates.
3. Able to analyse protein structure and sequence using methods like Sanger and Edman degradation and explain protein denaturation.
4. Explain the structure and function of nucleic acids and describe the molecular mechanisms of replication, transcription, and translation in prokaryotes.

UNIT-1 CARBOHYDRATES

Structure and biological functions of important monosachharides (excluding detailed conformational analysis) and derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars-*N*-acetylmuramic acid and sialic acid. Disaccharides- sucrose, lactose and maltose. Structure and biological functions of Structural polysaccharides (cellulose and chitin) and Storage polysaccharides (starch and glycogen). Heteropolysaccharides-glucosaminoglycans/mucopolysaccharides. Glycoconjugates-glyco proteins and glycolipids.

UNIT-2 CELL STRUCTURE AND METABOLISM

Intracellular organelles and their functions. Overview of metabolic processes-catabolism and anabolism. ATP - the biological energy currency. Carbohydrate metabolism: glycolysis and Kreb's cycle.

Lipids

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids. Lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism-β-oxidation of fatty acids.

UNIT-3 AMINO-ACIDS, PEPTIDES AND PROTEIN

Peptide bond, Chemical and enzymatic hydrolysis of proteins to peptides, Sanger method and Edman degradation method for amino acid sequencing. Secondary structure of proteins-α-helix, β-sheet, forces responsible for holding the secondary structures of proteins. Denaturation of Proteins.

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UNIT-4 NUCLEIC ACIDS AND GENETIC CODE

Structure and functions of nucleotides, nucleosides, DNA (Watson-Crick model, Chargaff's rules) and RNA (m RNA, r-RNA and t-RNA). Genetic code and its characteristics, codon-anticodon pairing (Wobble hypothesis).

Replication, Transcription and Translation (Prokaryotes only)

Replication of DNA: Maselson-Stahl experiment, mechanism of replication (Initiation, Elongation and Termination). Transcription: Promoters site, Initiation, Elongation, Termination. Translation: Activation of amino acids, Initiation, Elongation, Termination.

References:

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.

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PCDSE-01B: MATHEMATICS FOR CHEMIST

Learning Outcomes

After the completion of this course, the students will be able to:

1. Demonstrate proficiency in performing vector operations, including addition, subtraction, multiplication, and differentiation, and apply these concepts to problems in spectroscopy and quantum chemistry.
2. Able to perform matrix operations and use determinants to solve linear equations, applying these concepts to relevant chemical problems.
3. Proficiently use logarithms and graphical techniques to solve chemical problems and analyse experimental data.
4. Able to apply calculus techniques to analyse and solve mathematical problems in chemistry, demonstrating proficiency in differentiation, integration, and differential equations.

UNIT-1 VECTORS

Examples of scalar and vectors, definitions of vectors in two, three spaces, representation and simple properties of vectors, addition and subtraction of vectors, vector addition by the method of triangles, resolution of vectors into rectangular components, addition of vectors by components, multiplication and differentiation of vectors. Scalar product of vectors, vector product, concept of normalization, orthogonality and complete set of unit vectors. Illustration of applications to spectroscopy and quantum chemistry.

UNIT-2 MATRICES AND DETERMINANTS

Definition of matrix, types of matrices, viz. row matrix, column matrix, null matrix, square matrix, diagonal matrix, addition, subtraction and multiplication by a number, matrix multiplication. Transpose and adjoint of matrix, elementary transformation, representation and applications (without development of theory) to solution of linear equations. Definition of determinant, properties of determinants, evaluation of determinants. Illustration or applications to group theory, problems in chemistry.

UNIT-3 LOGARITHM AND GRAPHICAL REPRESENTATION OF EQUATIONS

Need for logarithm in chemistry. Theory and application of logarithms for solving general and chemical problems.

Rectangular coordinates, straight lines, slope and intercept of the equation, slope and point equation, two point equation, parallel lines, points of intersection, distance between two points, change of origin. Examples from problems in chemistry, curve fitting for least squares method. Data analysis, mean and standard deviation, Absolute and Relative errors

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UNIT-4 CHEMICAL MATHEMATICS: FUNCTIONS, DERIVATIVES AND EQUATIONS

Elements of Algebraic and Trigonometric Functions

The binomial expansion, some example from chemistry, sines, cosines and tangents, trigonometric identities, polar coordinates in trigonometric functions.

Differential Calculus

Theory, graphical significance of differentiation, rules of differentiation, Algebraic simplification, Partial differentiation, Exact and inexact differential with their application to thermodynamic principles.

Integral Calculus

Integral theory, methods of integration, viz. algebraic simplifications, substitution, integration by parts, integration by partial fractions, integration between limits, curve sketching, integral as area, , Illustration of application in chemistry.

Differential Equation

Simple differential equations, separable variables, homogeneous equations, exact differential equations, linear differential equations, partial differential equations, application to physico-chemical problems

References

1. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
2. Mathematical Preparation for General Physics, J.B. Marian, R.C. Davidson Saunder Company.
3. Mathematical Methods for Science Students, G. Stephemen, ELBS.
4. Chemical Thermodynamics, R.C. Reid.

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PCMDC-01: CHEMISTRY OF MATERIALS

Learning Outcomes:

After the completion of this course, student will be able to:

1. Understand the basic principles and importance of materials chemistry.
2. Compare the structures, properties, and applications of metals, ceramics, polymers, composites, and nanomaterials..
3. Explain various synthesis and characterization techniques used in materials chemistry..
4. Evaluate the applications of materials in energy, electronics, and medicine, and assess their environmental impact and sustainability.

UNIT-1 INTRODUCTION TO MATERIALS CHEMISTRY

Definition and importance of materials chemistry; Classification of materials: metals, ceramics, polymers, composites, and nanomaterials; Structure-property relationships in materials; Basic concepts of crystallography: unit cell, crystal systems, Bravais lattices.

UNIT-2 CLASSES OF MATERIALS AND THEIR PROPERTIES

Metals and Alloys Structure, properties, and applications; Ceramics: Structure, properties, and applications; Polymers: Types of polymers, polymerization mechanisms, properties, and applications; Composites: Types, properties, and applications; Nanomaterials: Unique properties, synthesis methods, and applications.

UNIT-3 SYNTHESIS AND CHARACTERIZATION OF MATERIALS

Synthesis Techniques

Solid-state synthesis, sol-gel process, hydrothermal synthesis, chemical vapor deposition (CVD), and physical vapor deposition (PVD);

Characterization Techniques:

X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA)

~~UNIT-3~~ 4 APPLICATIONS AND SUSTAINABILITY OF MATERIALS

Applications in Electronics: Semiconductors, conductors, and insulators; Applications in Energy: Batteries, fuel cells, and solar cells; Applications in Medicine: Biomaterials and drug delivery systems; Environmental and Sustainability Aspects: Recycling and waste management of materials; Green chemistry approaches in material synthesis.

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References:

1. Materials Science and Engineering: An Introduction by William D. Callister Jr., Wiley.
2. Introduction to Solid State Chemistry by Michael J. Van Valkenburg, Prentice Hall.
3. The Science and Engineering of Materials by Donald R. Askeland and Pradeep P. Phule, Cengage Learning.
4. Nanostructures and Nanomaterials: Synthesis, Properties, and Applications by Guozhong Cao and Ying Wang, Imperial College Press.
5. Fundamentals of Materials Science and Engineering by William D. Callister Jr. and David G. Rethwisch, Wiley.
6. Material Science and Metallurgy for Engineers by Dr. V.D. Kodgire and S.V. Kodgire, Everest Publishing House.
7. Materials Science and Engineering by V. Raghavan, Prentice-Hall of India.

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PCVAC-01: GREEN CHEMISTRY

Learning Outcomes:

After the completion of this course, student will be able to:

1. Understanding of the fundamental principles of green chemistry.
2. Ability to design and develop sustainable chemical processes.
3. Apply green chemistry principles to design sustainable reactions using alternative solvents, energy-efficient methods, and atom-economical strategies.
4. Understanding of the industrial applications and future aspects of green chemistry.

UNIT-1 GREEN CHEMISTRY: PRINICIPALS AND PRACTICES

Definition and principles of green chemistry, twelve principles of green chemistry, History and evolution of green chemistry, Benefits of green chemistry, Green chemistry metrics: Atom economy, Efactor, Role of green chemistry in sustainable development

UNIT-2 GREEN SYNTHESIS AND CATALYSIS

Green solvents: Supercritical fluids, Ionic liquids, Water, Green reagents and catalysts, Biocatalysis in green chemistry, Microwave and ultrasonic-assisted synthesis, Photocatalysis and electrocatalysis, Case studies of green synthesis in industry

UNIT-3 GREEN TECHNOLOGY

Reactions under aqueous medium: Enhancement of selectivity, efficiency and industrial applicability. Solvent free reactions in solid & liquid phase, Ionic liquids; Supercritical fluids, Microwave and Ultrasound assisted reactions; photochemical reactions using sunlight. Atom economy.

UNIT-4 FUTURE TRENDS

Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrin and supported catalyst; Phase-transfer catalysis; Biocatalysis using enzymes; Biomass conversion to fine chemicals. Flow techniques; combinatorial green chemistry

References:

1. New Trends in Green Chemistry, V.K. Ahluwalia and M. Kidwai, Kluwer Academic Publishers.
2. Handbook of Green Chemistry and Technology, James Clark and Duncan Macquarrie, Blackwell Publishing
3. An Introductory Text on Green Chemistry, Indu Tucker Sidhwani and Rakesh K. Sharma, Wiley Publisher

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PCSC-04: INORGANIC CHEMISTRY - II
(Transition and organometallic complexes)

Learning Outcomes:

After completing this course, students will be able to:

1. Forecast the electronic and magnetic properties of coordination compounds.
2. Have a good overview of the fundamental principles of organotransition-metal chemistry and know how chemical properties are affected by metals and ligands
3. Understand fundamental reaction types and mechanisms of organometallic compounds and how to combine these to understand efficient catalytic processes.
4. Describe the roles of organometallic ions in biological systems and explain the function of metalloproteins and metalloenzymes.

UNIT-1 ELECTRONIC SPECTRA AND MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES

Electronic arrangements of microstates, calculation of the number of microstates in various electronic arrangements, spectroscopic term symbols and splitting of terms in free atoms, determining the ground state terms, correlation and spin-orbit coupling in free ions for I^{st} series of transition metals. Interpretation of electronic spectra; Orgel (d^1 – d^9 states) and Tanabe-Sugano diagrams (d^2 and d^3 octahedral) for transition metal complexes, Spectrochemical and nephelauxetic series, calculation of Dq, B, β parameters, charge transfer spectra, magnetic properties; anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT-2 ORGANOMETALLIC CHEMISTRY

Synthesis and applications of BuLi, Grignard, organoaluminum and organozinc reagents. 18 electron rule. Metal carbonyls and nitrosyls: bonding and infrared spectra. Spectator ligands: Phosphines and NHC's, Alkenes and alkynes, carbenes and carbynes, Hapto ligands with hapticity from 2-8.

Metal alkyls, allyls and cyclopentadienyl derivatives. Hydrides, Metallocenes, Metal arene complexes. Carbonylate anions, agostic interaction. Fluxional molecules. Metal-Metal bonding and Metal clusters. Synthesis and reactivity of Fischer and Schrock carbenes.

UNIT 3: REACTIONS ORGANOMETALLIC COMPLEXES

Oxidative addition, reductive elimination, 1,1 and 1,2-migratory insertions and beta hydrogen elimination, insertion and deinsertion. Mechanism of substitution reactions, fluxionality and hapticity change, organometallic clusters, C-H activation- agostic and anagostic interactions.

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Homogeneous catalysis: hydrogenation, hydroformylation, methanol to acetic acid processes, Wacker oxidation.

UNIT 4: ROLE OF ORGANOMETALLIC CHEMISTRY IN BIOINORGANIC CHEMISTRY

Metal ions in biological systems- heme proteins, hemoglobin, myoglobin, ferritin, transferrin, cytochromes and vitamin B_{12}; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems. Porphyrin systems: Dioxygen Transport- Hemoglobin, Hemerythrin and Hemocyanin. Cooperativity in O_2 binding, O_2 and CO discrimination. Oxygen Metabolism - Oxygen atom transfer by cytochromes-P_{450} - Nitrogenases - Carbonic anhydrase – Carboxypeptidase-Alcohol dehydrogenase - Photosystem.

References

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, Harper & Row.
3. Modern Aspects of Inorganic Chemistry; H.J. Emeleus and Sharpe.
4. Organometallic Chemistry; R.C. Mehrotra and A. Singh, New Age International.
5. The Organometallic Chemistry of the Transition Metals; R.H. Crabtree, John Wiley.
6. Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition Metals, Universities Press, by B.D. Gupta and A.J. Elias.
7. Bio Inorganic Chemistry, Ellis Horwood, 1987 by R.W. Hay,
8. Bioinorganic Chemistry, John Wiley, 2002 by R.M. Roat-Malone,
9. Bioinorganic chemistry, Oxford University Press India, by D. Rehder and E. Nordlander.
10. Bioinorganic Chemistry by A.K. Das.

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PCSC-05: PHYSICAL CHEMISTRY - II
(Thermodynamics, Kinetics and Polymerization)

Learning Outcomes:

Upon successful completion of this course, students will be able to:

1. Utilize thermodynamic laws to determine entropy and other state functions.
2. Analyze the behavior of solutions using activity, fugacity, and phase rule concepts.
3. Interpret complex chemical reaction mechanisms using kinetic theories and approximations like steady-state and transition state theory
4. Explain the kinetics and mechanisms of polymerization processes and determine polymer molecular weights using various techniques.

UNIT-1 THERMODYNAMICS CONCEPTS:

Statements of the Third Law of Thermodynamics, Nernst Heat Theorem and its application to noncondensed systems, Determination of entropy from the Third Law using the correction due to gas imperfections. Calorimetric entropy, Spectroscopic entropy, Comparison of calorimetric and Spectroscopic entropies, Raoult's laws, Henry's law, solubility behaviour of ideal solutions.

UNIT-2 ACTIVITY, FUGACITY, PHASE RULE

Concepts of fugacity, fugacity of gases and its determination. Activity and activity coefficient, choice of standard states, determination of activity coefficient for solute and solvent.

Phase Rule

Phase Rule and its determination, application, Phase diagram for one component system, for two completely miscible components systems like Pb-Ag system, KI+ H_2O system, Bi-Cd system, Ferric chloride + water system, Sodium chloride + water system, Na_2SO_4-H_2O system

UNIT-3 CHEMICAL KINETICS-I

Empirical rate laws and temperature dependence; kinetics of complex reactions; equilibrium state and steady state approximation; determination of reaction mechanisms; theories of chemical reaction rates: collision theory, transition state theory, comparison of collision and absolute reaction rate theory, transition state theory in solution.

Chain Reactions: Hydrogen-bromine reaction, Pyrolysis of acetaldehyde, Decompositions of ethane. Photochemical reactions (hydrogen-bromine and hydrogen-chlorine reactions).

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General treatment of chain reaction (hydrogen- bromine reactions), Apparent activation energy of chain reactions, Chain length, Rice-Herzfeld mechanism of organic molecules decomposition (acetaldehyde).

UNIT-4 POLYMERIZATION

Basics of Polymers and Polymerization, Kinetics of Polymerization: Mechanism and Kinetics of chain-growth polymerization: free-radical, cationic, anionic, and coordination polymerization. Mechanism and Kinetics of step-growth polymerization. Comparison between step-growth and chain polymerization.

Molecular mass of Polymers: Concept of number average and mass average molecular weights, Methods of determination of molecular weights (1) viscometry (2) osmometry (3) sedimentation (4) Light Scattering methods (5) GPC method.

References

1. Chemical Bonding and Molecular Structure by M. L. McKee (Wiley, 2020).
2. Modern Thermodynamics: From Heat Engines to Dissipative Structures by Dilip Kondepudi and Ilya Prigogine (Wiley, 2014).
3. Introduction to Chemical Engineering Thermodynamics by J. M. Smith, Hendrick Van Ness, and Michael Abbott (McGraw-Hill, 2005).
4. Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon (University Science Books, 1997).
5. Physical Chemistry by Peter Atkins and Julio de Paula (Oxford University Press, 2014).
6. Principles of Physical Chemistry by Puri, Sharma and Pathania (Vishal Publishing Co.).
7. A Textbook of Physical Chemistry by K. L. Kapoor (McGraw Hill Education).

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PCSC-06: ORGANIC CHEMISTRY - II
(Reaction Mechanism-II and Stereochemistry)

Learning Outcomes:

After the completion of this course, the students will be able to:

1. Utilize addition reactions to carbon-heteroatom multiple bonds and key condensation reactions to synthesize and modify functionalized organic compounds.
2. Evaluate the structure, stability, and reactivity of free radicals, and carbocations to rationalize reaction outcomes and Interpret the role of neighbouring group participation in rearrangement reactions.
3. Able to analyse and interpret the stereochemical properties and configurations of organic molecules, including simple, cyclic, and acyclic systems.
4. Accurately analyse and determine the stereochemistry of complex molecules, including sugars and decalins

UNIT-1 ADDITION TO CARBON-HETERO ATOMS MULTIPLE BONDS

Addition to Carbon-Hetero Atoms Multiple Bonds

General mechanistic considerations and reactivity, Hydration and Addition of Alcohols to Aldehydes, Ketones and Acids. Addition -Elimination Reactions of Ketones and Aldehydes, Reactivity of carbonyl compounds towards Addition.

Lithium aluminium hydride reduction- carbonyl compounds, acids, esters, nitriles. Additions of Grignard reagents. Reformatsky reaction, Wittig reaction, Claisen condensation, Dieckman reaction, Aldol condensation, Knoevenagal condensation, Perkin reaction, Cannizzaro reaction, Benzoin condensation, Mannich Reaction, Robinson-Mannich reaction, Ester hydrolysis, aminolysis of esters, amide hydrolysis.

UNIT-2 NGP, CARBOCATION REARRANGEMENTS AND FREE RADICALS

Neighbouring Group Participation and Carbocation Rearrangements

Anchimeric assistance, neighbouring group participation by non-bonding electrons, sigma and π-bonds, classical and non-classical carbocations.

Carbocations rearrangements: migratory aptitudes, Wagner Meerwein rearrangement, pincol pinacolone rearrangement, Demjanove rearrangement, Tiffeneau-Demjanov ring expansion, aldehyde-ketone rearrangement, dienone-phenol rearrangement and trans-annular rearrangements.

Free Radicals

General aspects of generation, structure, stability and reactivity of free radicals, types of free radical reactions, halogenation including allylic halogenation (NBS), auto-oxidation,

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decomposition of azo compounds and peroxides, coupling of alkynes, homolytic aromatic substitution, Sandmeyer reaction and Hunsdiecker reaction

UNIT-3 STEREOCHEMISTRY-I

Symmetry elements, D-L, R-S, E-Z and threo-erythro nomenclature, interconversion of Fischer, Newman, Sawhorse and flying wedge formulae. conformational analysis, enantiomerism and diastereomerism of simple, cyclic (chair and boat configuration) and acyclic systems. Axial and planer chirality, optical isomerism in allenes, biphenyls (atropoisomerism), spiranes, hemispiranes.

UNIT-4 STEREOCHEMISTRY-II

Topicity of ligands and faces, their nomenclature and prostereoisomerism, stereogenecity, chirogenicity, pseudoasymmetry and prochiral centre. stereospecific and stereoselective reaction. Elementary idea of principle categories of asymmetric synthesis, Cram's rule and its modification, Prelog rule and horeaus rule. Stereochemistry of sugars-C1 and 1C conformations of hexoses, c_2'-endo and c_3'-endo conformation of pentoses, homomorphous sugars, abnormal mutarotation and Δ-2 instability factor. Stereochemistry of decalins

Reference:

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. O. House, Benjamin.
7. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
9. Organic Reactions and their Mechanisms (Multi Colour Edition), New Age International Private Limited, 5th Edition, 2020, P.S. Kalsi
10. Stereochemistry of Organic Compounds; Wiley: London. Eliel, E.L., Wilen, S.H. (1994)

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PCLAB-02 CHEMISTRY LAB-II

Learning Outcomes

1. Examine the given inorganic mixture qualitatively.
2. Perform and interpret experiments involving calorimetry, phase behavior, and thermodynamic measurements.
3. Perform qualitative analysis of organic binary mixtures using systematic separation and identification techniques.

"Students assigned to inorganic, physical, and organic laboratory work will perform at least nine experiments—three from each section."

A. INORGANIC PRACTICALS:

Qualitative analysis:

Total five radicals to be given containing two less common metal ions, one insoluble and two acid radicals: $CH_3COO^-, BO_3^{3-}, PO_4^{3-}, CO_3^{2-}, HCO_3^-, NO_2^-, NO_3^-, Cl^-, Br^-, I^-, S^{2-}, SO_3^{2-}, SO_4^{2-}, S_2O_3^{2-}, F^-, C_2O_4^{2-}$.

Less common metal ions – W, Tl, Mo, Se, Ti, Zr, Th, V, U, Ce, Be (two metal ions in cationic and anionic forms)

Insoluble: Halides (AgCl, AgBr, AgI); Sulphates ($PbSO_4$, $BaSO_4$) and Oxides (Al_2O_3, Cr_2O_3, SnO_2, TiO_2, SiO_2)

B. PHYSICAL PRACTICALS

1. To draw the mutual solubility curve of two immiscible liquids and find out the critical solution temperature of phenol-water system.
2. To obtain the phase diagram of water–ethanol-benzene system at room temperature.
3. To verify the Debye-Huckel-Onsager law for strong electrolytes using conductometer.
4. To determine the partial molar volume of urea and ethanol in aqueous solution from density measurements..
5. To determine the heat of neutralization of sulphuric acid using calorimeter.
6. To determine the heat of ionization of a weak base i.e. NH_4OH using calorimeter.
7. To find surface tension/interfacial tension between two immiscible liquids.
8. To determine the percentage composition of a given mixture of two liquids say CCl_4 and Toluene by surface tension method.

C. ORGANIC PRACTICALS

Organic Mixture Analysis

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1. Qualitative Analysis: Demonstrations of separation of binary mixtures (Solid-Solid): using H_2O, HCl, NaOH, $NaHCO_3$, Ether or other reagent as may be necessary along with required conditions for their use.

Systematic identification of organic mixtures: separation and identification of binary mixtures including derivatives, in the formation of individual components.

2. Spectroscopic confirmation of the binary mixtures using IR and NMR (IR & NMR spectra will be provided).

Note: Any experiment can be introduced or deleted in the practical class on the basis of availability of instruments/chemicals.

References

1. Qualitative Inorganic Analysis by Arthur I. Vogel and F.G. Svehla
2. Practical Inorganic Chemistry by O.P. Pandey, D.N. Bajpai, S. Giri
3. Advanced Practical Inorganic Chemistry by Gurdeep Raj
4. Qualitative Chemical Analysis and Instrumental Methods by G. Chatwal and S. Anand
5. Comprehensive Practical Chemistry by N.K. Verma, S.K. Khanna, and B. Kapila
6. Advanced Practical Physical Chemistry by J.B. Yadav, 20th Edition, Goel Publishing House.
7. Experiments in Physical Chemistry by Carl W. Garland, Joseph W. Nibler, and David P. Shoemaker, 8th Edition, McGraw-Hill Education.
8. Experimental Physical Chemistry by Farrington Daniels and J.H. Mathews, 7th Edition, McGraw-Hill Education.
9. Practical Physical Chemistry by Alexander Findlay, 9th Edition, Longmans, Green and Co.
10. Vogel's Textbook of Quantitative Chemical Analysis by G.H. Jeffery, J. Bassett, J. Mendham, and R.C. Denney, 6th Edition, Pearson.
11. Experimental Physical Chemistry by Arthur M. Halpern and George C. McBane, 3rd Edition, W.H. Freeman and Company.
12. "A Handbook of Organic Analysis Qualitative and Quantitative" by H.T. Clarke and revised by B.Maynes, Edward Arnold (Pub.). Ltd. London, 1975).
13. "Systematic Qualitative Organic Analysis" by H.Middleton, Edward Arnold (Publishers) Ltd., London 1959.
14. "A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis" by Arthur I. Vogel, Longmans Green and Co., Ltd., London 1966.
15. "Elementary Practical Organic Chemistry" by Arthur I. Vogel, CBS Publishers & Distributors.
16. "A Guide to spectroscopy in Organic Chemistry' by PAVY

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17. "Organic Spectroscopy', 3rd Ed., by William Kamp. John Wiley & Sons.
18. "Spectroscopic" Methods in Organic Chemistry, D.H. William & Ian Fleming.
19. Vogel's Text Book of Practical Organic Chemistry by B.S. Furnerset. al., Longman Group Ltd.

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PCDSE-02: SPECTROSCOPIC METHODS IN CHEMISTRY-I

Learning Outcomes

1. Identify and differentiate between various electronic transitions ($\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$) in organic molecules.
2. Interpret chemical shift values and correlate them with proton environments in various organic compounds.
3. Fundamental principles of IR spectroscopy and interpret characteristic vibrational frequencies of functional groups.
4. Differentiate between proton-coupled and proton-decoupled ^{13}C-NMR spectra and assign chemical shifts to various carbon environments.

UNIT 1: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

Introduction and understanding of UV phenomenon, Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds.

UNIT 2: INFRARED SPECTROSCOPY

Principle and Theory, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance. FT-IR.

UNIT-3 NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY-I

Basic principles of NMR, theory of nuclear magnetic resonance, spin lattice relaxation, spin-spin relaxation, experimental techniques chemical shift, the δ-scale of chemical shift, the origin of shielding constant, pattern of coupling, origin of spin-spin coupling, Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic).

UNIT-4 NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY-II

Chemical shift values and correlation for protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), complex spin-spin interaction between two, three, four and five nuclei (first order spectra), spin system-Pople notation, Karplus curve - variation of coupling constant with dihedral angle. Fourier transform technique.

Carbon-13 NMR Spectroscopy

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References:

1. Handbook of Molecular Spectroscopy, From Radio waves to gamma rays, By D.N. Sathyanarayana, I.K international Publishing House Pvt. Ltd, 2015.

2. Fundamentals of Molecular Spectroscopy, By C.N. Banwell Tata McGraw Hill, 4th Edition, 1996.

3. NMR Spectroscopy by Gunther John Wiley and Sons, 2nd Edition, 1995.

4. Organic Spectroscopy by Kemp. ELBS-Macmillan, 2nd Edition, 1987.

5. Spectra of Atoms and Molecules by P.F. Bernath, Oxford University Press, 2nd Edition, 2005

6., High-Resolution NMR Techniques on Organic Chemistry by D.W. Claridge, Pergamon, New York, 3rd Edition, 2016.

7. A Complete Introduction to Modern NMR Spectroscopy, By R. S. Macomber Wiley, 1st Edition, 1997.

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PCSEC-01: ANALYTICAL TECHNIQUES IN CHEMISTRY

Learning Outcomes:

After the completion of this course, student will be able to:

1. Basic understanding of analytical chemistry.
2. Use of thermogravimetric, imaging and polarization techniques in daily life.
3. Skills for analyzing and developing new sustainable methods.
4. Skills for developing industrially important analytical methods.
5. Development of alternate analytical methods.
6. Use of advanced and recent techniques in analytical chemistry.

UNIT 1: STATISTICAL ANALYSIS

Errors: Precision and accuracy, Classification of errors, methods of minimization and elimination of errors; Statistical methods: Treatment of random errors, reliability of results, rounding up of results from chemical computation, confidence interval, Normal error curve and its importance; Comparison of results: students t-test, F-test and linear regression for deriving calibration plots.

UNIT 2: ANALYTICAL TECHNIQUES

Chromatography - Fundamentals, working Principles, classification, optimization of chromatographic conditions; Gas chromatography - Instrumentation and working principle. Applications; High-Performance Liquid Chromatography (HPLC): Principles and Components, Instrumentation, principles of preparative HPLC, applications; Electrophoresis and capillary *electrophoresis* - Principle, Classification, instrumentation and applications

UNIT 3: ADVANCED SPECTROSCOPIC

Principle, instrumentation; Spectral and chemical interferences, applications in qualitative and quantitative analysis (determination of metal in blood serum, Mg/Ca in hard water, Pb in petrol etc.); Atomic Emission Spectroscopy: Principles, Instrumentation and applications; Flame emission spectrometry: Principles, instrumentation and interferences, applications (determination of alkali metals, iron in non-ferrous alloys etc.) and Limitations. Inductively coupled plasma (ICP) spectrometry: Principles, Instrumentations and applications.

UNIT 4: THERMAL ANALYSIS TECHNIQUES

Introduction to thermogravimetry; Principles and applications of TGA and DTA, decomposition analysis curve of $MgC_2O_4.H_2O$ and $Ca(OOCCH_3)_2.H_2O$; Simultaneous DTA

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and TGA curves. *DSC*- Principles, Instrumentation, and application; Comparison of DTA and DSC. Electrogravimetry: Principles, Instrumentation, Electro gravimetric determination with constant applied voltage and at constant current and applications.

Reference Books

1. Fundamentals of analytical Chemistry By D.A. Skoog, D.M. West, and F.J. Holler, Cengage Learning India Pvt. Ltd.; 10th Edition, 2022.

2 Analytical Chemistry By R.A. Day, Jr. and A.L. Underwood Pearson, 6th Edition, 2015.

3. Instrumental methods of chemical analysis By H. Kaur Pragati Prakashan, 12th Edition, 2016.

4. Vogel's Textbook of Quantitative By G.H. Jeffery, J. Bassett, J. Mendham, and R.C. Denney, Chemical Analysis, Longman Scientific and Technical, 6th Edition, 2008.

5. Basic Concepts of Analytical Chemistry by S.M. Khopkar, New Age International Ltd, 3rd Edition, 2011.

6. Modern Analytical Chemistry by D. Harvey,, McGraw-Hill Education, 1st Edition, 1999.

7. Analytical Chemistry by G.D. Christian, P.K. Dasgupta, K.A. Schug, Wiley, 7th Edition, 2020

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PCMDC-02: DRUG DESIGN AND DISCOVERY

1. Understand the principles of drug classification, discovery, and design, including structure-activity relationships (SAR) and mechanisms of drug action.
2. Gain knowledge of drug development processes such as screening, isolation, purification, and the role of pharmacokinetics and prodrugs.
3. Acquire insights into the synthesis, mechanisms, and therapeutic uses of antineoplastic agents and antimalarials.
4. Develop a comprehensive understanding of the synthesis, action, and medicinal uses of analgesics, antipyretics, and anti-inflammatory agents.

UNIT-1 FUNDAMENTALS OF DRUG DESIGN

Classification and discovery of new drugs, Drug development: screening of natural products, isolation and purification, structure determination, structure-activity relationships (SAR), synthetic analogues, isosteres, and bioisosteres, Concept of lead compounds, therapeutic index, LD_{50}, and ED_{50}, Elementary idea about drug action: receptor role, neurotransmitters and receptors, ion channels, and their control, Membrane-bound enzymes: activation/deactivation.

UNIT-2 DRUG DEVELOPMENT

Screening of natural products, isolation and purification, structure determination structure-activity relationships (SAR), synthetic analogues, isosteres and bioisosteres, concept of lead compounds. Brief overview of pharmacokinetics and pharmacodynamics, concept of prodrugs.

UNIT-3 SPECIALIZED DRUGS AND THEIR APPLICATIONS-I

Antineoplastic Agents: Synthesis, general mode of action and medicinal uses of Mechlorethamine, Chlorambucil, Cyclophosphamide, Carmustine, Aminopterin, 6-Mercaptopurine, Paclitaxel (synthesis of paclitaxel excluded).

Antimalarials: Synthesis, general mode of action and medicinal uses of Chloroquine, Primaquine, Chloroguanide, Pyrimethamine.

UNIT-4 SPECIALIZED DRUGS AND THEIR APPLICATIONS-II

Analgesics, Antipyretics, and Anti-inflammatory Agents: Synthesis, general mode of action and medicinal uses of Morphine and related compounds (Codeine and Heroin), Meperidine, Methadone, Aspirin, Acetaminophen, Phenylbutazone, Mefenamic Acid, Ibuprofen, Diclofenac, Naproxen, Celecoxib.

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References

1. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
2. Burger's Medicinal Chemistry and Drug Discovery Vol-I Ed. M.E. Wolf, John Wiley.
3. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
4. Organic Chemistry Vol.-2 I. L. Finar, ELBS.
5. R. B. Silverman, The Organic Chemistry of Drug Design and Drug Action, 3rd Edition. Academic Press, 2014.
6. G. L. Patrick, an Introduction to Medicinal Chemistry, 5th Edition. Oxford University Press, 2013.
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