Cotton University

Panbazar, Guwahati–781001

Syllabus for Four-Year UG Programme (FYUGP) in Chemistry

January, 2024

Programme Learning Objectives (PLOs):

PLO-1: To provide broad and balanced knowledge in chemistry in addition to understanding of key chemical concepts, principles and theories.

PLO-2: To develop students' ability and skill to acquire expertise over solving both theoretical and applied chemistry problems.

PLO-3: To educate and prepare graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic laboratories.

PLO-4: To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of all branches of chemistry involving applied organic, inorganic, physical, analytical, quantum, industrial, pharmaceutical, polymer, Nanoscience & technology.

PLO-5: To expose the students to a breadth of experimental techniques using modern instrumentation.

PLO-6: To mould a responsible citizen who is aware of the most basic domain-independent knowledge, including of critical thinking and communication.

PLO-7: To enable the graduate, prepare for national as well as international competitive examinations, especially UGC-CSIR NET, GATE and UPSC Civil Services Examination.

PROGRAMME SPECIFIC OUTCOMES (PSOs)

The student graduating with the Degree B.Sc. (Chemistry Core) will be able to acquire:

PSO-1: Systematic and coherent understanding of the fundamental concepts in Physical Chemistry, Organic Chemistry, Inorganic Chemistry, Analytical Chemistry and all other related allied chemistry subjects.

PSO-2: Students will be able to use the evidence-based comparative chemistry approach to explain the chemical synthesis and analysis.

PSO-3: Students will be able to understand the characterisation of materials.

PSO-4: Students will be able to understand the basic principles of equipments/instruments used in the chemistry laboratory.

PSO-5: Students will be able to demonstrate the experimental techniques and methods encountered in their course in chemistry.

PSO-6: Discipline's Knowledge and Skills – A graduate student is expected to be capable of demonstrating comprehensive understanding of both theoretical and experimental/applied chemistry knowledge in various fields of interest like Analytical Chemistry, Physical Chemistry, Inorganic Chemistry, Organic Chemistry, Material Chemistry, etc. Further, the student will be capable of using of advanced instruments and related software for in-depth characterisation of materials/chemical analysis and separation technology.

PSO-7: Skilled Communicator – The course curriculum incorporates basics and advanced training in order to make a graduate student capable of expressing the subject through technical writing as well as through oral presentation.

PSO-8: Critical Thinker and Problem Solver – The course curriculum also includes components that is helpful for graduate students to develop critical thinking ability by way of solving numerical/non-numerical problems using basic chemistry knowledge and concepts.

PSO-9: Sense of Inquiry – It is expected that the course curriculum will develop an inquisitive characteristic among the students through appropriate questions, planning and reporting experimental investigation.

PSO-10: Team Player – The course curriculum has been designed to provide opportunity to act as team player by collaborating in laboratory, field-based situations and industry.

PSO-11: Skilled Project Manager – The course curriculum has been designed in such a manner as to enable a graduate student to become a skilled project manager by acquiring knowledge about chemistry project management, writing, planning, study of ethical standards, and rules and regulations pertaining to scientific project operation.

PSO-12: Digitally Literate – The course curriculum has been so designed to impart a good working knowledge in understanding and carrying out data analysis, use of online library search tools, and use of chemical simulation software and related computational work.

PSO-13: Ethical Awareness – A graduate student requires to understand and to develop ethical awareness which the course curriculum adequately provides.

PSO-14: Lifelong Learner – The course curriculum is designed to inculcate a habit of learning continuously through use of advanced ICT techniques and other available techniques/books/journals for personal academic growth as well as for increasing employability opportunity.

Mapping of PSO and Chemistry Courses

Table-1

	Core-1	Minor – I	MDE - I	AEC	SEC - I	Core-2	Minor - II	MDE - II	AEC	SEC - II	Core-3	Core-4	Minor-III	MDE - III	AEC	SEC - III	Core - 5	Core - 6	Core - 7	Minor - IV	AEC	Summer Internship
	Chemistry	Chemistry	Molecular Basis of Matter	English Comm. 1	Chemical Analysis for Everyday Life	Chemistry	Chemistry	Fuels and Pollutants	MIL 1	Tools in Computational Chemistry	Inorganic Chemistry - I	Organic Chemistry - I	Chemistry	Chemistry in Daily Life	English Comm. 2	Chemistry Tools for Pollution Studies	Inorganic Chemistry – II	Organic Chemistry – II	Physical Chemistry -1	Chemistry	MIL 2	
														√	√		√	√	√		√	
PSO1	√	√	√		√	√	√		√	√	√	√	√	√	√		√	√	√		√	
PSO2	√	√	√		√	√	√		√	√	√		√	√	√		√	√	√		√	
PSO3	√	√	√		√	√	√		√	√	√		√	√	√		√	√	√		√	
PSO4	√	√	√		√	√	√		√	√	√		√	√	√		√	√	√		√	
PSO5	√	√	√		√	√	√		√	√	√		√	√	√		√	√	√		√	
PSO6	√	√	√		√	√	√		√	√	√	√	√	√	√		√	√	√		√	
PSO7	√	√	√		√	√	√		√	√	√		√	√	√		√	√	√		√	
PSO8	√	√	√		√	√	√		√	√	√	√	√	√	√		√	√	√		√	
PSO9	√	√	√		√	√	√		√	√	√	√	√	√	√		√	√	√		√	
PSO10	√	√	√		√	√	√		√	√	√		√		√	√			√	√		
PSO11			√	√			√	√				√	√			√				√		
PSO12				√				√				√	√	√	√	√	√	√	√	√	√	
PSO13	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	√	
PSO14	√	√	√	√	√	√	√	√	√	√	√	√	√				√	√	√	√	√	

Table- 2

	Core-8 Inorganic Chemistry- III	Core-9 Organic Chemistry- III	Core-10 Physical Chemistry - II	Core-11 Quantum Chemistry	Minor - V Chemistry	Core-12 Inorganic Chemistry - IV	Core-13 Organic Chemistry - IV	Core-14 Physical Chemistry - III	Core-15 Molecular Spectroscopy	Minor- VI Chemistry	Core-16 Group Theory and Spectroscopy of Inorganic Compounds	Core-17 Advanced Organic Chemistry	Core-18 Research Methodology	Core-18* Chemistry of Nanomaterials	Core- 21*/Core 21** Industrial Chemistry / Heterogeneous Catalysis	Minor - VII Chemistry	Core-19 Advanced Physical Chemistry	Core- 20 Analytical and Instrumental Method of Chemical Analysis	Core – 22* Environmental and Green Chemistry	Core -23*/Core-23** Natural Products and Medicinal Chemistry / Supramolecular Chemistry	Minor - VIII Chemistry
PSO1	√	√	√			√	√	√			√	√	√	√	√						√
PSO2	√	√	√			√	√	√			√	√	√		√	√	√	√	√	√	√
PSO3	√	√	√			√	√	√			√	√	√		√	√	√	√		√	√
PSO4	√	√	√			√	√	√			√	√	√		√	√	√	√		√	√
PSO5	√	√	√			√	√	√			√	√	√		√	√	√	√		√	√
PSO6	√	√	√			√	√	√			√	√	√	√	√	√	√	√		√	√
PSO7	√	√	√			√	√	√			√	√	√		√	√	√	√	√	√	√
PSO8	√	√	√			√	√	√			√	√	√	√	√	√	√	√		√	√
PSO9	√	√	√			√	√	√			√	√	√	√	√	√	√	√	√	√	√
PSO10	√	√	√			√	√	√			√	√	√		√	√	√	√	√	√	√
PSO11			√	√				√	√					√	√	√	√	√		√	
PSO12				√					√					√	√				√	√	
PSO13	√	√	√	√		√	√	√	√		√	√	√	√	√				√	√	√
PSO14	√	√	√	√		√	√	√	√		√	√	√	√	√	√	√	√	√	√	√

Semester-wise Course and Credit distribution for FYUGP at Cotton University:

Minimum Credit required for the complete programme: 160

Semester	Major (Core) Each paper is of 4 Credits	Minor Each Paper of 4 Credits	MDE Each paper of 3 Credits	AEC Each Paper of 2 Credits	SEC Each paper of 3 Credis	Summer Internship 2 Credits	VAC Each paper of 2 Credits	Total Credits
I	Core 1 (Level 100)	Minor - I (Level 100)	MDE - I	AEC English Comm. 1	SEC - I		VAC 1 VAC 2	20
II	Core 2 (Level 100)	Minor - II (Level 100)	MDE - II	AEC MIL 1	SEC - II		VAC 3 VAC 4	20
III	Core 3 (Level 200) Core 4 (Level 200)	Minor - III (Level 200)	MDE - III	AEC English Comm. 2	SEC - III			20
IV	Core 5 (Level 200) Core 6 (Level 200) Core 7 (Level 200)	Minor - IV (Level 200)		AEC MIL 2		Summer Intern		20
V	Core 8 (Level 300) Core 9 (Level 300) Core 10 (Level 300) Core 11 (Level 300)	Minor - V (Level 200)						20
VI	Core 12 (Level 300) Core 13 (Level 300) Core 14 (Level 300) Core 15 (Level 300)	Minor - VI (Level 200)						20
VII	Core 16 (Level 400) Core 17 (Level 400) Core 18 (Level 400) Core 18* (Level 400)	Minor - VII (Level 300)			Dissertation/Project of 12 credits over semester VII and VIII, for Honours with Research Degree, only if CGPA ≥ 7.5 up to semester VI. In semester VII, evaluation of 4 credits *Students without research must take Core 18* and			20

	Core 21*/Core21** (Level 400)				Core 21*/Core 21** in VII semester	
VIII	Core 19 (Level 400) Core 20 (Level 400) Core 22* (Level 400) Core 23*/Core 23** (Level 400)	Minor - VIII (Level 300)			Dissertation/Project Evaluation of the remaining 8 credits in semester VIII *Students not having dissertation/Project must take Core 22* and Core23*/Core 23** in this semester	20

Cotton University

Syllabus for Four-Year UG Programme in Chemistry

List of Contents

Topics

19. Core 18 (Research Methodology) for Semester VII
20. Core 18* (Chemistry of Nanomaterials) for Semester VII
21. Core 21* (Industrial Chemistry) for Semester VII
22. Core 21** (Heterogeneous Catalysis) for Semester VII
23. Core 19 (Advanced Physical Chemistry) for Semester VIII
24. Core 20 (Analytical and Instrumental Method of Chemical Analysis) for Semester VIII
25. Core 22* (Environmental and Green Chemistry) for Semester VIII
26. Core 23* (Natural Products and Medicinal Chemistry) for Semester VIII
27. Core 23** (Supramolecular Chemistry) for Semester VIII
28. Minor 1 for Semester I
29. Minor 2 for Semester II
30. Minor 3 for Semester III
31. Minor 4 for Semester IV
32. Minor 5 for Semester V
33. Minor 6 for Semester VI
34. Minor 7 for Semester VII
35. Minor 8 for Semester VIII
36. MDE – 1 for Semester I
37. MDE – 2 for Semester II
38. MDE – 3 for Semester III
39. SEC – 1 for Semester I
40. SEC – 2 for Semester II
41. SEC – 3 for Semester III

Cotton University: Department of Chemistry
NEP UG Syllabus: Core Courses

Semester I

Paper: Core 1 **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. Familiarization with the various states of matter, and laws and concepts needed to describe the states.
2. Understanding kinetic theory model of gases, Maxwell distribution and collisions.
3. Learn the basic properties of organic molecules, and understand their structure and bonding.
4. To appreciate the electronic effects, acid-base properties and reaction intermediates in organic compounds.
5. To understand about evolution of atomic theory, the scientific theory of atoms and concept of wave function.
6. To know about the arrangement of elements in periodic table; physical and chemical characteristics of elements and their periodicity.

Unit 1: States of Matter **(15 lectures)**

Gases: Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor and its variation with pressure for different gases. Causes of deviation from ideal behaviour. The van der Waals equation of state, its application in explaining real gas behaviour. Boyle temperature. Critical state, critical constants and van der Waals constants, Andrews' isotherms of CO_2.

Kinetic molecular theory of a gas, its postulates, derivation of the kinetic gas equation. Maxwell speed distribution, its use in evaluating the mean molecular speeds (average, root mean square and most probable speeds) and average kinetic energy, law of equipartition of energy, degrees of freedom (with lack in expression of vibrational ones at room temperature), molecular basis of heat capacities. Collision cross section, collision frequency and mean free path of gases.

Liquids: Structure and physical properties of liquids; vapour pressure, surface tension, viscosity, their dependence on temperature and their determinations. Effect of addition of various solutes on surface tension, cleansing action of detergents. Elementary ideas of liquid crystals.

Solids: Forms of solids. Elementary ideas of symmetry, symmetry elements and symmetry operations, unit cells, crystal systems, Bravais lattices. Laws of Crystallography – Law of constancy of interfacial angles, Law of rational indices. Weiss and Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl. Defects in crystals.

Unit 2: Basics of Organic Chemistry **(15 lectures)**

(a) Hybridization, Shapes of molecules, Influence of hybridization on bond properties.
(b) Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications;
(c) Organic acids and bases; their relative strength.
(d) Homolytic and Heterolytic fission with suitable examples.
(e) Electrophiles and Nucleophiles; Nucleophlicity and basicity;
(f) Reaction intermediates: Types, shape and relative stabilities of Carbocations, Carbanions, Free radicals and Carbenes.
(g) Types of Organic reactions: Addition, Elimination and Substitution reactions.
(h) Aromaticity: Hückel's rule; aromatic, non-aromatic and anti-aromatic compounds.

Unit 3: Atomic Structure **(9 lectures)**

Concept of atom in ancient India, Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Time-independent Schrödinger's wave equation, significance of ψ and $|\psi|^2$. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals (Contour boundary and probability diagrams). Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau principle and its limitations.

Unit 4: Periodicity of Elements **(6 lectures)**

The s, p, d, f block elements, the long form of periodic table. Discussion of the following properties with reference to s and p-block elements:
(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
(b) Concept of Atomic radii (van der Waals, covalent, ionic and metallic).
(c) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy.
(d) Electron gain enthalpy, trends of electron gain enthalpy.
(e) Electronegativity, Pauling, Mullikan, Allred Rachow scales, electronegativity and bond order, Partial charge.

Recommended Textbooks/ References:

1. P.W. Atkins and J. de Paula. Atkins' Physical Chemistry 8th Ed., Oxford University Press (2006)

2. D. W. Ball. Physical Chemistry Thomson Press, India (2007)
3. G. W. Castellan. Physical Chemistry 4th Ed. Narosa (2004)
4. R. G. Mortimer. Physical Chemistry 3rd Ed. Elsevier, Noida (UP). (2009).
5. I. N. Levine. Physical Chemistry 6th Ed., Tata McGraw-Hill, 2011.
6. Lee, J. D. Concise Inorganic Chemistry, Wiley, 5th Edition.
7. Douglas, B.E., McDaniel, D.H., Alexander J.J., Concepts & Models of Inorganic Chemistry, (Third Edition) John Wiley & Sons, 1999.
8. Atkins, P. W., Overton, T., Rourke, J., Weller, M., and Armstrong, F. Shriver. Atkins' Inorganic Chemistry, Fifth Edition, Oxford University Press, 2010.
9. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4th ed.
10. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
11. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.
12. Sarkar, R. P., General and Inorganic Chemistry (Part I and II), New Central Book Agency, 2012.
13. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
14. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
15. Clayden, J., Greeves N., Warren, S., Organic Chemistry, Oxford University Press 2nd Ed., 2012.
16. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
17. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
18. S. Sengupta, Organic Chemistry, Oxford University Press; First Edition, 2014.

Lab Experiments for Chemistry Core 1:

Physical Chemistry Lab

1. Determination of surface tension for three aqueous solutions of ethanoic acid (with concentrations not beyond 25% w/w) by drop number method to judge its change with increasing concentration.
2. Determination of coefficient of viscosity of three aqueous solutions of ethanol (with concentrations not beyond 30% w/w) using Ostwald viscometer to judge its change with increasing concentration.

Organic Chemistry Lab

1. Purification of organic compounds by crystallization using the following solvents:

a. Water   b. Alcohol   c. Alcohol-Water

2. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds.

3. Chromatography: Separation of a mixture of organic compounds by thin layer chromatography (TLC).

Recommended Books/References:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand, New Delhi, 2011.

2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, Eighth Edition, McGraw-Hill (2003).

3. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry, Third Edition, W, H. Freeman (2003).

4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)

5. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Course Outcomes:

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

1. Know about kinetic molecular theory of gases, molecular collisions in gases, mean free path and their interrelations, and to perform numerical calculations on these topics. Also to recognise real gas behaviour as different from ideal gas behaviour.

2. Know about the structure and various physical properties of liquids, along with how the surface tension depends on solutes, and experimentally determine surface tension and coefficient of viscosity of liquids.

3. Understand the crystal structure and symmetry in crystalline solids and perform numerical calculations on these.

4. Understand the basic properties of organic molecules, and their structure and bonding.

5. Apply the knowledge of various electronic effects in determining reactivity organic compounds.

6. Know about structure of atom, classical and quantum mechanical models and theories of atomic structure, dual behavior of electrons and concept of atomic orbitals.

7. Understand about arrangement of elements in periodic table, periodic variation of element's properties.

Cotton University: Department of Chemistry
NEP UG Syllabus: Core Courses

Semester II

Paper: Core 2 **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. Understanding the fundamentals of chemical kinetics: concepts of rate, differential and integrated rate equations, half-life, order and molecularity, temperature dependence of rate.
2. Determination of progress of reaction, rate, rate constant and order.
3. Understanding the fundamentals of catalysis – types of catalysis, cause of catalytic action, mechanism of heterogeneous catalysis, introduction to acid-base catalysis and enzyme catalysis.
4. Learn 3-D structure and concept of chirality in organic molecules.
5. Learn properties and reactions of saturated and unsaturated hydrocarbon
6. Understand the concept of ionic bonding, lattice energy using Born-Landé equation, Born Haber Cycle and Solvation Energy.
7. Learn about VSEPR theory, VBT and MOT (homo- & hetero- nuclear diatomic molecules).
8. Understand the theory and application of acid-base and redox chemistry.

Unit 1: Chemical Kinetics **(10 Lectures)**

The concept of reaction rates. Effect of concentration, temperature and catalyst on reaction rates. Differential rate equation and the order of a reaction. Methods of experimental determination of the progress of a reaction and of the rate constant. Concept of molecularity, comparison between order and molecularity. Derivation of integrated rate equations for zeroth, first and second order reactions. Half–life of a reaction and its dependence on initial concentration for different orders. Methods for determination of the order from the half-life for single-reactant systems. Temperature dependence of the reaction rate, Arrhenius equation. Concept of pre-exponential factor, activation energy and their calculation.

Qualitative ideas of the Collision theory and Activated Complex theory of bimolecular reactions.

Unit 2: Catalysis **(5 lectures)**

Types of catalysis – homogeneous and heterogeneous. Cause of catalytic effect on reaction rate. Introductory ideas of acid-base catalysis. Mechanism of catalysed reactions at solid surface, effect of particle size. Enzyme catalysis, its characteristics, Michaelis-Menten mechanism. Specificity and selectivity in enzyme catalysis.

Unit 3: Stereochemistry **(7 Lectures)**

(a) Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations.
(b) Conformations with respect to ethane, butane and cyclohexane.
(c) Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; *cis–trans* nomenclature; CIP Rules: R/ S and E / Z Nomenclature

Unit 4: Chemistry of Aliphatic Hydrocarbons **(8 Lectures)**

Alkanes:

(a) *Preparation:* Catalytic hydrogenation, Wurtz Reaction, Wurtz-Fittig Reaction, Kolbe reaction
(b) *Reactions*: Combustion reaction, Cracking, Free radical substitutions: Halogenation - relative reactivity and selectivity.

Alkenes:

(a) *Preparation*: Elimination reactions: Dehydration of alkenes anddehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction).
(b) *Reactions*: cis-addition (alk. $KMnO_4$)and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Unit 5: Chemical Bonding **(10 lectures)**

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Born-Landé equation with derivation. Madelung constant, Born-Haber cycle and its application, Solvation energy.

Covalent bond: Lewis structure, Valence Shell Electron Pair Repulsion Theory (VSEPR), Shapes of simple molecules and ions containing lone-and bond-pairs of electrons multiple bonding, sigma and pi-bond approach, Valence Bond theory (Heitler-London approach). Hybridization containing s, p and s, p, d atomic orbitals, shapes of hybrid orbitals, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of simple homonuclear and heteronuclear diatomic molecules, e.g., N_2, O_2, C_2, B_2, F_2, CO, NO (idea of s-p mixing and orbital interaction to be given).

Unit 6: Acid Base and Redox Chemistry (5 lectures)

Arrhenius, Brönsted and Lewis theories of acids and bases, Strength of Brönsted acids and bases in water, Strength of Lewis acids and bases. Hard and soft acid-base (HSAB) concept and its applications.

Redox equations, Standard electrode potential and its application to inorganic reactions.

Recommended Textbooks/ References:

1. P. W. Atkins and J. De Paula. Physical Chemistry (10th Ed.), Oxford University Press, 2014.
2. G.W. Castellan. Physical Chemistry, 4th Ed., Narosa, 2004.
3. T. Engel and P. Reid. P. Physical Chemistry, 3rd Edition, Prentice-Hall, 2012.
4. D.W. Ball. Physical Chemistry, Cengage India, 2012.
5. R. G. Mortimer. Physical Chemistry 3rd Ed., Elsevier: NOIDA (UP), 2009.
6. I. N. Levine. Physical Chemistry 6th Ed., Tata McGraw-Hill, 2011.
7. C. R. Metz. Physical Chemistry 2nd Ed., Tata McGraw-Hill, 2009.
8. E. L. Eliel & S. H. Wilen Stereochemistry of Organic Compounds, Wiley: London, 1994.
9. D. Nasipuri, Stereochemistry of Organic Compounds Principle of Application. New Age International Private Limited; 4^{th} edition (2020).
10. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
11. S. Sengupta, Basic Stereochemistry of Organic Molecules, Oxford Univ. Press; 2^{nd} Ed., 2018.
12. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
13. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
14. S. Sengupta, Organic Chemistry, Oxford University Press; First Edition, 2014.
15. J. D. Lee: A new Concise Inorganic Chemistry, E. L. B. S.
16. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4^{th} ed.
17. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33^{rd} Ed., 2020.
18. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.
19. Sarkar, R. P. General and Inorganic Chemistry (Part I & II), New Central Book Agency, 2012.

20. Douglas, B.E., McDaniel, D.H., Alexander J.J., Concepts & Models of Inorganic Chemistry, (3rd Ed.) John Wiley & Sons, 1999.
21. Rodger, G. E. Inorganic and Solid-State Chemistry, Cengage Learning, 2002.

Lab Experiments for Chemistry Core 2:

Physical Chemistry Lab

1. Study of the iodine clock reaction to judge the slowing down of the reaction rate with the passage of time.
2. To gauge the effect of added manganous ion catalyst to the initial rate of the titration process between oxalic acid solution versus permanganate ion in strong acidic medium done at room temperature.

Inorganic Chemistry Lab

1. Titrimetric Analysis
(i) Calibration and use of apparatus.
(ii) Preparation of solutions of different molarity/normality of titrants.
(iii) Use of primary and secondary standard solutions.

2. Acid-Base Titrations
(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.

3. Oxidation-Reduction Titrimetry
(i) Estimation of Fe(II) using standardized $KMnO_4$ solution involving oxalic acid solution.
(ii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine/ anthranilic acid) and external indicator.
(iii) Estimation of Fe(III) using standardized $KMnO_4$ solution.

Recommended Books/References:
1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand, New Delhi, 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, Eighth Edition, McGraw-Hill (2003).
3. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry, Third Edition, W, H. Freeman(2003).
4. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis Sixth Edition, Pearson, 2009.
5. Svehla G. and Sivasankar I. B, Vogel's Qualitative Inorganic Analysis, Pearson, India, 2012.

6. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
7. Barua, S., A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016
8. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed., 2014.
9. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013

Course Outcomes:

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

1. Know about and perform calculations on the rate laws for simple reactions of various orders and on temperature dependence of the reaction rate.
2. To learn about determination of the progress of a reaction and to experimentally perform such a determination.
3. To have an introductory understanding of the collision theory and the activated complex theory of chemical reactions.
4. Understand the types of catalysed reactions and the cause behind the catalytic effect, and the mechanisms of such reactions at solid surfaces, enzyme environments and acid-base mediums.
5. Understand the effect of spatial arrangements of atoms in organic molecules on their properties and reactivities.
6. Interpret reactions and properties of aliphatic hydrocarbons.
7. Have introductory idea about chemical bonding.
8. Calculate relevant bonding parameters, interpret trends, predict and draw molecular structures using various bonding theories.
9. Apply acid-base and redox concepts to inorganic compounds and reactions.
10. They will also have hands-on experience at learning titrimetric techniques.

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Semester III

Paper: Core 3 (Inorganic Chemistry - I) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To learn about the various bonding theories and weak chemical forces along with their applications.
2. To learn about the properties of s- and p- block elements and their compounds.
3. To learn about the classification, synthesis, structural aspects and applications of inorganic polymers.
4. To understand the underlying chemistry behind some metallurgical processes.

Unit 1: Chemical Bonding-II (10 lectures)

Covalent Bonding: Bent's Rule and the energetics of hybridization, MO diagrams of simple di, tri and tetra-atomic molecules and their ions: HCl, CO, BeF_2, BeH_2, CO_2, BF_3, HCHO. Covalent character in ionic compounds, polarizing power and polarizability. Fajan rules, polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Ionic character from dipole moment and electronegativities.

Metallic Bond: Qualitative idea of free electron model, Semiconductors, Insulators.

Weak Chemical Forces: van der Waals, ion-dipole, dipole-dipole, induced dipole, dipole-induced dipole interactions, Lenard-Jones 6-12 formula, hydrogen bond, effects of hydrogen bonding on melting and boiling points, solubility, dissolution.

Unit 2: Chemistry of s- and p- Block Elements (12 lectures)

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behavior of first member of each group. Allotropy and catenation. Complex formation tendency of s and p block elements. Hydrides and their classification – ionic, covalent and interstitial hydrides. Basic beryllium acetate and nitrate.

Structure, bonding, preparation, properties and uses of: Boric acid and borates, boron nitrides, borohydrides (diborane), carboranes and graphitic compounds, silanes, oxides and oxoacids of nitrogen, phosphorus and chlorine. Per-oxo acids of sulphur. Inter-halogen compounds, polyhalide ions, pseudo-halogens, properties of halogens.

Unit 3: Noble Gases **(6 lectures)**

Occurrence and uses, rationalisation of inertness of noble gases, clathrates, preparation and properties of XeF_2, XeF_4 and XeF_6. Bonding in noble gas compounds (Valence Bond and MO treatment for XeF_2), shapes of noble gas compounds (VSEPR theory).

Unit 4: Inorganic Polymers **(6 lectures)**

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates, phosphazenes, and polysulphates.

Unit 5: General Principles of Metallurgy **(11 lectures)**

Occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon or carbon monoxide as reducing agent. Electrolytic reduction, hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel - de Boer process and Mond's process, Zone refining.

Recommended Textbooks/ References:

1. Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry, 3rd Ed., John Wiley Sons, N.Y. 1994.
3. Greenwood, N.N., Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
5. Rodger, G.E. Inorganic and Solid-State Chemistry, Cengage Learning India Edition, 2002.
6. Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry Fourth Ed., Pearson, 2010
7. Atkins, P. W and Shriver D. N. Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
8. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4th ed.
9. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
10. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.

11. Sarkar, R. P., General and Inorganic Chemistry (Part I and II), New Central Book Agency, 2012.

Lab Experiments for Inorganic Chemistry - I

(A) Iodo / Iodimetric Titrations:
(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
(ii) Estimation of Cu(II) and Fe(II)/Fe(III) in a mixture Iodometrically.
(iii) Estimation of available chlorine in bleaching powder iodometrically.

(B) Inorganic Preparations:
(i) Cuprous chloride, Cu_2Cl_2
(ii) Preparation of aluminium potassium sulphate (potash alum) or chrome alum.

Recommended Books/References:
1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand, New Delhi, 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, Eighth Edition, McGraw-Hill (2003).
3. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry, Third Edition, W, H. Freeman (2003).
4. Mendham, J. A. I. Vogel's Quantitative Chemical Analysis Sixth Edition, Pearson, 2009.
5. Svehla, G. and Sivasankar, I. B. Vogel's Qualitative Inorganic Analysis, Pearson, India, 2012.
6. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
7. Barua, S. A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016.
8. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013.

Course Outcomes:
On completion of the course, the students will be able to:
1. Know the underlying principles of metallurgy and various methods of purification of metals.
2. Know the chemistry of s- and p- block elements including noble gases.
3. Get a deeper insight into the various types of inorganic polymers and compounds formed by s and p block elements.
4. Know about the iodometric and iodimetric methods for metal estimations in addition to performing a few inorganic syntheses.

Paper: Core 4 (Organic Chemistry – I) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To be conversant about the reactivity of alkynes.
2. To understand organic reaction mechanisms.
3. To know how to perform one step organic synthesis
4. To learn about different chromatographic techniques used for separation of binary mixtures of sugars and amino acids and detection of product of chemical reaction.

Unit 1: Alkynes (5 Lectures)

Reactions of alkynes:
(a) Addition reaction: Reduction, hydration, addition of hydrogen halide and halogen
(b) Acidity of alkynes
(c) Alkylation of terminal alkynes, introduction to multistep organic synthesis

Unit 2: Alkyl halides and alcohols (15 Lectures)

(a) Elimination reactions (E1, E2, E1cB) of alkyl halides and alcohols.
(b) Nucleophilic substitution reactions (S_N1, S_N2, S_Ni) alkyl halides and alcohols.
(c) Effect of substrate, leaving group, nucleophile/base and solvent in elimination and substitution reactions.
(d) Elimination vs substitution.
(e) Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.
(f) Organometallic compounds: Grignard reagent, Gilman reagent and organo-lithium reagents and their synthetic utility.

Unit 3: Electrophilic substitution reactions of aromatic compounds: (18 Lectures)

(a) Reactions of benzene and substituted benzene: Mechanism of Nitration, Halogenation, Friedel-Crafts alkylation and acylation, sulphonation; regioselectivity in electrophilic aromatic substitution reaction.
(b) Reactions of phenol (Kolbe-Schmitt reaction, Reimer-Tiemann reaction, Gattermann reaction, Hoesch reaction, halogenation, nitration); reactions of aromatic amines: halogenation, nitration, alkylation and acylation. (c) Reactions of pyrrole, furan, thiophene, indole, pyridine, pyridine *N*-oxide, Vilsmeier reaction.

Unit 4: Nucleophilic aromatic substitution reactions of aryl halides (7 Lectures)

(a) S_NAr (addition-elimination) mechanism, Influence of EWG, relative rates of different halides.
(b) Benzyne mechanism: Structure, stability and isolation of benzyne intermediate, regioselectivity.
(c) Nucleophilic aromatic substitution of pyridine, pyridine N-oxide.

Recommended Textbooks/ References:

1. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
3. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., (2012), Oxford University Press.
4. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
5. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
6. S. Sengupta, Organic Chemistry, Oxford University Press; First Edition, 2014.
7. D. R. Klein. Organic Chemistry, John Wiley & Sons Inc; 4th edition (Dec. 2020).
8. F. A. Carey, R. M. Giuliano. Organic Chemistry, McGraw Hill; 10th edition (Feb. 2016).
9. T. W. G. Solomons, C. B. Fryhle, S. A. Snyder, Solomons's Organic Chemistry, J Wiley; Global edition (Jan. 2017).
10. S. Sengupta, Reaction Mechanisms In Organic Chemistry, Oxford University Press; 1st Ed. (Jun. 2016).
11. P. S. Kalsi. Organic Reactions and Their Mechanisms, New Age International Private Limited; 5th edition (Jun. 2020).

Lab Experiments for Organic Chemistry – I:

(a) Separation of a mixture of two amino acids by paper Chromatography.
(b) Separation of a mixture of two sugars by paper Chromatography.
(c) Bromination of any one of the following:
   (i) Acetanilide by conventional methods
   (ii) Acetanilide using green approach (Bromate-bromide method)
(d) Nitration of any one of the following:
 Acetanilide/benzene/toluene/nitrobenzene by conventional method.
(e) Aldol condensation using either conventional or green method.
(f) Hydrolysis of amides/esters.
(g) Detection of product by TLC.

Recommended Books/References:

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Vogel's Practical Organic Chemistry, 5th Ed. Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
4. Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

Course Outcomes:

On completion of the course, the students will be able to:

1. Describe general reactivity of alkynes.
2. Understand basic aspects of organic reaction mechanism involving substitution, elimination reaction in both aliphatic and aromatic compounds.
3. Interpret formation of product and write probable mechanism of various organic reactions.
4. Design synthetic route for simple organic transformations.
5. Have in-hand experience of carrying out organic reaction and applying chromatographic technique for analysis and separation of mixture of compounds.

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Semester IV

Paper: Core 5 (Inorganic Chemistry – II) Credits: 3 + 0 + 1 = 4

Learning objectives:

1. To understand the trends in physical and chemical properties of transition and inner transition elements.
2. To learn about structure, bonding, nomenclature, and underlying principles of certain physical and chemical properties of coordination compounds.
3. To learn about the role of various metal ions in biomolecules and biological processes, and toxic effect of metals and their treatments.
4. To obtain hands on experience in basic synthetic inorganic chemistry, gravimetric estimation and chromatographic separation of metal ions.

Unit 1: Transition Elements (11 lectures)

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Frost-Ebsworth diagrams). Difference between the first, second and third transition series. Chemistry of Ti, V, Cr, Mn, Fe and Co in various oxidation states (excluding their metallurgy).

Unit 2: Coordination Chemistry (15 lectures)

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with the coordination number 4 and 6. Chelate effect.

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δ_o, Δ_t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry. Jahn-Teller theorem, square planar geometry. Qualitative aspects of Ligand Field and MO Theory, labile and inert complexes.

Unit 3: Lanthanides and Actinides (8 lectures)

Electronic configuration, oxidation states, colour, spectral and magnetic behaviour, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Unit 4: Bioinorganic Chemistry (11 lectures)

Metal ions present in biological systems, geochemical effect on distribution of metals. Classification of elements according to their action in biological system. Sodium/Potassium-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of Cu and Fe. Toxicity of metal ions (Hg, Pb, Cd and As), chelating agents in medicine. Iron and its application in biosystems, Myogloibin and Haemoglobin – Structure, Functions, Oxygen binding, Cooperativity, Bohr effect; Storage and transfer of iron – Structures and Functions of Ferritin, Transferrin, Siderophores.

Recommended Textbooks/References:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
2. Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry. Panima Publishing Company 1994.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
5. Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
6. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
7. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4^{th} ed.
8. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
9. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.
10. Sarkar, R. P., General and Inorganic Chemistry (Part I and II), New Central Book Agency, 2012

Lab Experiments for Inorganic Chemistry – II

Gravimetric Analysis**:**

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).

ii. Estimation of copper as CuSCN

iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

iv. Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

Inorganic Preparations**:**

(i) Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

(ii) *Cis*- and *trans*- $K[Cr(C_2O_4)_2(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)

(iii)Tetraamminecarbonatocobalt (III) ion

(iv) Potassium tris(oxalato)ferrate(III)

Chromatography of metal ions:
Principles involved in chromatographic separations.
Paper chromatographic separation of the following metal ions:
i. Ni(II) and Co(II)
ii. Fe(III) and Al(III)

Recommended Textbooks/References:

1. Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.
2. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
3. Barua, S., A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016
4. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed., 2014.
5. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013.

Course Outcomes:

On completion of the course, the students will be able to:

1. Know about chemistry of transition metals and their complexes and the theories associated with the structure, stereochemistry and properties of coordination compounds.
2. Know about the properties of transition and inner transition elements.
3. Familiarize about the role of metals, metal enzymes and metallo-proteins in biological processes.
4. Get laboratory experience on the synthesis of coordination compounds
5. Get laboratory experience on gravimetric estimation and chromatographic separation of metal ions.

Paper: Core 6 (Organic Chemistry – II) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To know about various oxidizing agents of alcohols and reducing agents of aldehydes, ketones and carboxylic acids and derivatives.
2. To understand reaction mechanism of various reactions of carbonyl compounds including carboxylic acids and their derivatives.
3. To know about chemistry of sulphur-containing compounds.
4. To acquire the skill of qualitative analysis of organic compounds.

Unit 1: Alcohols, Phenols, Ethers and Epoxides (10 Lectures)

(a) Oxidation reactions of alcohols: Oxidation by PCC, PDC, $KMnO_4$, CrO_3, Jones reagent, Swern oxidation, Oppenauer oxidation.
(b) Preparation, properties and reactions of glycols: Oxidation by periodic acid and lead tetraacetate.
(c) Acidity of phenol and factors affecting it.
(d) Williamson ether synthesis, reaction of ethers with acids.
(e) Preparation of epoxides, ring opening reactions (nucleophilic and acid catalyzed) of epoxides.

Unit 2: Carbonyl Compounds (20 Lectures)

(a) Nucleophilic addition reactions: cyanohydrin, bisulphite, hydrate and acetal/ketal formation.
(b) Nucleophilic addition-elimination reactions with ammonia derivatives, hydrazone formation, imine and enamine formation.
(c) Reaction of enol/enolate: Aldol reaction, Knoevenagel condensation, Claisen-Schmidt, Perkin reaction, Reformatsky reaction, Claisen ester condensation.
(d) Haloform reaction, Cannizzaro reaction.
(e) Reaction with ylid: Wittig reaction.
(f) Reduction reactions: Clemmensen, Wolff-Kishner, Meerwein–Pondorff–Verley reduction; McMurry reaction, reduction using hydride transfer reactions: $LiAlH_4$, $NaBH_4$, DIBAL
(g) Conjugate addition: Michael reaction, Robinson annulation reaction.
(h) Active methylene compounds: Synthetic applications of diethyl malonate and ethyl acetoacetate.

Unit 3: Carboxylic Acids and their Derivatives (10 Lectures)

(a) Nucleophilic substitution reactions at acyl group.
(b) Hydrolysis of ester, amide and nitrile. Mechanism of acidic and alkaline hydrolysis of esters, transesterification
(c) Comparative study of reactivity among carboxylic acids, acid chlorides, anhydrides, esters and amides.
(d) Inter conversion among different acid derivatives.
(c) Acidity of carboxylic acids and factors affecting it.

(e) HVZ reaction
(f) Reduction reactions of carboxylic acids, acid chlorides, esters and amides, selective reduction to aldehyde.
(g) Decarboxylation of 1,3-dicarbonyl compounds.

Unit 4: Sulphur Containing Compounds (5 Lectures)

(a) Preparation and reactions of thiols
(b) Acidity and nucleophilicity of thiols
(c) Disulfide formation and biological relevance of it
(d) Umpolung of carbonyl compounds using dithiane and synthetic utility
(e) Desulfurization reaction

Recommended Textbooks/References:

1. Morrison, R. N. and Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. McMurry, J. E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
3. Clayden, J., Greeves, N. and Warren, S. Organic Chemistry, 2nd Ed. (2012), Oxford University Press.
4. M. B. Smith, J. March. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
5. B. Y. Paula. Organic Chemistry, 8th edition, Pearson Education India.
6. S. Sengupta. Organic Chemistry, Oxford University Press; First Edition, 2014.
7. D. R. Klein. Organic Chemistry, John Wiley & Sons Inc; 4th edition (Dec. 2020).
8. F. A. Carey. Robert M. Giuliano, Organic Chemistry, McGraw Hill; 10th edition (Feb. 2016).
9. S. Sengupta. Reaction Mechanisms In Organic Chemistry, Oxford University Press; First Edition (Jun. 2016).
10. P. S. Kalsi. Organic Reactions And Their Mechanisms, New Age International Private Limited; Fifth edition (Jun. 2020).

Lab Experiments for Organic Chemistry – II

Analysis of organic compounds:

(i) Detection of elements (Nitrogen, sulphur and halogens)
(ii) Detection of functional groups- test for unsaturation, -COOH, -OH, phenolic –OH, amine, nitro, aldehyde, ketone, amide, ester, urea.
(iii) Determination of melting point.
(iv) Preparation of derivatives.

Recommended Textbooks/References:

1. Clarke, H. T. A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS.
2. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry, Pearson Education (2009).

3. Furniss, B. S., Hannaford, A. J., Smith, P. W. G. & Tatchell, A. R. Vogel's Practical Organic Chemistry, 5th Ed. Pearson (2012).

Course Outcomes:

On completion of the course, the students will be able to:
1. Appreciate the various oxidation reactions of alcohols and reduction reactions of aldehydes, ketones and carboxylic acids and their derivatives.
2. Classify various carbonyl compounds and distinguish their reactivity pattern
3. Know about preparation of thiols and their reactions and applications including biological applications of disulfides and reversal of polarity (umpolung) in organic synthesis.
4. To follow various organic reactions for the analysis and detection of simple organic compounds.

Paper: Core 7 (Physical Chemistry – I) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. Appreciating the basic concepts of thermodynamics such as system, variables, heat, work, and the laws that govern thermodynamics.
2. To be conversant with the concept of heat (enthalpy/ internal energy) of reactions and use of equations in calculations of bond energy, enthalpy, etc.
3. Realizing the concept of entropy; reversible and irreversible processes, and the calculation of entropy changes.
4. Understanding the concept of absolute zero of temperature, absolute and residual entropies.
5. Understanding thermodynamic theories of dilute solutions.
6. Appreciating the concepts of component, degrees of freedom and phases, The Gibbs phase rule and its applications, construction of phase diagram of different systems, and the application of phase diagram.
7. Understanding the phenomenon of adsorption and adsorption isotherms, their significance, monolayer and multilayer adsorption, their theory and significance.

Unit 1: Thermodynamics and Thermochemistry (20 lectures)

Introduction to thermodynamics: Systems and surroundings; isolated, closed and open systems; intensive and extensive properties; thermodynamic state, state functions and path functions – concepts of work done (w), heat transfer (q), internal energy (U) and enthalpy (H). Heat capacities and its two specific forms C_p and C_v. Concept of irreversible and reversible processes. Zeroth law of thermodynamics and the concept of temperature. First law of thermodynamics and its common mathematical form. Heat absorbed, work done, changes in internal energy (ΔU) and in enthalpy (ΔH) for reversible, irreversible and free expansion of ideal gases under isothermal and adiabatic conditions.

Thermochemistry: The concepts of standard states of substances and of standard enthalpy of a reaction, Hess's law relating various reaction enthalpies, relation between enthalpy of a reaction $\Delta_r H$ and the associated change $\Delta_r U$ in the internal energy. Specific standard enthalpy of reactions: for formation of compounds and ions from elements, for combustion, for acid-base neutralisation. Bond enthalpy and resonance enthalpy – their estimations from thermochemical data, uses of bond enthalpy data. Effect of temperature (Kirchhoff's equation) on the enthalpy of reactions.

Second and Third Laws of Thermodynamics: The second law of thermodynamics and its various formulations. Clausius inequality. Concept of entropy, molecular and statistical interpretations of entropy, entropy defining the arrow of time. Introductory idea of the Carnot engine and the thermodynamic scale of temperature. Calculation of entropy changes for reversible and irreversible processes. Statement of the third law of thermodynamics, concept of the absolute zero temperature, concepts of absolute and residual entropies. The concepts of Gibbs and Helmholtz free energy, and their use in discussing spontaneity of thermodynamic processes. Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equations of state.

Unit 2: Phase Equilibria (14 lectures)

Concept of phases, components and degrees of freedom, Gibbs phase rule for nonreactive and reactive systems. Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Binary solutions: Gibbs-Duhem equation, fractional distillation of binary miscible liquids (ideal and non-ideal), azeotropes, lever rule. Partial miscibility of liquids: CST – upper and lower. Steam distillation of immiscible liquid pair. Nernst distribution law: its derivation and applications.

Unit 3: Surface Chemistry (11 lectures)

Adsorption as a surface phenomenon, thermodynamics of adsorption. Physical and chemical adsorptions, their characteristics and differences, adsorption isotherms. Monolayer vs. multilayer adsorption. Derivation of the Langmuir adsorption isotherm, and determination of surface area. The Brunauer–Emmett–Teller (BET) theory of multilayer adsorption (derivation not required). Adsorption in solution such as acetic acid by activated charcoal.

Recommended Textbooks/References:

1. Atkins P. W. and De Paula J., Physical Chemistry, 10th Ed., Oxford University Press, 2014.

2 Castellan, G. W. Physical Chemistry, 4thEd., Narosa Publishing House, 2004.

3 McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books, 2004.

4 Engel, T. & Reid, P. Physical Chemistry, 3rd Ed., Prentice-Hall, 2012.

5. Zundhal, S.S. Chemistry Concepts and Applications, Cengage India, 2011

6. Ball, D. W. Physical Chemistry, Cengage India, 2012.

7. Mortimer, R. G. Physical Chemistry, 3rd Ed., Elsevier, 2009.

8. Levine, I. N. Physical Chemistry, 6th Ed., Tata McGraw-Hill, 2011.

9. Metz, C. R. Physical Chemistry, 2nd Ed., Tata McGraw-Hill, 2009.

10. Roy, B. N. Fundamentals of Classical and Statistical Thermodynamics, Wiley, 2001.

Lab Experiments for Physical Chemistry – I

1. Determination of heat capacity of a calorimeter by using water.
2. Determination of heat capacity of a calorimeter using known enthalpy of neutralisation data for strong acid and strong alkali.
3. Determination of heat capacity of the calorimeter and enthalpy of neutralisation of hydrochloric acid with sodium hydroxide.
4. Determination of heat capacity of the calorimeter and enthalpy of neutralisation of acetic acid with sodium hydroxide.
5. Determination of critical solution temperature and composition of the phenol-water system.
6. Verification of Freundlich adsorption isotherm for adsorption of acetic acid in activated charcoal.

Recommended Textbooks/References:

1. Khosla, B. D., Garg, V. C. and Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co., New Delhi (2011).

2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).

3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3 rd Ed.; W.H. Freeman & Co.: New York (2003).

Course Outcomes:

On completion of the course, the students will be able to:

1. Know about the basic concepts of thermodynamics such as state and path and recognise its various laws.
2. Calculate the heat and work transfers and energy/enthalpy changes in ideal gas processes and in chemical reactions.

3. Judge the spontaneity of physical/chemical processes and their entropy and free energy changes.

4. Calculate the absolute entropy as per the third law, and estimate the residual entropy of imperfectly crystalline substances.

5. Know about, inter-relate and calculate the free energy functions, chemical potentials in solutions, equilibrium constants and colligative properties of solutions.

6. Know the theoretical aspects of phase equilibria such as Gibbs phase rule and Clausius-Clapeyron equation, and understand the specific cases of one-component phase equilibria, two-component solid-liquid equilibria of various types and three-component liquid-liquid ones.

7. Know phase equilibrium of partially miscible binary-liquid mixtures and liquid-vapour transition of various types of binary liquid mixtures.

8. Distinguish between physical and chemical adsorptions and know about various popular monolayer adsorption isotherms and about multi-layer isotherms, along with numerical aspects.

Cotton University: Department of Chemistry
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Semester V

Paper: Core 8 (Inorganic Chemistry – III) **Credits – 3 + 0 +1 = 4**

Learning Objectives:

1. To learn about structure, reactions, chemical properties and applications of organometallic compounds
2. To learn about structures and properties of simple solids, Inorganic cages and clusters
3. To learn about the various metalloenzymes usage of metal complexes in medicine
4. To learn about systematic qualitative analyses of inorganic salt mixtures

Unit1: Organometallic Compounds **(10 Lectures)**

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18-electron rule, electron count of mononuclear and polynuclear metal carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Isolobal analogy.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multi-centre bonding in these compounds. Role of triethyl aluminium in polymerisation of ethene (Ziegler – Natta Catalyst).

Unit 2: Catalysis by Organometallic Compounds **(5 Lectures)**

Study of the following industrial processes and their mechanisms:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)

5. Synthesis gas by metal carbonyl complexes

Unit 3: Structure of Simple Solids (10 Lectures)

Packing of spheres – hexagonal and cubic close packing, tetrahedral and octahedral holes in close-packed structures- metals and alloys, solid solutions. The ionic model for the description of bonding in ionic solids. Characteristic structures of ionic solids- the NaCl and CsCl types, the sphalerite and wurtzite types of ZnS, the NiAs structure type, the perovskite and spinel structure types of mixed-metal oxides- importance ionic radii and the radius ratios in determining structure type among ionic solids.

Unit 4: Inorganic Chains, cages, and clusters (10 Lectures)

Catenation, Heterocatenation, Zeolites, Intercalation, Structure, and bonding in polyhedral boranes, carboranes, metalloboranes and metallocarboranes, Styx notation, Wade's rules, Synthesis and electron count in polyhedral boranes. Inorganic clathrates. Synthesis and bonding in metal clusters. Metal-metal quadruple bonding in Re_2Cl_8, $Mo_2Cl_8^{4-}$.

Unit 5: Bioinorganic Chemistry – II (10 Lectures)

Metalloenzymes: Chlorophyll, Photosynthesis, Catalase, Peroxidase, Superoxide Dismutase, Iron-Sulphur Proteins, Cytochrome P-450, Cytochrome C Oxidase, Electron Transport Chain, Nitrogen Fixation and Nitrogenase, Coenzyme Vitamin B_{12}.

Metal Complexes in Medicine: Cisplatin, Carboplatin, Oxaliplatin, Gold compounds in Rheumatoid Arthritis, Gd(III) and Mn(II) complexes as MRI Contrast Agents.

Reference Books:

1. Cotton, F. A., Wilkinson, G.; & Gaus, P. L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
2. Huheey, J. E.; Keiter, E. A. & Keiter, R. L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
3. Sharpe, A. G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
4. Douglas, B.E.; Mc Daniel, D. H. & Alexander, J. J. Concepts and Models in Inorganic Chemistry 3rdEd., John Wiley and Sons, NY, 1994.
5. Lee, J. D. Concise Inorganic Chemistry 5thEd., John Wiley and sons 2008.
6. Powell, P. Principles o*f* Organometallic Chemistry, Chapman and Hall, 1988.
7. Shriver, D. D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
8. Purcell, K.F. & Kotz, J. C., Inorganic Chemistry, W. B. Saunders Co. 1977
9. Miessler, G. L. & Donald, A. Tarr, Inorganic Chemistry 4th Ed., Pearson, 2010.

10. Collman, James P. et. al. Principles and Applications of Organotransition Metal Chemistry
11. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. J New York, NY: John Wiley, 2000.
12. Spessard, Gary O., & Gary L. Miessler. Organometallic Chemistry. Upper Saddle River, N J: Prentice-Hall, 1996.
13. Gray, H. B., Stiefel, E. I., Valentine, J. S. & Bertini, I. Biological Inorganic Chemistry: Strucutre and Reactivity 1st Ed., University Science Book, 2006
14. Bertini, I., Gray, H. B., Lippard, S. & Valentine, J. S. Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi
15. Wilkins P. C. & Wilkins R. G. Inorganic Chemistry in Biology: Oxford Chemistry Primers, Oxford University Press, 1997.
16. Housecroft, C. E., Sharpe, A. J. Inorganic Chemistry 5th Ed. Pearson 2018.

Inorganic Chemistry - III Lab

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations: Emphasis should be given to the understanding of chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO^{2-}, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, $CH3COO^{-}$, F^{-}, Cl^{-}, Br^{-}, I^{-}, NO^{3-}, SO_4^{2-}, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^{+},

K^{+}, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, $Ca^{2+,}$ Mg^{2+}

Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3), or combination of anions, e.g., CO_3^{2-} and SO_3^{2-}, $NO_2^{-}$and NO_3^{-}, Cl^{-} and Br^{-}, Cl^{-} and I^{-}, Br^{-} and I^{-}, $NO_3^{-}$and Br^{-}, NO_3^{-} and I^{-}.

[Spot tests should be done whenever possible.]

Reference Books:

1. Vogel, A. I. Qualitative Inorganic Analysis, Longman, 1972
2. Svehla, G. Vogel's Qualitative Inorganic Analysis, 7th Edition, Prentice Hall, 1996-03-07.
3. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
4. Barua, S., A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016
5. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed., 2014.

6. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013.
7. Marr, G., Rockett, B. W. Practical Inorganic Chemistry, Van Nostrand Reinhold Company, 1972.

Course Outcomes:

On completion of the course the students will:

1. Understand the bonding, structures, reactivities, chemical properties and applications of significant organometallic compounds having historical and industrial relevance.
2. Have an idea about structures, bonding and properties of inorganic simple solids, chains, cages and clusters.
3. Understand the structures of active sites, mechanisms of actions and underlying principles of various metalloenzymes and medicinal metal complexes.
4. Have a hands-on experience of performing qualitative analyses of inorganic salt mixtures.

Paper: Core 9 (Organic Chemistry – III) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To learn the various structural forms of carbohydrates and reactions of carbohydrates
2. To learn about the structural properties of amino acids and proteins, synthesis of amino acids and peptides, separation of amino acids and peptides by electrophoresis and sequencing of polypeptides.
3. To learn the mechanism of enzyme action, factors that affect enzyme activity and enzyme inhibition.
4. To learn about the different types of nucleic acids and their functions, components of nucleic acids, reactions of nucleobases, DNA replication and biosynthesis of proteins.
5. To learn the fundamentals of fats and oils and mechanism of generation of energy in biosystems.

Unit 1: Carbohydrates (10 Lectures)

Occurrence, classification and their biological importance.
Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani-Fischer synthesis and Ruff degradation.

Disaccharides –Structure elucidation of maltose, lactose and sucrose.
Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Unit 2:Amino Acids, Peptides and Proteins (8 Lectures)

Amino acids, Peptides and their classification.
α-Amino Acids - Synthesis, ionic properties, p*K*a values, isoelectric point and electrophoresis.
Study of peptides: Determination of their primary structures through end group analysis; Synthesis of dipeptides using N-protecting, C-protecting and C-activating groups (solution phase and solid-phase synthesis)
Primary, secondary, tertiary and quaternary structure of proteins.

Unit 3:Enzymes (6 Lectures)

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes.

Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition).

Unit 4:Nucleic Acids **(7 Lectures)**

Components of nucleic acids: Nucleobases, Nucleosides and nucleotides
Structure of Adenine, Guanine, Cytosine, Uracil and Thymine;
Structure of polynucleotides, Double-helix structure of DNA
Types and structures of RNAs
Elementary ideas of DNA replication, Transcription (biosynthesis of RNA) and Translation (biosynthesis of proteins)

Unit 5: Lipids **(4 Lectures)**

Definition of lipids, Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, iodine number, Reversion and rancidity
Phospholilpids and cell membrane.

Unit 6: Energy in Biosystems **(10 Lectures)**

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD.
Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle, oxidative phosphorylation, production of ATP, electron transport chain and ATP synthase.
Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types

Recommended Textbooks/ References:

1. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. 4th Edition. W.H. Freeman and Co.
2. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. 28th Edition. Lange Medical Books/ McGraw-Hill.
3. McMurry, J. (2014) Organic Chemistry with Biological Applications. 2nd Edition, Brooks/Cole
4. Voet, D., Pratt, C. W. and Voet, J. G. (2012) Principles of Biochemistry. 4th Edition. Wiley.
5. Berg, J. M., Stryer, L., Tymoczko, J. and Gatto, G. (2019) Biochemistry, 9th Edition, WH Freeman
6. Carey, F. A. and Giuliano, R. M. (2011) Organic Chemistry, 8th Edition, McGraw Hill

Lab experiments for organic Chemistry – III

1. Estimation of glycine by Sorenson's formalin method.
2. Study of the pH metric titration curve of glycine.
3. Estimation of glucose by Fehling solution.
4. Determination of saponification value of an oil or a fat.
5. Determination of Iodine number of an oil/ fat.
6. Study of the effect of temperature on the action of salivary amylase.

Recommended Books/References:

1. Arthur, I. V. Quantitative Organic Analysis, Pearson.
2. Mann, F. G. and Saunders, B. C. Practical Organic Chemistry.
3. Vogel's Textbook of Practical Organic Chemistry

Course outcomes:

On completion of the course, the students will be able to:

1. Understand the various structural forms of carbohydrates and their reactions
2. Learn synthesis and ionic properties of amino acids, separation of amino acids by electrophoresis, end group analysis of peptides and various structures of proteins.
3. Know the mechanism of enzyme action, factors affecting enzyme activity and enzyme inhibition.
4. Know the different types of nucleic acids, components of nucleic acids, reactions of the nucleobases, DNA replication and stages of protein biosynthesis.
5. Understand the various pathways involved in oxidation of food thereby producing energy.
6. Understand some fundamentals of fats and oils such as hydrogenation, rancidity etc.
7. Experiments involving quantitative estimation of amino acids and glucose, saponification value and iodine number of fat.

Paper: Core 10 (Physical Chemistry – II) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To learn about the thermodynamic properties of liquid mixtures including colligative properties.
2. To get familiar with colloids and their preparation, purification and properties.
3. To familiarize with chemical equilibria in ideal gases and solutions, and concepts of equilibrium constants.
4. To understand about electrolytes and their ionization properties and terms like pH, buffers and indicators.
5. To know about the conductivity of electrolytes and their related laws and applications.
6. To comprehend the ionic mobilities and transference numbers and their determinations.

Unit I: Solutions, colligative properties and colloids (15 lectures)

Liquid mixtures, concept of partial molar properties, ideal solutions, Raoult's law and Henry's Law and their applications. Activity and activity coefficients. Excess thermodynamic functions.

Thermodynamic derivations using chemical potential to derive relations between the four colligative properties (i) relative lowering of vapour pressure, (ii) elevation of boiling point,
depression of freezing point, and (iv) osmotic pressure. Applications in calculating molar masses.

Colloids, lyophobic and lyophilic colloids; preparation and purification of colloids, structure and stability of colloids, electrical double layer and electrokinetic phenomena. Surface-active agents (surfactants), micelle formation, critical micelle concentration.

Unit II: Chemical and ionic equilibria (15 lectures)

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature. Thermodynamic derivation of relations between the various equilibrium constants K_p and K_c. Examples and numerical problems of various chemical equilibrium. Le Chatelier's principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Theory of acid–base indicators; selection of indicators and their limitations.

Unit III: Electrical Conductance (15 lectures)

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) solubility and solubility product of sparingly soluble salts, (iii) conductometric titrations.

Physical Chemistry Lab (any five)

(1) Determination of the dissociation constant of a weak acid using Hendersen's equation.
(2) Verification of the Debye-Huckel-Onsager equation for aqueous solutions of a strong electrolyte.
(3) Verify the Ostwald dilution law by conductance measurement of a weak electrolyte and determine the dissociation constant of the electrolyte.
(4) Investigate the solubility of a sparingly soluble salt by conductance measurements.
(5) Study of the equilibrium between iodine, iodide ion and tri-iodide ion by distribution method and determine the equilibrium constant of the reaction.
(6) Determination of the equilibrium constant of an esterification reaction between acetic acid and ethanol.
(7) Study the inversion of cane sugar (sucrose) in presence of an acid.
(8) Determine the CMC of a surfactant by surface tension (conductivity or viscosity) measurements.

Textbooks and References

1. Atkin's Physical Chemistry, 10th Ed., PW Atkins and J De Paula, Oxford University Press, 2014.
2. Physical Chemistry, 4th Ed., GW Castellan, Narosa, 2004.
3. Physical Chemistry, 3rd Edition, T. Engel and P. Reid, Prentice-Hall, 2012.
4. Physical Chemistry, DW Ball, Cengage, India, 2012.
5. Physical Chemistry, 3rd Ed., RG Mortimer, Elsevier: Noida, 2009.
6. Physical Chemistry, 6th Ed., IN Levine, Tata McGraw-Hill, 2011.
7. Physical Chemistry, 2nd Ed., CR Metz, Tata McGraw-Hill, 2009.
8. Physical Chemistry by GW Castellan, Addison-Wesley.
9. Physical Chemistry, A Molecular approach, DA Mcquarrie and JD Simon, University Science Books, 1997.
10. A Textbook of Physical Chemistry (Volume 1, 2, 3, 4 & 5) by K.L. Kapoor (MacMillan)
11. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand, New Age International, 2014.
12. Principles of Physical Chemistry, by BR Puri, LR Sharma, and MS Pathania, Vishal Publishing Co, 2016.
13. Physical Chemistry, by PC Rakshit, Sarat Book Distributors, 2016.
14. The Physical Chemist's Toolbox, by RM Metzger, Willey, 2012.
15. Advanced Practical Physical Chemistry, by JB Yadav, Krishna Publications, 2012.
16. Advanced Practical Chemistry, J Singh, RKP Singh, J Singh, LDS Yadav, IR Siddiqui, J Shrivastava, Pragati Prakashan, 2017.
17. Experimental Physical Chemistry, by RC Das and B Behera, Tata McGrow-Hill Publishing, 1983.

Course Outcomes:

On completion of the course, the students will be able to:

1. Comprehend about the thermodynamic properties of liquid mixtures including colligative properties.
2. Understand the colloids, their preparation and purification based on structural stability. And micelle formation.
3. Familiarize with chemical and ionic equilibria in ideal gases and solutions including equilibrium constants.
4. Understand about electrolytes and their ionizations to understand the terms pH, buffers and indicators.
5. Know about the conductivity of electrolytes and pertinent laws and applications.
6. Achieve ideas on mobilities and transference numbers of ions and their determinations.

Paper: Core 11 (Quantum Chemistry) Credits: 4 + 0 + 0 = 4

Learning Objectives:
1. Familiarization with basic ideas of quantum mechanics – its postulates, operators, Schrodinger equation, wave functions, probability interpretation, etc.
2. Knowing forms of the Schrodinger equation and its solutions for simple model systems such as particle in a box, harmonic oscillator, rigid rotor, etc.
3. Understanding quantum mechanical treatment of hydrogen-like atomic systems in terms of radial and angular wavefunctions, nodes, representation of orbital shapes along with electron-nuclear distance quantifications.
4. Following the electronic structure of many-electron atoms in terms of their spin-included wavefunctions, using variation theory and involving spectroscopic atomic terms and levels.
5. Following quantitative MO and VB treatments of chemical bonding in simple molecules and Huckel MO treatments of conjugated organic compounds.

Unit 1: Basic principles of quantum mechanics (12 Lectures)

Postulates of quantum mechanics. Schrödinger wave equation – both time dependent and time independent forms. Wave functions of one-particle and many-particle systems, their Born interpretation. Well-behaved functions and normalized functions. Orthogonal functions and Schmidt's orthogonalization technique. Physical observables and corresponding quantum mechanical operators. Eigenvalues and eigenfunctions of quantum mechanical operators, the physical significance of the eigenvalues. Expectation values of observable properties.

Hermitian operators and their real eigenvalues. Concept of degeneracy. Compatible and incompatible observables and the (generalised) uncertainty principle (derivation not required). Basic ideas about the theory of angular momenta – spin and orbital angular momenta, ways of their coupling.

Unit 2: Some Model Systems with Exact Solutions (14 Lectures)

Discussion of the Schrödinger time-independent equations and their solutions for:

(i) Particle in a one-dimensional box and in a three-dimensional box.
(ii) Linear harmonic oscillator, vibrational energy levels of diatomic molecules.
(iii) Rectangular potential barrier problem, concept of quantum mechanical tunnelling.

(iv) Problem of two interacting particles: separating centre of mass and relative motion.

(v) The two-particle rigid rotor problem, rotational energy levels of a diatomic molecule.

Unit 3: Quantum Mechanics of Hydrogen Atom and Hydrogen-Like Ions (12 Lectures)

Setting up of Schrödinger equation for relative motion of electron in Cartesian and spherical polar coordinates, obtaining radial equation and angular equation (solution procedures not required for both equations). Radial solution: radial wavefunction and radial probability distribution function, average and most probable distances of electron from nucleus. Angular solution: the angular wavefunction and the representation of the shapes of atomic orbitals.

Unit 4: Electronic Structure of Many-Electron Atoms (8 Lectures)

Setting up of Schrödinger equation for many-electron atoms (He, Li, etc.). Product wave functions: complete many-electron wave functions involving atomic orbitals along with spin functions. Pauli's anti-symmetry and exclusion principles. Spin states of the He atom: singlet and triplet states. Need for approximation methods. Statement of variation theorem and its application to the ground electronic state of He atom. Spectroscopic term symbols for the s^1p^1, p^2 and d^2 configurations – splitting of the energy of a configuration due to inter-electronic repulsion (into terms) and spin-orbit coupling (into levels).

Unit 5: Chemical Bonding in Molecules (14 Lectures)

The hydrogen molecule ion (H_2^+): LCAO-MO theory, ground and excited electronic states of H_2^+.
The H_2 molecule: LCAO-MO and valence bond (VB) treatments. Refinements of the two approaches (configuration interaction for MO, ionic-covalent resonance for VB). Equivalence of the improved MO and the improved VB methods for H_2.
Extension of the LCAO-MO method to other homonuclear and heteronuclear diatomic molecules.
Term symbols for diatomic molecular electronic states, their symmetry classification. Correlation diagrams and the non-crossing rule.
The π-electron theory: Hückel molecular orbital (HMO) method for conjugated carbon compounds with chain and ring structures; introduction to extended Hückel theory.

Recommended Textbooks/References:

1. Levine, I.N. *Quantum Chemistry*, 7th Ed., Pearson, 2016.

2. Lowe, J. P. & Peterson, K. *Quantum Chemistry*, 3rd Ed., Academic Press, 2005.
3. Sen, B. K. *Quantum Chemistry Including Spectroscopy*, Kalyani Publishers, 2011.
4. Szabo, A. and Ostlund, N. S., *Modern Quantum Chemistry,* 1st Ed., Dover Publications, 1996.
5. Engel, T. and Reid, P. *Quantum Chemistry and Spectroscopy*, 4th Ed., Pearson, 2018.
6. Atkins, P. W and Friedman, R. S. *Molecular Quantum Mechanics,* 5th Ed., OUP (Oxford), 2010.

Course Outcomes:

On completion of the course, the students will be able to:

1. Understand and internalise the basic concepts of quantum mechanics such as postulates, operators, Schrodinger equation, wave functions and their probability aspects.
2. Appreciate the form of the Schrodinger equation and become knowledgeable about its application in various simple model systems.
3. Follow the quantum mechanical treatment of one-electron atoms with quantifications.
4. Recognise the extension of the one-electron atom treatment to many-electron atoms using approximation theory and electron spin concept.
5. Appreciate the quantitative aspects of MO and VB treatments for molecules that are already theoretically familiar to them, and of the Huckel MO treatment for conjugated organic molecules.

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Semester-VI

Paper: Core 12 (Inorganic Chemistry - IV) **Credits 3 + 0 + 1 = 4**

Learning Objectives:

1. To learn about inorganic reaction mechanisms and kinetics
2. To learn about the electronic spectroscopy and magnetic behavior of transition metal complexes
3. To learn about the symmetry operations and point group determination of molecules
4. To learn about the basics of radioactivity, nuclear chemistry and related applications
5. To learn about synthesis of some metal complexes and their characterizations

Unit 1: Reaction Kinetics and Mechanism **(11 Lectures)**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedralcomplexes. Inner sphere and outer sphere mechanisms of Redox Reactions, Marcus Theory.

Unit 2: Electronic spectra of Transition metal complexes **(10 lectures)**

d-d transition, charge transfer transition, colour, intensity and origin of spectra, term symbols and splitting of terms in different geometries, selection rules for electronic transitions, correlation, Orgel and Tanabe-Sugano diagrams, calculation of Dq and Racah parameters, Nephelauxetic series.

Unit 3: Magnetic Properties of Transition Elements (8 lectures)

Ferro and antiferro-magnetism, temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation, experimental measurement, magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling, spin crossover. Temperature dependence of magnetic susceptibility, exchange coupling effects.Magnetic properties of second and third transition series.

Unit 4: Molecular symmetry and symmetry groups (8 lectures)

Concept of group theory, Symmetry elements and symmetry operations, Classesof symmetry operation, Symmetry point groups, Assignment of point groups to simplemolecules, Structure and symmetry of Inorganic complexes (coordination number 2-6), Shapes and Symmetry of s, p and d orbitals.

Unit 5: Nuclear Chemistry (8 lectures)

Introduction, Nuclear binding energy, Mass defect and binding energy, Radioactivity, Nuclear emissions (a-decay, b-decay, g-decay, neutron emission, positron emission, electron capture), Nuclear transformations, The kinetics of radioactive decay, half lives, Units of radioactivity, Artificial isotopes, Nuclear fission, The fission of uranium, Nuclear fusion, Applications of isotopes, Kinetic isotope effects, Radiocarbon dating.

Reference Books:

1. Cotton, F.A. Wilkinson G.; & Gaus, P. L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
2. Huheey, J. E.; Keiter, E. A. & Keiter, R. L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins1993, Pearson, 2006.
3. Sharpe, A. G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
4. Douglas, B. E.; McDaniel, D. H. & Alexander, J. J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
5. Greenwood, N. N. & Earnshaw, A. Chemistry o*f* the Elements, Elsevier 2nd Ed, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
6. Lee, J. D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.

7. Shriver, D. D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
8. Basolo, F. & Person, R. Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.
9. Purcell, K.F. &Kotz, J. C., Inorganic Chemistry, W. B. Saunders Co. 1977
10. Miessler, G. L. & Donald, A. Tarr, Inorganic Chemistry 4th Ed., Pearson, 2010.
11. Dutta, R. L. & Shyamal, A., Elements of Magnetochemistry 2nd Ed., Affiliated East-West Press
12. Arnikar, H. J. Essentials of Nuclear Chemistry 4th Ed., New Age International Pvt. Ltd., 2011
13. Housecroft, C. E., Sharpe, A. J. Inorganic Chemistry 5th Ed. Pearson 2018
14. Figgis, B. N., Hitchman, M. A., Ligand Field Theory and Its Applications, Wiley India Pvt. Ltd. 2010
15. Cotton, F.A., Chemical Applications to Group Theory 3rd Ed.; Wiley India,
16. Reddy, K. V., Symmetry and Spectroscopy of Molecules 2nd Ed.; New Age International Publishers, 2020

Inorganic Chemistry - IV Laboratory:

(i) Measurement of 10Dq by spectrophotometric method

(ii) Verification of spectrochemical series.

(iii) Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs. thermodynamic factors.

(iv) Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complexes.

(v) Synthesis of ammine complexes of Ni (II) and its ligand exchange reactions (e.g., bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Reference Books:

1. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
2. Barua, S., A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016
3. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed.,

2014.
4. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013.
5. Marr, G., Rockett, B. W.Practical Inorganic Chemistry, Van Nostrand Reinhold Company, 1972.

Course Outcomes:

After the completion of the course, the students will acquire knowledge of:

1. Inorganic reaction mechanisms and their kinetic behaviors
2. Electronic spectra and magnetic properties of metal complexes
3. Symmetry elements, symmetry operations and point group determination of molecules
4. Radioactivity and basic aspects of nuclear chemistry along with specific examples
5. Basic aspects of inorganic synthesis and some characterization techniques

Paper: Core 13 (Organic Chemistry – IV) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To learn about the methods of preparation of amines, nitro compounds, nitriles and isonitriles and their reactions.
2. To know the synthesis of the five and six membered heteroaromatic compounds.
3. To learn the photochemical reactions of carbonyl compounds, alkenes and polyenes and photochemistry involved in vision and singlet oxygen quenching in biological systems.
4. To learn about the fundamentals of cycloaddition, electrocyclic and sigmatropic reactions with simple examples.
5. To learn about reaction intermediates and rearrangement reactions involving rearrangement to electron deficient C, N and O atoms and electron rich C atoms.
6. To do simple synthesis involving pericyclic reaction and rearrangement reaction

Unit 1. Nitrogen containing functional groups (8 Lectures)

Amines: Basicity of alkyl amines, aryl amines, amidine bases
Preparation: Gabriel phthalimide synthesis, Hoffmann bromamide reaction, Mannich reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent, nitrous acid and carbylamines reaction.
Diazonium Salts: Preparation and their synthetic applications.
Preparation and important reactions of nitro compounds, nitriles and isonitriles.

Unit 2. Heterocyclic compounds (7 Lectures)

Classification, nomenclature and structure.
Aromaticity in 5-numbered and 6-membered rings

Synthesis: Furan, Pyrrole and Thiophene (Paal-Knorr synthesis), Pyridine (Hantzsch synthesis), Indole (Fischer synthesis), Quinoline (Skraup synthesis synthesis), Isoquinoline (Bischler-Napieralski reaction).
Synthesis and aromaticity in pyrimidine and purine.

Unit 3. Photochemical reactions **(6 Lectures)**

Basics of photochemistry: Introduction to organic photochemical and photophysical processes, chemiluminescence, photosensitization.
Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, Paterno-Buchi reaction and photoreduction.
Photochemistry of alkenes and polyenes: Geometrical isomerization, photostereomutation of *cis-trans* isomers, optical pumping.
Other photochemical reaction – Barton reaction, di-π-methane rearrangement
Reaction of singlet oxygen, singlet oxygen quenching in biological systems, photochemistry of vision.

Unit 4. Pericyclic reactions **(7 Lectures)**

Molecular orbital symmetry, Frontier molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Pericyclic reactions and their classification; Cycloaddition reactions: [2+2] and [4+2] cycloaddition, dienes and dienophiles, suprafacial and antarafacial orbital overlap, FMO approach. Regeo and stereoselectivity. Electrocyclic reactions: conrotation and disrotation. Sigmatropic reactions: [1,3] hydride shift and alkyl shift.

Unit 5. Reaction intermediates (7 **Lectures**)

Carbocations, carbanions, free radicals, carbenes and nitrenes: Generation – structure and stability.
Reactions – Wagner-Meerwein rearrangement – neighbouring group participation of σ and π bonds, non-classical carbocations, Whitmore 1,2-shift, Wolff rearrangement, Simmons-Smith reaction, Curtius rearrangement, Hofmann–Löffler–Freytag reaction.

Unit 6. Rearrangement reactions **(10 Lectures)**

General concept, electrophilic, nucleophilic and radical rearrangement.
Rearrangement to electron deficient carbon: Pinacol-pinacolone rearrangement, Tiffeneau-Demjanov Rearrangement, Benzilic acid rearrangement. Arndt-Eistert Homologation Reaction.
Rearrangement to electron rich carbon: Favorskii rearrangement
Rearrangement to electron deficient nitrogen: Beckmann rearrangement, Hofmann rearrangement, Schmidt rearrangement.
Rearrangement to electron deficient oxygen: Baeyer-Villiger Oxidation, Dakin reaction
Migratory aptitudes of groups, Stereoelectronic effects in rearrangement reactions.

Recommended Textbooks/ References:

1. Turro, N.J., Ramamurthy, V. and Scaiano, J. C. Principles of Molecular Photochemistry, An Introduction, University Science Books, 2008.
2. Gilbert, A. and Baggott, J. "Essentials of Molecular Photochemistry," CRC Press, London, UK, 1991
3. Mattay, J. and Griesbeck, A. eds., "Photochemical Key Steps in Organic Synthesis", VCH, New York, 1994, 4.
4. Coyle, J. D. ed., "Photochemistry in Organic Synthesis", Royal society of Chemistry, London, 1986
5. Wayne, R. P. Principles and Applications of Photochemistry, Oxford Science Publications, Oxford University Press, Oxford
6. Norman, R.O.C. and Coxon, C. M. Principles of Organic Synthesis, CRC Press, New York, 2009.
7. Mundy, B. P., Ellerd,M. G., Favaloro, F. G. Jr. Name Reactions and Reagents in Organic Synthesis, Wiley Interscience, New Jersey, 2005.
8. Sankararaman, S. Pericyclic Reactions – A textbook. Wiley-VCH, 2005.
9. Fleming, I. Pericyclic Reactions, Oxford University Press, 1999.
10. March's Advanced Organic Chemistry,: Reactions, Mechanisms and Structure, 7th Edn. Wiley Interscience, Yew York, 2015
11. Clayden, J.; Greeves, N. and Warren S. (2012), Organic Chemistry, 2nd Edition, Oxford Publishers

Lab experiments for organic Chemistry – IV

1. Green synthesis of acetanilide
2. Preparation of methyl orange
3. Preparation of benzilic acid from benzil
4. Diels-Alder reaction between furan and maleic acid
5. Preparation of benzanilide from benzophenone

Recommended Books/References:

1. Mann, F. G. and Saunders, B. C. Practical Organic Chemistry.
2. Vogel's Textbook of Practical Organic Chemistry

Course outcome:

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

1. Know the methods of preparation of amines and their derivatives and synthetic utilities of the azo compounds.
2. Know the methods of preparation of the five and six membered heteroaromatic compounds.

3. Understand the photochemical reactions of alkenes and carbonyl compounds, photochemistry involved in vision.
4. Understand the stereochemistry of the product formed in simple cycloaddition, electrocyclic and sigmatropic reactions.
5. Know reaction intermediates and some rearrangement reactions involving migration to electron deficient and electron rich centres.
6. Appreciate involvement of pericyclic and rearrangement reactions in synthesis of some simple products.

Paper: Core 14 (Physical Chemistry – III) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To gain sound knowledge about various electrodes and electrochemical cells including fuel cells.
2. To familiarize with EMF measurements and their applications.
3. To comprehend about the basics of bimolecular transition state theory and the unimolecular reaction theories.
4. To acquire knowledge of different complex reactions and steady state treatment to understand the kinetics of complex reactions.
5. To attain knowledge about the polymers, their classifications and structure in solutions.
6. To comprehend about the concept of average molecular weight of polymers and their determinations.

Unit I: Electrochemical Cells (15 lectures)

Chemical cells, reversible and irreversible cells. Measurement of electrode and cell potential (EMF), Standard hydrogen electrode, standard electrode (reduction) potential, different classes of electrodes and reference electrodes. Nernst equation and equilibrium constants. Application of EMF measurements: (i) Free energy, enthalpy and entropy of cell reaction, (ii) Equilibrium constants, (iii) pH, using hydrogen, quinine-hydroquinone and glass electrode, and (iv) Potentiometric titrations (acid-base and redox).

Concentration cells, cells with and without transference. Liquid junction potential, determination of activity coefficients and transference numbers.
Primary cells: construction and working of zinc-graphite dry cells. Secondary cells: construction and working of lead storage battery. Fuel cells, their applications and reason behind their high efficiency.

Unit II: Advanced Chemical Kinetics **(15 lectures)**

Transition State theory – statistical mechanical formulations. Applications of Transition state theory – reactions between atoms and molecules. Theory of unimolecular reactions (Lindemann theory) – dynamic molecular collisions – potential energy surfaces.

Consecutive, concurrent and opposing reactions. Steady state treatment, kinetics of decomposition of N_2O_5 and ozone. Kinetics of chain reactions, H_2-Br_2 reaction, branching and non-branching chain reaction, H_2-O_2 reaction, concept of explosion limits.

Reactions in solution, Bronsted-Bjerrum equation, Kinetic salt effect. Linear free energy relationship, Hammett equation and Taft equation.

Unit III: Introduction to Polymers **(15 lectures)**

Monomers, repeat units, degree of polymerization, concepts of linear, branched and network polymers with examples. Classifications of polymers on the basis of origin, properties and uses with examples. Introductory concepts of free-radical, cationic, anionic and coordination chain polymerizations, ring-scission polymerization and copolymerization.

Dispersity and average molecular weight concept. Number, weight and viscosity average molecular weights – numerical calculations, dispersity index. Determination of molecular weights: viscosity, osmotic pressure and light scattering methods. Free-radical chain polymerization kinetics, chain length, kinetics of step polymerization and of chain copolymerization.

Structure and configuration of polymer chains – root mean square end to end distance and radius of gyration; random flight model, unperturbed dimension, short-range and long-range interactions; chain stiffness and theta solvent concepts.

Physical Chemistry Lab (any five)

(1) Determination of the viscosity-average molecular weight of a polymer by viscometric method.
(2) Verification of the proportionality of the rate constant for acid-catalyzed hydrolysis of methyl acetate to the concentration of the mineral acid catalyst (graphical method).
(3) Study of the progress of the autocatalytic reaction between oxalic acid and $KMnO_4$ with time and identification of its autocatalytic nature.
(4) Study of the complex formation between Cu^{2+} ion and ammonia by distribution method using water-chloroform mixtures and hence to find the composition of the complex.
(5) Study the kinetics of the reaction between potassium persulphate and potassium iodide. Verify the influence of ionic strength on the rate constant.

(6) Potentiometric titration of acetic acid with NaOH and determination of the dissociation constant of acetic acid using Quinhydrone electrode.
(7) Titrate a mixture of HCl and CH_3COOH potentiometrically by NaOH.
(8) Calculations of potential energy surface for ethane molecule.

Textbooks and References

1. Atkin's Physical Chemistry, 10th Ed., PW Atkins and J De Paula, Oxford University Press, 2014.
2. Physical Chemistry, 4th Ed., GW Castellan, Narosa, 2004.
3. Physical Chemistry, 3rd Edition, T. Engel and P. Reid, Prentice-Hall, 2012.
4. Physical Chemistry, DW Ball, Cengage, India, 2012.
5. Physical Chemistry, 3rd Ed., RG Mortimer, Elsevier: Noida, 2009.
6. Physical Chemistry, 6th Ed., IN Levine, Tata McGraw-Hill, 2011.
7. Physical Chemistry, 2nd Ed., CR Metz, Tata McGraw-Hill, 2009.
8. Physical Chemistry by GW Castellan, Addison-Wesley.
9. Physical Chemistry, A Molecular approach, DA Mcquarrie and JD Simon, University Science Books, 1997.
10. A Textbook of Physical Chemistry (Volume 1, 2, 3, 4 & 5) by K.L. Kapoor, MacMillan.
11. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand, New Age International, 2014.
12. Principles of Physical Chemistry, by BR Puri, LR Sharma, and MS Pathania, Vishal Publishing Co, 2016.
13. Physical Chemistry, by PC Rakshit, Sarat Book Distributors, 2016.
14. Textbook of Polymer Science, by FW Billmeyer, Wiley, 1994.
15. Polymer Science, by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, New Age International.
16. Chemical Kinetics, by KJ Laidler, Pearson, 2013.
17. The Physical Chemist's Toolbox, by RM Metzger, Willey, 2012.
18. Electrochemistry, PH Rieger, Prentice-Hall International.
19. Advanced Practical Physical Chemistry, by JB Yadav, Krishna Publications, 2012.
20. Advanced Practical Chemistry, J Singh, RKP Singh, J Singh, LDS Yadav, IR Siddiqui, J Shrivastava, Pragati Prakashan, 2017.
21. Experimental Physical Chemistry, by RC Das and B Behera, Tata McGrow-Hill Publishing, 1983.

Course Outcomes:

On completion of the course, the students will be able to:

1. Understand various electrodes and electrochemical cells including fuel cells.
2. Acquire knowledge on EMF measurements and their applications.

3. Comprehend about the basics of bimolecular transition state theory and the theories of unimolecular reaction.
4. Familiarize with different complex reactions and steady state treatment to understand the kinetics of complex reactions.
5. Understand about the polymers, their classifications and structure in solutions.
6. Attain knowledge on the concept of average molecular weight of polymers and their determinations.

Paper: Core 15 (Molecular spectroscopy) Credits-4 + 0 + 0 = 4

Learning Objectives:

1. This course will introduce basics of various spectroscopic techniques used for analysis of organic and inorganic molecules.
2. Idea of interaction of electromagnetic radiation with molecules to generate spectra, knowing about characteristics of rotational, vibrational and Raman spectra of molecules.
3. Introduction to electronic transitions, Frank-Condon principle, dissociation and electronic spectra of molecules.
4. Principles, characteristic parameters and characterising features of ^{1}H NMR, ^{13}C NMR and ESR spectroscopy.
5. To introduce basic principles and instrumentation used in mass spectrometry and to explain important features in mass spectra
6. To understand and acquire knowledge on the application of these techniques

Unit 1: Principles of Spectroscopy (5 Lectures)

The nature of electromagnetic radiation. Regions of the electromagnetic spectrum. Mechanism of interaction of electromagnetic radiation with matter. Absorption and emission spectroscopy. Representation of spectrum, signal-to-noise ratio, the width of spectral lines, intensity of spectral lines, Beer-Lambert's law, molar extinction coefficient, concept of selection rules.

Unit 2: Rotational, Vibrational and Raman spectroscopy (12 Lectures)

Classification of molecules according to their moments of inertia. Rotational spectra of diatomic molecules – rigid rotor approximation. Determination of bond length, effect of isotopic substitution, spectra of non-rigid rotor.

Vibrational spectra of diatomic molecules – harmonic and anharmonic oscillator model, Morse potential. Calculation of force constants, effect of isotopic substitution on vibrational frequency.

Vibrations of polyatomic molecules, fundamental vibrations and their symmetry, normal modes of vibration (in H_2O, CO_2), overtone and combination bands (in H_2O, CO_2), Fermi resonance, Hot bands.

Diatomic vibrating rotator, P, Q, R branches, vibration-rotation spectrum of CO.

Stretching frequencies of bonds and functional groups (examples from both organic and inorganic molecules), concept of fingerprint region. Correlation of infrared spectra with molecular structure – effects of conjugation, hydrogen bonding and coordination to metals on IR spectra.

Principle of Raman spectroscopy: rotational and vibrational Raman spectra of linear molecules. Selection rules for infrared and Raman spectra, rule of mutual exclusion, stokes'and anti-stokes' lines.

Unit 3: Electronic spectroscopy (6 Lectures)

Electronic transition in diatomic molecules: selection rules, Born-Oppenheimer approximation, vibrational structure, Franck-Condon principle, electronic transitions in polyatomic molecules. Chromophores (conjugated systems, carbonyl compounds), auxochrome, absorption due to ethylenic chromophore – Woodward-Fieser rules. d-d transitions and charge transfer transitions. Effect of solvents on electronic transition, quantitative estimations by spectrophotometry.

Basic concepts of photoelectron spectroscopy.

Unit 4: Spin resonance spectroscopy (12 Lectures)

Interaction between spin and the magnetic field, nuclear spin, nuclear magnetic resonance spectroscopy, ^1H NMR spectroscopy, chemical shift, concept of shielding and deshielding,

splitting and integration of peaks, chemical equivalence and magnetic equivalence, approximate chemical shifts for simple organic molecules (alkanes, alkenes, alkynes, arenes, aldehydes, carboxylic acids and esters).
Spin-spin coupling and coupling constant, Karplus equation, first order and non-first order spectra, high resolution ^{1}H NMR spectrum of few organic compounds.
Basic outlines of ^{13}C NMR spectroscopy, spin decoupling and its applications.
Basic concept of electron spin resonance (ESR) spectroscopy, hyperfine structures, ESR of few simple inorganic and organic ions and radicals.

Unit 5: Mass spectrometry (6 Lectures)

Mass spectrometry: principlesof mass spectrometry, components of mass spectrometer, ionization techniques, base peak, molecular ion peak, pseudo molecular ion peak and isotope peak, fragmentation patterns. Applications in structure elucidation of simple organic molecules, McLafferty rearrangement (hexanoic acid, pentanal etc.), nitrogen rule.

Unit 6: Structure elucidation using various spectroscopic techniques (4 Lectures)

Determination of chemical structure of organic compounds by analyzing UV-Visible, IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry data.

Course outcomes:

1. Students will understand the fundamentals of spectroscopic technique.
2. Know how electromagnetic radiation interacts with molecules to generate spectra, with illustration of molecular rotational, vibrational and Raman spectra. Understand how electronic transitions happen, leading sometimes to dissociation and generally to spectra.
3. This course will also make the students capable to assign spectroscopic bands and to understand their underlying features.
4. Elucidate the structure of simple organic molecules from the chemical shift and coupling constant values
5. Interpret the structure of a molecule from ^{13}C NMR spectra
6. Determine the structure from the ESR spectra of simple organic and inorganic molecules
7. Relate the molecular structure with the mass spectra

8. Students will be able to solve problems relating to structure elucidation using the information obtained from rotational, vibrational and Raman spectroscopic techniques.

Books/References:

1. Fundamentals of molecular spectroscopy by C.N.Banwell and E. M. Mc Cash (Tata Mcgraw Hill)
2. Quantum chemistry and spectroscopy by B.K. Sen (Kalyani publishers)
3. Organic spectroscopy by W. Kemp (Mcmillan)
4. Introductory organic spectroscopy by B.K. Sen and Mausumi Ganguly (Kalyani)
5. Inorganic spectroscopic methods by A.K. Bridson (Oxford Chemistry Primers)
6. Spectroscopy in inorganic chemistry by C.J. Ballhausen (Academic Press)
7. Introduction to Spectroscopy by D.L. Pavia (Cengage India)
8. Spectrometric identification of organic compounds by R. Silverstein (Willey)
9. Spectroscopy of organic compounds by P.S. Kalsi (New Age Publishers)

Cotton University: Department of Chemistry
NEP UG Syllabus: Core Courses

Semester-VII

Paper: Core 16 (Group Theory and Spectroscopy of Inorganic Compounds)

Credits – 3 + 0 + 1 = 4

Learning Objectives:

1. To learn about group theory and its applications in chemistry
2. To learn about determination of symmetry properties and their application in elucidation of certain spectral behaviors
3. To learn about the applications of IR, ESR, NMR and Mossbauer spectroscopic techniques on inorganic molecules
4. To learn about synthesis inorganic metal complexes and their characterizations using IR, UV-vis, NMR, ESR, magnetic and conductometric measurements

Unit 1: Introduction to Group Theory in Chemistry (12 lectures)

Matrix representation of symmetry operations, The Great Orthogonality Theorem, Reducible and Irreducible representation of groups, Features and Construction of

Charactertables (*C_{2v}*, *C_{3v}*, *C_{2h}* and *D_3*).Group theory and Quantum Mechanics- wave functions as bases for irreducible representations, the direct product and its importance in predicting spectral transition probabilities.

Unit 2: Chemical Applications of Group Theory (15 lectures)

Molecular Vibrations- determining symmetry types of normal modes of vibrations with selected examples, Selection rules for Fundamental Vibrational Transition (IR and Raman).

Symmetry properties of atomic orbitals, molecular orbitals for and bonding in AB_4 molecules, Bonding in polyatomic molecules (H_2O, BeH_2, H_2O, CO_2, NO_2, NH_3) based on the concept of hybridization and SALC. MO treatment of bonding in Ferrocene. Ligand field states, constructon of correlation diagram for d^2 configuration in an octahedral environment.

Unit 3: ESR and NMR Spectroscopy (10 lectures)

Applications of NMR spectroscopy to diamagnetic and paramagnetic inorganic compounds; paramagnetic shifts, ^{11}B, ^{15}N, ^{19}F, and ^{31}P NMR in inorganic compounds.

Electron Spin Resonance (ESR spectroscopy): Basic principles, factors affecting g-tensors, hyperfine splitting in free radicals and metal complexes, zero field splitting, application of ESR for $d^1$and d^9complexes.

Unit 4: Infrared and Mössbauer Spectroscopy of Inorganic Compounds (8 lectures)

Infrared Spectroscopy of inorganic/coordination and organometallic representative compounds.

Basic principles, isomer shift, quadrupole splitting and effect of magnetic field. Mössbauer Spectra of high-spin and low-spin iron complexes.

Reference Books:

17. Cotton, F.A., Chemical Applications to Group Theory 3rd Ed.; Wiley India,

18. Reddy, K. V., Symmetry and Spectroscopy of Molecules 2nd Ed.; New Age International Publishers, 2020
19. Drago, R. S., Physical Methods in Inorganic Chemistry; Affiliated East-West Press Pvt. Ltd., 2012
20. Drago, R. S.,Physical Methods for Chemists 2nd Ed.; Affiliated East-West Press Pvt. Ltd., 2016
21. Figgis, B. N., Hitchman, M. A., Ligand Field Theory and Its Applications, Wiley India Pvt. Ltd. 2010
22. Bridsdon, A. K., Inorganic Spectroscopic Methods: 62 (Oxford Chemistry Primers) 1st Ed.; Oxford Science Publications. 1998.
23. Cotton, F.A. Wilkinson G.; & Gaus, P. L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
24. Huheey, J. E.; Keiter, E. A. &Keiter, R. L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins1993, Pearson, 2006.
25. Sharpe, A. G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
26. Douglas, B. E.; McDaniel, D. H. & Alexander, J. J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
27. Lee, J. D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
28. Powell, P. Principles o*f* Organometallic Chemistry, Chapman and Hall, 1988.
29. Shriver, D. D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
30. Basolo, F. & Person, R. Mechanisms o*f* Inorganic Reactions: Study o*f* Metal Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.
31. Purcell, K.F. & Kotz, J. C., Inorganic Chemistry, W. B. Saunders Co. 1977
32. Miessler, G. L. & Donald, A. Tarr, Inorganic Chemistry 4th Ed., Pearson, 2010.
33. Collman, James P. *et. al.* Principles and Applications o*f*Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
34. Crabtree, Robert H. The Organometallic Chemistry o*f* the Transition Metals. J New York, NY: John Wiley, 2000.
35. Spessard, Gary O., & Gary L. Miessler. Organometallic Chemistry. Upper Saddle River, N J: Prentice-Hall, 1996.
36. Housecroft, C. E., Sharpe, A. J. Inorganic Chemistry 5th Ed. Pearson 2018

Inorganic Chemistry Laboratory:

Preparation of selected inorganic complexes (Linkage isomers, Cis-Trans isomers etc.) and their physico-chemical characterization by elemental analysis, IR, NMR, ESR and electronic spectroscopic techniques, magnetic susceptibility measurements, and solution conductivity measurements wherever appropriate and possible.

Reference Books:

6. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
7. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed., 2014.
8. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013.
9. Marr, G., Rockett, B. W. Practical Inorganic Chemistry, Van Nostrand Reinhold Company, 1972.

Course Outcomes:

On completion of the course students will be able to:

1. Understand the underlying principles of group theory and their applications in chemistry
2. Utilize IR, ESR, NMR, MS and Mossbauer in structure elucidations of inorganic molecules
3. Apply spectroscopic and spectrometric techniques for characterization of synthesized metal complexes

Paper: Core 17 (Advanced Organic Chemistry) Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To learn basic concepts of how stereoselective synthesis can be done
2. To learn how C-C, C=C and C-N bond can be formed in organic reactions with some simple examples which find application in organic synthesis.
3. To learn fundamentals of how to find out simple raw materials for construction of organic molecules through disconnection of chemical bond
4. To learn protection-deprotection of functional groups which is frequently applied in organic synthesis
5. To learn fundamentals of click chemistry and metathesis reactions.
6. To learn synthesis a few organic molecules which involve formation of C-C, C=C and C-heteroatom bonds.

Unit 1. Introduction to asymmetric synthesis (10 Lectures)

Stereoselective and racemization reactions, Explanation of stereoselectivity through energy profile diagram. Use of chiral auxiliary, chiral reagent and chiral catalyst for asymmetric synthesis. Merits and demerits of using chiral inducing agents. Evans oxazolidinones for enantioselective alkylation, Sharpless asymmetric epoxidation, CBS catalyst. Resolution of racemic mixture through diastereomeric recrystallization and kinetic resolution. Asymmetric synthesis using chiral pool.

Unit 2. C-C, C=C and C-heteroatom bond forming reactions (17 Lectures)

Concept of the rection between electrophilic and nucleophilic centres with examples.

C-C Bond forming reactions: Alkylation of enamines and enolates (both kinetic and thermodynamic enolates) of ketones, esters and nitriles. Reaction of enolate with aldehydes, ketones – aldol reaction - use of boron enolates and silyl enol ethers; directed aldol reaction. Michael reaction. Darzen's reaction, Henry reaction, Reformatsky reaction.
C-C bond formation through transition metal catalyzed reactions – general mechanism and examples (Heck, Suzuki, Stille, Sonogashira).
C=C Bond forming reactions: Pyrolytic syn elimination- pyrolyses of carboxylic esters and xanthate esters (Chugaev reaction) and amine oxides (Cope elimination reaction). Wittig reaction- use of stabilized and unstabilized phosphorus ylides, Peterson reaction. Shapiro reaction.
Metathesis reactions: Definition, Olefin metathesis – cross metathesis, ring closing metathesis, ring opening metathesis, the Chauvin mechanism of metathesis reaction, catalysts used in metathesis reactions.
C-heteroatom bond forming reactions: Reaction of nucleophilic nitrogen with electrophilic carbon - Gabriel Synthesis, Strecker synthesis, Ritter reaction; Reaction of electrophilic nitrogen with nucleophilic carbon – nitrosation and nitration of active methylene compounds.

Unit 3. Retrosynthesis (5 Lectures)

Retrosynthesis- disconnection approach, synthons and synthetic equivalents; umpolung; Functional Group Interconversions (FGI); One group C-C disconnections, One group C-X disconnections, retrosynthesis of some simple organic compounds.

Unit 4. Protection-deprotection strategy (8 Lectures)

Protecting groups, criteria of a protecting group to be useful in synthesis, protection – a necessary evil; orthogonal protecting groups, permanent and temporary protection groups.
Protection and deprotection of hydroxyl groups – silicon based protecting groups, benzyl ether protecting groups, trifluoroacetate; protection and deprotection of aldehydes and ketones – acetals, 1,3-dioxolanes and 1,3-dithianes; Protection and deprotection of carboxylic acids – t-butyl ester, benzyl ester (Mitsunobu Reaction); Protection and deprotection of amines – t-Boc, Fmoc, Cbz

Unit 5. Click Chemistry (5 Lectures)

Definition, characteristics of click chemistry reactions and connection with green chemistry, click chemistry –an inspiration from nature's organic synthesis, Azide-alkyne cycloaddtion, thiol-X click reactions, Tetrazole cycloaddition and nitrile oxide cycloaddition; application of click chemistry in bioconjugation – modification of protein and application of click chemistry in drug discovery.

Recommended Textbooks/ References:

1. Clayden, J.; Greeves, N. and Warren S. (2012), Organic Chemistry, 2nd Edition, Oxford Publishers
2. Smith, M. B. (2016), Organic Synthesis, 4th Edition, Academic Press, Inc.
3. Warren, S. (2010), Organic Synthesis: The Disconnection Approach, 1st Edition, Wiley
4. Kalsi, P.S. (2022), Organic Synthesis through Disconnection Approach, 3rd Edition, MedTech Science Press

5. Coxon, J. M. and Norman, R.O.C. (1993), Principles of Organic Synthesis, 3rd Edition, CRC Press.
6. Carruthers, W. and Coldham, I (2004), Moder Methods of Organic Synthesis, 4th Edition, Cambridge University Press
7. Kolb, H.C.; Finn, M.G. and Sharpless, K. B. (2001), Click Chemistry: Diverse Chemical Function from a Few Good Reactions. Angewandte Chemie International Edition, 48, 2004-2021
8. Shirame, S. P. and Bhosale, R. B. (2018), Green Approach in Click Chemistry. Book Chapter in Green Chemistry. Editors: Saleh, H. M. and Koller, M.
9. Xi, W.; Scott, T. F.; Kloxin, C. J. and Bowman, C. N. (2014), Click Chemistry in Material Science. Advanced Functional Materials, 24, 2572-2590
10. Click Chemistry and Bioorthogonal Chemistry. Nobel Prize in Chemistry 2022
11. Moses, J. E. and Moorhouse A. D. (2007). The growing applications of click chemistry. Chemical Society Review, 36, 1249-1262
12. Caron, S. (2011). Editor of Practical Synthetic Organic Chemistry: Reactions, Principles and Techniques. Wiley.

Lab experiments for organic Chemistry – V

1. Synthesis of coumarin by Pechmann condensation and study of the absorption and fluorescence spectra of the synthesized coumarine
2. Synthesis of dibenzalpropanone
3. Synthesis of benzoin (thiamine catalyzed synthesis)
4. Synthesis of dihydropyrimidinone
5. Solvent free aldol condensation between acetophenone and 3,4-dimethoxybenzaldehyde
6. Any other synthesis may be given time to time.

Recommended Books/References:

1. Monograph on Green Chemistry Laboratory Experiments
2. Palleros, D. R. (2004). Solvent-Free Synthesis of Chalcones. Journal of Chemical Education, 81, 1345-1347.

Course outcomes:

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

1. Understand the role of the chiral-inducing agents in stereoselective synthesis
2. Know fundamentals of C-C bond formation through the chemistry of enolates and enamines and Pd-catalyzed coupling reactions, C=C bond formation though syn elimination and C-N bond formation through simple examples.
3. Find out the simple starting materials for the construction of small target molecules.

4. Understand why the protection of functional groups is necessary in organic synthesis and know some of the protecting groups used for protection of alcohol, carbonyl, carboxylic acid and amine.
5. Appreciate the fundamentals of click chemistry and metathesis reactions and understand remarkable chemistry which they serve in organic synthesis.
6. Learn synthesis of a few molecules whose synthesis involves formation of C-C, C=C and C-heteroatom bond through green chemistry.

Paper: Core 18 (Research Methodology) Credits: 4 + 0 + 0 = 4

Learning Objectives:

1. To understand about different print and digital sources for literature survey on a research topic.
2. Learning how to write a scientific paper.
3. To learn about analysis and presentation of data.
4. To understand the basics about research ethics

Unit 1. Introduction to research methodology (8 lectures)

Meaning and objectives of research, Types of Research, Qualitative and Quantitative approaches of research, Criteria of good research.

Research problem, Importance of defining the research problem, Techniques involved in defining a research problem, Illustration of research problem

Unit 2: Literature Survey (14 lectures)

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples Digital: Web resources, E-journals, Journal access, Citation index, Impact factor, H-index, Search engines, Google Scholar, Science Direct, SciFinder, Scopus. Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

Unit 3. Data Analysis (12 lectures)

Information and data, Scientific method and design of experiments. Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Student's t test, P value, Dixon's Q test, Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases.

Unit 4. Methods of Scientific Research and Writing Scientific Papers (14 lectures)

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work.

Unit 5. Ethics in Research, Copyright and Intellectual Property Rights (12 lectures)

Brief introduction to ethics and etiquettes in research, Research misconduct: fabricating, falsifying, and manipulating data.

Plagiarism: Definition, various forms of plagiarism, self-plagiarism, software for checking plagiarism

Intellectual property rights: Intellectual property and intellectual property rights, patent, trade mark, industrial design, geographical indication, copyright laws, world intellectual property organization.

Course Outcomes:

This course will help the students in planning a smooth, effective and manageable research work and becoming a successful researcher.

Books:

1. Kothari C.R. Research Methodology: Methods and Techniques. New Age International Publishers.
2. Research Methodology: A Step by Step Guide for Beginners 2/e by R. Kumar,

Pearson India, 2005.

3. Statistics By T. R. Jain & S. C. Aggarwal, VK Enterprises, India.

Paper: Core 18* (Chemistry of Nanomaterials) Credits- 4 + 0 + 0 = 4

Learning Objectives:

1. Know about the nomenclature of nanomaterials and how properties changes in nanomaterials as compared to their bulk counterpart.
2. Learn how nanomaterials will grow by bottom-up methods and self-assembled in beautiful morphologies using different physical and chemical methods.
3. Students will get familiar with how to make single walled and multi walled carbon nano tubes.
4. Differentiate the nanomaterials according to their confinements in 1-D, 2-D and 3-D.
5. Classification of nanostructures and nanomaterials, Bio-inorganic nanomaterials, DNA and nanomaterials
6. Learn the working and principles of various analytical tools such as XRD, UV-VIS spectroscopy, FT-IR, Raman spectroscopy and Electron Microscopy required for the characterization of nanomaterials.

7. Understand the novel properties like optical, magnetic and catalytic.
8. Understand about the environmental impact and toxicity of nanomaterials.

Unit 1: Introduction (8 Lectures)

Concept of nanoscale, Introduction of nanomaterials, nanoscience and nanotechnology, History of nanomaterials, Quantum confinement, Quantum dots, Surface Plasmon Resonance, Nanotechnology in nature.

Unit 2: Synthesis of Nanomaterials (22 Lectures)

Top- down and Bottom-up approaches of fabricating nanomaterials, Different physical and chemical methods of synthesizing nanomaterials, Brust-Schiffrin method, colloidal route, sol-gel methods, co-precipitation method. Templated synthesis using frameworks, supports and substrates: physical vapour deposition(PVD) and chemical vapour deposition(CVD). Challenges in the synthesis of nanoparticles, Ostwald ripening, electrostatic and steric stabilization.

One-dimensional control: carbon nanotubes and inorganic nanowires. Two-dimensional control: graphene and quantum wells. Three dimensional control: mesoporous materials and composites.

Unit 3: Characterization of nanomaterials (14 Lectures)

Electron Microscopy- Scanning Electron Microscope/Electron Diffraction X-Ray (SEM/EDX), Transmission Electron Microscope/ Selected Area Electron Diffraction(TEM/SAED). Surface Probe Microscopy- Scanning Tunneling Microscope (STM) and Atomic Force Microscope(AFM). UV- Vis Spectrophotometry, X-Ray Diffraction (XRD)-Scherrer Equation, Dynamic Light Scattering (DLS), Fourier Transform Infrared (FT-IR) Spectroscopy

Unit 4: Properties and applications of nanomaterials (12 Lectures)

Special properties and applications of metal & metal oxide nanoparticles, semiconducting nanoparticles, biomimetics, bio nanocomposites and other natural and artificial nanomaterials in industrial, environmental, and medical fields.

Unit 5: Toxicity of nanomaterials (4 Lectures)

Toxicity of nanomaterials, effects of inhaled nanosized particles, skin exposure to nanoparticles, impact of CNTs on respiratory systems, environmental impact of nanomaterials.

Course outcomes:

1. The students will also be benefited by gaining knowledge on different aspects of nanomaterials like classification and properties.
2. Students will get knowledge about how to synthesize nanomaterials and learn about their potential applications.
3. They will also get familiar with characterization tools like UV-Vis spectroscopy, FTIR, Electron Microscopy and XRD.
4. Will get familiar with nanomaterial toxicity.

Books/References:

1. Inorganic Chemistry by Weller Overton, Rourke, Armstrong, Oxford University Press.
2. Nanochemistry: A Chemical Approach to Nanomaterials – Royal Society of Chemistry, Cambridge UK 2005.
3. Chemistry of Nanomaterials: Synthesis, properties and applications, CNR Rao et. al.
4. Characterization of Nanophase materials – Z.L Wang (ed), Wiley-VCH, New York, 2000
5. Nanoparticles: From theory to applications – G. Schmidt, Wiley Weinheim, 2004.
6. Properties of Materials, Robert E. Newnham, Oxford University Press, 2005.

Paper: Core 21* (Industrial Chemistry) Credits- 4 + 0 + 0 = 4

Learning objectives:

1. To learn about different types of polymers and their applications.
2. To understand colour mixing, different dyes and their colours.
3. To know the process of preparation of cosmetics and perfumes.
4. To be familiar with pesticides and their beneficial and adverse effects.
5. To learn about different fractions of petroleum and uses of those.

Unit 1 Review of basic concepts of polymers and polymeric reactions (12 Lectures)

Preparation and applications of:
Plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);
Fabrics – natural and synthetic (acrylic, polyamido, polyester)
Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives;
Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples.

Unit 2 Dyes and Pigments (10 Lectures)

Colour and constitution; Complementary colours, additive and substractive colours (RGB and CMYK color system)
Classification, Mordant and Vat Dyes; Chemistry of dyeing;
Synthesis and applications of:
Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling);
Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet;
Phthalein Dyes – Phenolphthalein and Fluorescein;
Natural dyes –Alizarin and Indigotin;
Edible Dyes with examples.
Inorganic pigments; TiO_2, lithopone, ZnS, ZnO and Fe_2O_3; Corrosion protection pigments; Luminescent and magnetic pigments.

Unit 3 Cosmetics & Perfumes (8 Lectures)
A general study including composition and preparation of the following: Hair dye, hair spray, shampoo, suntan lotions, lipsticks, talcum powder, nail enamel, toothpaste.

Extraction and isolation of essential oils, their composition and uses in cosmetic industries: sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Unit 4: Pesticides (8 Lectures)
General introduction; natural and synthetic pesticides; benefits and adverse effects, changing concepts of pesticides,
Preparation and analysis of Organochlorines (Gammexene), Organophosphates (Malathion, Parathion), Carbamates (Carbofuran and carbaryl), Anilides (Alachlor and Butachlor).

Unit 5: Enamel and Ceramics (7 Lectures)
Ceramics: Manufacturing, Classification, Properties and Applications; Specialty ceramic products.
Enamel: Introduction, Process of Enameling, Properties and Uses.

Lab Experiments
1. Preparation and characterization of urea-formaldehyde resin
2. Preparation and characterization of simple azo-dye
3. Preparation of indigo dye
4. Preparation of simple organophosphates/ phosphonates/ thiophosphates
5. Preparation of shampoo/enamels/talcum powder/nail polish and nail polish remover

Course outcomes:
On completion of the course, the students will be able to:
1. Understand different types of industrial organic chemicals.
2. Draw structures; know utilities of industrial organics.
3. Gain adverse effect of using organic chemicals and importance of reducing those.
4. Get practical knowledge of synthesis and characterization of industrially important organic chemicals.

Recommended Text Books / References:

- F. W. Billmeyer, *Textbook of Polymer Science*, John Wiley & Sons, Inc.
- V. R.Gowariker, N. V. Viswanathan, &J. Sreedhar, *Polymer Science*, New Age International (P) Ltd. Pub

- M.A. Benvenuto, *Industrial Organic Chemistry,*Walter de Gruyter GmbH
- K.Weissermel, H-J. Arpe, *Industrial Organic Chemistry,* Wiely VCH 3rd edition
- M. F. Ali, B. M. Ali and J. G. Speight, *Handbook of industrial Chemistry (organic chemicals)*, McGraw-Hill

Paper: Core 21** (Heterogeneous Catalysis) Credits- 4 + 0 + 0 = 4

Learning Objectives:

1. Knowing about chemisorption pathway for heterogeneous catalysts and determining their surface area and porosity so as to identify potential good catalysts.
2. Appreciating the special characteristics and various applications of zeolites and clays.
3. Knowing about the applicability of catalysis in various processes in petroleum industry.
4. Having ideas about the role of catalysis in controlling automobiles exhausts and industrial plants.

Unit 1: Heterogeneous Catalysts and Catalysis (20 Lectures)

Characteristics of a good catalyst. Catalyst design methods, catalyst support and preparation of industrial catalyst, supported and unsupported metal catalysts, bimetallic catalysts.
Effect of temperature on rates of catalysed reactions, mass transport limitation of catalysed reactions. Surface dependence of reaction rates.
Surface area determination of solid catalysts from Langmuir and BET adsorption isotherms, porosity determination by volumetric and gravimetric methods. Chemisorption on metals, semi-conducting oxides and insulator oxides. Volcano principle.

Unit 2: Zeolites and Clays (15 Lectures)

Natural and synthetic zeolites, shape selectivity properties, solid acids, acidity of zeolites and clays. Mesoporous materials, poorly crystalline silicates and aluminosilicates.
Applications of zeolites and clays as heterogeneous catalysts in cracking, reforming and olefin reactions. Zeolites as catalyst supports.

Unit 3: Catalysis in Petroleum Industry (15 Lectures)

Synthesis gas and production of chemicals from it. Hydrodesulphurization process and catalysts involved. Lewis acid catalysts, hydrogenation catalysts and bi-functional catalysts. Selective oxidation of hydrocarbon compounds – production of various petrochemicals. Manufacture and transformation of hydrocarbons – hydrogenation and isomerisation. Catalytic deactivation and reactivation.

Unit 4: Heterogeneous Catalysts and Environment (10 Lectures)

Control of pollution from automobile exhaust, catalytic converters – use of non-selective oxidation. Abatement of nitrogen oxides and industrial odours, cleaning of industrial effluents.

Course Outcomes:

On completion of the course, the students will be able to:

1. Be aware of chemisorption action of heterogeneous catalysts and determination of their surface area, porosity etc., and identify potential good catalysts.
2. Understand the properties of zeolites and clays with applications in different industrial fields.
3. Appreciate the use of heterogeneous catalysts in petroleum industries.
4. Recognise the role of heterogeneous catalysts in cleaning automobile and industrial exhausts.

Cotton University: Department of Chemistry
NEP UG Syllabus: Core Courses

Semester VIII

Paper: Core 19 (Advanced Physical Chemistry) Credits: 4 + 0 + 0 = 4

Learning Objectives:

1. To understand the terms of macrostate, microstate, partition functions and the concept of distribution of gas molecules in various energy levels.
2. To comprehend about non-equilibrium thermodynamics and Onsager's reciprocal relations.
3. To learn the principles, instrumentation and applications of voltametric techniques - polarography, linear sweep and cyclic voltammetry.
4. To gain knowledge on electrified interfaces and electrode kinetics leading to the deduction of the Butler-Volmer equation.
5. To comprehend on theories of unimolecular reactions including RRK and RRKM

theories.

6. To learn the techniques to investigate fast reactions and heterogeneous catalysis.
7. To familiarize with the laws of photochemistry, photophysical kinetics and quenching phenomena.

Unit 1: Statistical and non-equilibrium thermodynamics **(18 lectures)**

Molecular energy levels and concept of distribution of gas molecules in energy levels. Concept of macrostate (thermodynamic state) and microstate (quantum mechanical state) for a gaseous system. Molecular significance of heat and work. The Boltzmann distribution in a gaseous system, the molecular partition function and its significance. Translational, electronic, rotational and vibrational partition functions of gas molecules. Statistical thermodynamics of monatomic and diatomic gases, Sackur-Tetrode equation. Applications of statistical mechanics for calculation of equilibrium constants of gaseous reactions.

Non-equilibrium thermodynamics, Concept of internal entropy production in irreversible processes. Generalized forces and flows, coupled forces and flows, phenomenological relations, statement of Onsager's reciprocal relation.

Unit 2: Advanced electrochemistry **(20 lectures)**

Dynamic electrochemistry, electrified interfaces, polarizable and non-polarizable interfaces, concentration polarization, concept of overvoltage. Voltammetry, polarography, linear sweep and cyclic voltammetry – principle, instrumentation and applications, formal and half-wave potential, mass transport by migration, convection and diffusion, reversible and irreversible processes, faradaic and non-faradaic processes.

Kinetics of electrode reactions, the Butler-Volmer equation and its field approximations, Tafel plots. Homogeneous and heterogeneous electrocatalysis, volcano relationship.

Unit 3: Molecular reaction dynamics **(14 lectures)**

Unimolecular reactions, drawbacks of Lindemann theory, Hinshelwood treatment, introduction to RRK theory and RRKM theory. Effect of solvent dielectric constant on reaction rates, Double-sphere model; electron transfer reactions in solution – the Marcus theory.

Fast reaction kinetics: Introduction to relaxation and flow methods, idea of relaxation kinetics and stopped flow technique. Kinetics of heterogeneous catalysis – Langmuir-Hinselwood and Eley-Rideal models.

Oscillating reactions: Belousov-Zhabotinski reaction, concept of chemical chaos.

Unit 4: Photochemistry (8 lectures)

Laws of photochemistry, quantum yield, actinometry, photophysical kinetics of fluorescence and phosphorescence, low and high quantum yield reactions, photostationary states, kinetics of H_2-Cl_2 reactions, photosensitized reactions, chemiluminescence, the mechanism and kinetics of fluorescence quenching – Stern-Volmer equation. Introduction to lasers and flash photolysis.

Course Outcomes:

On completion of the course, the students will be able to:

1. Understand the terms of macrostate, microstate, partition functions and the concept of distribution of gas molecules in various energy levels.
2. Comprehend about non-equilibrium thermodynamics and Onsager's reciprocal relations.
3. Attain knowledge on the principles, instrumentation and applications of voltametric techniques - polarography, linear sweep and cyclic voltammetry.
4. Gain knowledge on electrified interfaces and electrode kinetics including the deduction of the Butler-Volmer equation.
5. Comprehend on theories of unimolecular reactions including RRK and RRKM theories.
6. Learn the techniques to investigate fast reactions and heterogeneous catalysis.
7. Familiarize with the laws of photochemistry, photophysical kinetics and quenching phenomena.

Textbooks and References

1. Atkin's Physical Chemistry, 10th Ed., PW Atkins and J De Paula, Oxford University Press, 2014.
2. Physical Chemistry, 4th Ed., GW Castellan, Narosa, 2004.
3. Physical Chemistry, 3rd Edition, T. Engel and P. Reid, Prentice-Hall, 2012.
4. Physical Chemistry, DW Ball, Cengage India, 2012.
5. Physical Chemistry, 3rd Ed., RG Mortimer, Elsevier: Noida, 2009.
6. Physical Chemistry, 6th Ed., IN Levine, Tata McGraw-Hill, 2011.
7. Physical Chemistry, 2nd Ed., CR Metz, Tata McGraw-Hill, 2009.
8. Physical Chemistry by GW Castellan (Addison-Wesley).
9. Physical Chemistry, A Molecular approach, DA Mcquarrie and JD Simon, University Science Books, 1997.

10. A Textbook of Physical Chemistry (Volume 1, 2, 3, 4 & 5) by K.L. Kapoor (MacMillan)
11. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand, New Age International, 2014.
12. Principles of Physical Chemistry, by BR Puri, LR Sharma, and MS Pathania, Vishal Publishing Co, 2016.
13. Physical Chemistry, by PC Rakshit, Sarat Book Distributors, 2016.
14. Chemical Kinetics, by KJ Laidler, Pearson, 2013.
15. The Physical Chemist's Toolbox, by RM Metzger, Willey, 2012.
16. Fundamentals of Photochemistry, by KK Rohatgi-Mukherjee, New Age International.
17. The Modern Electrochemistry 1, Ionics, JO'M Bockris and AKN Reddy, Springer, 2012.
18. The Modern Electrochemistry 2A, Fundamental of Electrodics, JO'M Bockris, AKN Reddy and M. Gamboa-Aldeco, Kluwer Academic, 2012.
19. Electrochemistry, PH Rieger, Prentice-Hall International.
20. Electrochemical Methods, Fundamentals and applications, by AJ Bard and LR Faulkner, Wiley, 2006.
21. Statistical Thermodynamics, MC Gupta, New Age International 1995.

Paper: Core 20 (Analytical and Instrumental Method of Chemical Analysis)

Credits: 4 + 0 + 0 = 4

Learning Objectives:

1. To familiarize with various errors in measurements and analysis.
2. To comprehend the knowledge on various separation techniques such as chromatography and solvent extraction.
3. To have sound knowledge on spectroscopic techniques – UV-Vis, FT-IR and flame spectrophotometry.
4. To understand the principle and applications of voltametric techniques.

Unit 1 Errors and Statistical data treatment in Chemical analysis (8 Lectures)

Errors and deviations in measurements of physical quantities; accuracy and precision. Absolute, relative and mean errors. Relative and standard deviations. Significant figures in reporting measurements. Determinate and indeterminate errors, various types of determinate errors. Propagation of errors in calculations. Reliability of Results (Q Test), Confidence limit and interval.

Unit 2 Chromatography **(15 Lectures)**

Chromatography: General Principles, Classification of Chromatographic Techniques: adsorption, partition and ion exchange. Principles of Paper and Thin Layer Chromatography, Principles of Column Chromatography, the chromatograph (elution time and volume), capacity factor, column efficiency and resolution, sample preparation
Various Chromatographic Technique: Gas Chromatography (GC), Gas Chromatography-Mass Spectrometry (GCMS), Liquid Chromatography- Mass Spectrometry (LCMS), High Performance Liquid Chromatography (HPLC), Gel permeation chromatography (GPC): Techniques, Instrumentation and Applications.

Unit 3 Solvent Extraction **(7 Lectures)**
Distribution law, Determination of distribution ratio, Batch extraction, continuous extraction, discontinuous extraction, counter current extraction.

Unit 4 Spectroscopic methods

UV-Visible Spectrophotometry **(8 Lectures)**
Basic principles, Beer-Lambert law and instrumentation (light source, monochromator and detector) for single and double beam instrument. Estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

FT-Infrared Spectroscopy **(5 Lectures)**
Basic principles and instrumentation (choice of source, monochromator & detector); sampling techniques. Structural illustration through interpretation of data.

Flame Atomic Absorption and Emission Spectrometry **(7 Lectures)**
Origin of atomic spectra and instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs). Atomic fluorescence spectrometry. Techniques of atomization and sample introduction; Quantitative estimation of trace level of metal ions from water samples.

Unit 5 Thermal methods of analysis **(3 Lectures)**
Basic principles and instrumentation of thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC).

Unit 6 Electrochemical methods **(7 Lectures)**
Voltammetry: voltametric cells, formal and half-wave potential, reference electrodes, Potentiostat /Galvanostat, linear sweep and cyclic voltammetry and their applications; Controlled potential coulometry and its applications.

Course Outcomes:
On completion of the course, the students will be able to:
1. Familiarize with various errors in measurements and analysis.
2. Understand and use various separation techniques such as chromatography and

solvent extraction.
3. Employ various spectroscopic techniques – UV-Vis, FT-IR and flame spectroscopy – in their routine analysis.
4. Have sound knowledge on the principle and applications of voltametric techniques.

Books and references

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman.
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7 th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
7. Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
8. Ditts, R.V. Analytical Chemistry – Methods of separation.
9. Skoog, D.A., West, DA, Holler F.J. and Crouch, SR. Fundamentals of Analytical Chemistry, Eight Eds, Thomson, 2004.

Paper: Core 22* (Environmental and Green Chemistry)

Credits: 3 + 0 + 1= 4

Learning objectives:

1. To make the students aware of environmental pollution and understand the role of chemistry in mitigating it.
2. To understand the utilization of green chemistry from the industrial perspective.
3. To understand the impact of chemicals on society, economy and the environment.
4. To learn about the tools to measure sustainability.

Unit 1: Chemistry of air pollution (10 Lectures)

Parameters of air quality and their permissible limits. Contaminants and Pollutants. Primary air pollutants and formation of secondary air pollutants, smog formation. Automobile vehicles as a source of air pollution and its control using catalytic converters. Increasing level of CO_2 in the air and greenhouse effect, measures (such as shifting to greener energy sources, afforestation, preventing deforestation, etc.) to control CO_2 pollution. CFCs as pollutants, ozone layer depletion, and measures for its mitigation.

Unit 2: Chemistry of Soil and Water Pollution (10 Lectures)

Parameters of water and soil, and their permissible limits. Soil and water pollution due to anthropogenic sources: changes in pH in both cases, reclamation of problem soil, adverse effects of petroleum exploration and processing on soil and water, increase of BOD in water, decrease of dissolved oxygen in water, effect of industrial effluents and thermal pollution on aquatic life, pesticides in soil and water, its trophic level biomagnification. Groundwater pollution by pesticides and heavy metals. Fertilizers, detergents and sewage as water pollutants, eutrophication of water bodies.

Unit 3: Introduction to Green Chemistry (5 Lectures)

The essentials of green chemistry: definitions, adverse effects of chemicals on health and the environment, Accidents with Chemicals Wastes and Minimization, history of the development of Green Chemistry, sustainability as it relates to GC, and ethical awareness. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit 4: Designing a Chemical Synthesis Using Principles of Green Chemistry (10 lectures)

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

1. Designing a Green Synthesis using these principles; Prevention of Waste/ by-products; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
2. Prevention/ minimization of hazardous/ toxic products reducing toxicity
3. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, and solventless processes.
4. Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy. Photochemical synthesis.
5. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.
6. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, heterogeneous and homogeneous catalysis, biocatalysis.

Unit 5: Examples of Green Synthesis and some real-world cases (5 Lectures)

Green Synthesis of the following compounds: adipic acid, catechol, disodium Iminodiacetate, Ibuprofen.

New insecticides that are relatively non-toxic; (mode of action of traditional insecticides)
An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.
Healthier fats and oil by Green Chemistry: Enzymatic interesterification for production of no Trans-Fats and Oils

Unit 6: Chemical technologies using renewable feed stocks (5 Lectures)

Raw materials from nature: Introduction, basic "biorefinery" concepts, lignocellulose as potential raw materials, new chemistry required for using new feedstocks (contrast with oil/alkenes). Real-world examples of the use of renewable feedstocks.

Lab experiments for Environmental and Green Chemistry

1. Preparation of biodiesel from vegetable/ waste cooking oil.
2. Solventless formation of dibenzyl amines via reductive amination.
3. Reaction between furan and maleic acid in water and at room temperature rather than
   in benzene and reflux.
4. Photoreduction of benzophenone to benzo pinacol in the presence of sunlight
5. Bromination of acetanilide.

Course Outcomes:

On completion of the course,

1. Students will acquire adequate knowledge about the chemicals and chemical phenomena related to environmental pollution.
2. Students will understand and apply knowledge of the common metrics used in Green Chemistry applications
3. Students will understand and apply knowledge of introductory green chemical synthetic methods, choice of solvents, atom economy, and sustainable raw materials.
4. Students will understand and apply the concepts of biocatalysis.

Recommended Text Books / References:

1. S.E. Manahan, Fundamentals of Environmental Chemistry, Lewis Publishers
2. G. W. Vanloon, S. J. Duffy, Environmental Chemistry, 3rd Edison, Oxford University Press
3. Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice,* Oxford University Press (1998).
4. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition,

2010.
5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
6. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).

Paper: Core 23* (Natural Products and Medicinal Chemistry)

Credits: 4 + 0 + 0 = 4

Learning objectives:
1. To learn about different natural products.
2. To understand cell signaling molecules like hormones and neurotransmitters.
3. To know the process of drug design and development.
4. To be familiar with commonly used drugs of different pharmacological classes.

Unit 1: Alkaloids and Terpenoids (12 Lectures)
General idea, classification of natural products, primary and secondary metabolites

Occurrence, general structural features, isolation and biological functions of alkaloids
Hoffmann's exhaustive methylation, Emde's modification
Structure elucidation and synthesis of nicotine.
Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

Occurrence, classification, isoprene rule of terpenes, essential oils

Structure elucidation and synthesis of citral,

Unit 2: Hormones and Neurotransmitters (7 Lectures)

Endocrine glands in human, classification, structures, functions and therapeutic uses of hormones (emphasis on insulin, thyroid hormones, steroid hormones)

Classification, structures, functions, mechanism of action, therapeutic uses of neurotransmitters (emphasis on GABA, nitric oxide, dopamine, serotonin, histamine)

Unit 3: Drug discovery, design and development (18 Lectures)

Definition and classification of drugs, prodrugs,
History of drug development: Aspirin, paracetamol, sulpha drugs.
Phases in drug development
Receptors, drug-receptor interaction, agonist, antagonist
Chemotherapeutic index & therapeutic index, IC50, EC50, LD50 values
Clark's occupancy theory
Lead compound, structure activity relationship
Quantitative structure activity relationships (QSAR).
Pharmacokinetics and pharmacodynamics
Combinatorial library and molecular modeling in drug discovery,

Unit 4: Drugs of the different pharmacological classes (23 Lectures)

Structures, synthesis and mode of actions of following drugs
Antibiotics: Penicillins, macrolides (Azithromycin), fluoroquinolones (ciprofloxacin); oxazolidone (Linezolid). Bacterial resistance
Antifungal: Clotrimazole
Antiviral and anti HIV-AIDS: Acyclovir, Zidovudine
Antimalarials: Chloroquine, HCQ
Anthelmintic: Albendazole
Analgesics and antipyretics: Aspirin, paracetamol, lbuprofen
Anticancer: Fluorouracil, Vinblastine, Doxorubicin
Anxiolytic: Diazepam
Anti-diabetic: Metformin
Antihistamine and antacid: Ranitidine, Omeprazole
Antilaprosy: Dapsone

Course outcomes:

On completion of the course, the students will be able to:

1. Understand and classify natural products.
2. Drawstructures;know functions and importance of alkaloids, terpenes, hormones and neurotransmitters.
3. Realize and appreciate the process of drug discovery and development process and the connection of it with natural products.
4. Expand their knowledge about commonly used drugs in their life and drugs used in other lethal diseases.

Recommended Text Books / References:

- G. L. Patrick, *An introduction to medicinal chemistry*, Oxford university press, 1995

- G. Thomas, *Fundamentals of medicinal chemistry*, John Wiley and Sons, 2004
- J. M. Beale, Jr., J. H. Block, *Wilsomn and Gisvold's textbook of Organic medicinal and pharmaceutical chemistry*, Wolters Kluwer, 2011
- I. L. Finar, *Organic chemistry, volume 2*, PEARSON

Paper: Core 23** (Supramolecular Chemistry) Credits: 4 + 0 + 0 = 4

Learning Objectives:

1. To learn the basics and principles of supramolecular chemistry
2. To understand the importance and relevance of supramolecules and supramolecular chemistry in biological systems
3. To learn about the applications of supramolecules in medicines
4. To learn about the usage of computational approaches in supramolecular chemistry

Theory:

Unit 1: Introduction to Supramolecular chemistry (10 Lectures)

Basic concept and principles, History, Fundamental supramolecular interactions (H-bonding, π-π interactions, lone pair-π interactions, σ- and π hole interactions, dipole-dipole interactions etc), Supramolecular Host Guest: Definition, Synthesis and applications of molecular host, Supramolecular Synthons, Molecular recognition.

Unit 2: Supramolecular assembly of biomolecules (12 Lectures)

Biological supramolecular systems: Ionophores, cryptands, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA, rotaxanes and catenanes: as artificial molecular machine, and Biochemical Self-assembly.

Unit 3: Supramolecular catalysis and Enzyme mimics (12 Lectures)

Supramolecular interactions in enzyme catalysis: lock and key vs. induced fit models, Enzymes and their supramolecular models, Structural and functional models of hemoglobin, Esterase and its cyclodextrin-based mimics, ATPase and its corand-based ATPase mimics, Ion channel mimics.

Unit 4: Supramolecular Diagnostics and Therapeutics (12 Lectures)

Macrocyclic complexes for radiotherapy (DOTA, Texaphyrin), Photodynamic Therapy (PDT) agents, Cyclams in anti-HIV therapy, Supramolecular antibiotics.

Optical and fluorescent biosensors for metal detection, Supramolecular magnetic resonance imaging (MRI) contrast agents: Omiscan, Magnavist.

Unit 5: Computational Approaches in Supramolecular Chemistry (15 Lectures)

Concept of potential energy surface. Energy landscape of a molecule. Calculation of vertical and adiabatic ionization potential and electron affinity of a molecule. Computational tools such as quantum theory of atoms in molecules (QTAIM) and non-covalent interaction (NCI) index for characterizing non-covalent interaction. Concept of molecular electrostatic potential.

References:

1. Supramolecular Chemistry: Concepts and Perspectives by J-M. Lehn (Wiley-VCH Verlag GmbH; 1st edition, 6 June 1995)
2. Supramolecular Chemistry from Biological Inspiration to Biomedical Applications by Peter J. Cragg. (Spinger)

3. Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace. (John Wiley and Sons, Ltd)
4. Encyclopedia of Supramolecular Chemistry, vol 1 edited by J. L. Atwood, J. Steed. (Taylor & Francis).
5. Supramolecular Chemistry Second Edition by J. L. Atwood, J. Steed. (John Wiley and Sons, Ltd).
6. Supramolecular Chemistry– Fundamentals and Applications. Advanced Textbook by T. Kunitake, K Ariga, Berlin: Springer-Verlag Heidelberg, 2006. 208 p. ISBN 978-3- 540- 01298-6
7. Introduction to Supramolecular Chemistry by H. Dodziuk, Kluwer Academic Publishers, The Netherlands (2002).

Course Outcomes:

On completion of the course,

1. Students will be able to learn the basics and underlying principles involved in supramolecular chemistry
2. Students will be able to realize the importance and relevance of supramolecules and supramolecular chemistry in biological systems
3. Students will know about real life applications with examples from medicinal of supramolecules
4. Students will be familiar with the use of computational approaches in supramolecular chemistry

Chemistry Minor Courses

Semester I

Paper: Chemistry Minor – I **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. Familiarization with the various states of matter, and laws and concepts needed to describe the states.
2. Understanding kinetic theory model of gases, Maxwell distribution and collisions.
3. Learn the basic properties of organic molecules, and understand their structure and bonding.
4. To appreciate the electronic effects, acid-base properties and reaction intermediates in organic compounds.

5. To understand about evolution of atomic theory, the scientific theory of atoms and concept of wave function.
6. To know about the arrangement of elements in periodic table; physical and chemical characteristics of elements and their periodicity.

Unit 1: States of Matter (15 lectures)

Gases: Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor and its variation with pressure for different gases. Causes of deviation from ideal behaviour. The van der Waals equation of state, its application in explaining real gas behaviour. Boyle temperature. Critical state, critical constants and van der Waals constants, Andrews' isotherms of CO_2.

Kinetic molecular theory of a gas, its postulates, derivation of the kinetic gas equation. Maxwell speed distribution, its use in evaluating the mean molecular speeds (average, root mean square and most probable speeds) and average kinetic energy, law of equipartition of energy, degrees of freedom (with lack in expression of vibrational ones at room temperature), molecular basis of heat capacities. Collision cross section, collision frequency and mean free path of gases.

Liquids: Structure and physical properties of liquids; vapour pressure, surface tension, viscosity, their dependence on temperature and their determinations. Effect of addition of various solutes on surface tension, cleansing action of detergents. Elementary ideas of liquid crystals.

Solids: Forms of solids. Elementary ideas of symmetry, symmetry elements and symmetry operations, unit cells, crystal systems, Bravais lattices. Laws of Crystallography – Law of constancy of interfacial angles, Law of rational indices. Weiss and Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl. Defects in crystals.

Unit 2: Basics of Organic Chemistry (15 lectures)

(a) Hybridization, Shapes of molecules, Influence of hybridization on bond properties.
(b) Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications;
(c) Organic acids and bases; their relative strength.
(d) Homolytic and Heterolytic fission with suitable examples.
(e) Electrophiles and Nucleophiles; Nucleophlicity and basicity;
(f) Reaction intermediates: Types, shape and relative stabilities of Carbocations, Carbanions, Free radicals and Carbenes.
(g) Types of Organic reactions: Addition, Elimination and Substitution reactions.
(h) Aromaticity: Hückel's rule; aromatic, non-aromatic and anti-aromatic compounds.

Unit 3: Atomic Structure (9 **lectures**)

Concept of atom in ancient India, Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Time-independent Schrödinger's wave equation, significance of ψ and $|\psi|^2$. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals (Contour boundary and probability diagrams). Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau principle and its limitations.

Unit 4: Periodicity of Elements (6 lectures)

The s, p, d, f block elements, the long form of periodic table. Discussion of the following properties with reference to s and p-block elements:

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Concept of Atomic radii (van der Waals, covalent, ionic and metallic).

(c) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy.

(d) Electron gain enthalpy, trends of electron gain enthalpy.

(e) Electronegativity, Pauling, Mullikan, Allred Rachow scales, electronegativity and bond order, Partial charge.

Recommended Textbooks/ References:

1. P.W. Atkins and J. de Paula. Atkins' Physical Chemistry 8th Ed., Oxford University Press (2006)
2. D. W. Ball. Physical Chemistry Thomson Press, India (2007)
3. G. W. Castellan. Physical Chemistry 4th Ed. Narosa (2004)
4. R. G. Mortimer. Physical Chemistry 3rd Ed. Elsevier, Noida (UP). (2009).
5. I. N. Levine. Physical Chemistry 6th Ed., Tata McGraw-Hill, 2011.
6. Lee, J. D. Concise Inorganic Chemistry, Wiley, 5th Edition.
7. Douglas, B.E., McDaniel, D.H., Alexander J.J., Concepts & Models of Inorganic Chemistry, (Third Edition) John Wiley & Sons, 1999.
8. Atkins, P. W., Overton, T., Rourke, J., Weller, M., and Armstrong, F. Shriver. Atkins' Inorganic Chemistry, Fifth Edition, Oxford University Press, 2010.
9. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4th ed.
10. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
11. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.
12. Sarkar, R. P., General and Inorganic Chemistry (Part I and II), New Central Book Agency, 2012.
13. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt.

Ltd. (Pearson Education).
14. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
15. Clayden, J., Greeves N., Warren, S., Organic Chemistry, Oxford University Press 2nd Ed., 2012.
16. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
17. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
18. S. Sengupta, Organic Chemistry, Oxford University Press; First Edition, 2014.

Lab Experiments for Chemistry Minor – I:

Physical Chemistry Lab

1. Determination of surface tension for three aqueous solutions of ethanoic acid (with concentrations not beyond 25% w/w) by drop number method to judge its change with increasing concentration.
2. Determination of coefficient of viscosity of three aqueous solutions of ethanol (with concentrations not beyond 30% w/w) using Ostwald viscometer to judge its change with increasing concentration.

Organic Chemistry Lab

1. Purification of organic compounds by crystallization using the following solvents:
a. Water b. Alcohol c. Alcohol-Water
2. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds.
3. Chromatography: Separation of a mixture of organic compounds by thin layer chromatography (TLC).

Recommended Books/References:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand, New Delhi, 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, Eighth Edition, McGraw-Hill (2003).
3. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry, Third Edition, W, H. Freeman (2003).
4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
5. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Course Outcomes:

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

1. Know about kinetic molecular theory of gases, molecular collisions in gases, mean free path and their interrelations, and to perform numerical calculations on these topics. Also to recognise real gas behaviour as different from ideal gas behaviour.
2. Know about the structure and various physical properties of liquids, along with how the surface tension depends on solutes, and experimentally determine surface tension and coefficient of viscosity of liquids.
3. Understand the crystal structure and symmetry in crystalline solids and perform numerical calculations on these.
4. Understand the basic properties of organic molecules, and their structure and bonding.
5. Apply the knowledge of various electronic effects in determining reactivity organic compounds.
6. Know about structure of atom, classical and quantum mechanical models and theories of atomic structure, dual behavior of electrons and concept of atomic orbitals.
7. Understand about arrangement of elements in periodic table, periodic variation of element's properties.

Semester II

Paper: Chemistry Minor – II **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. Understanding the fundamentals of chemical kinetics: concepts of rate, differential and integrated rate equations, half-life, order and molecularity, temperature dependence of rate.
2. Determination of progress of reaction, rate, rate constant and order.
3. Understanding the fundamentals of catalysis – types of catalysis, cause of catalytic action, mechanism of heterogeneous catalysis, introduction to acid-base catalysis and enzyme catalysis.

4. Learn 3-D structure and concept of chirality in organic molecules.
5. Learn properties and reactions of saturated and unsaturated hydrocarbon
6. Understand the concept of ionic bonding, lattice energy using Born-Landé equation, Born Haber Cycle and Solvation Energy.
7. Learn about VSEPR theory, VBT and MOT (homo- & hetero- nuclear diatomic molecules).
8. Understand the theory and application of acid-base and redox chemistry.

Unit 1: Chemical Kinetics (10 Lectures)

The concept of reaction rates. Effect of concentration, temperature and catalyst on reaction rates. Differential rate equation and the order of a reaction. Methods of experimental determination of the progress of a reaction and of the rate constant. Concept of molecularity, comparison between order and molecularity. Derivation of integrated rate equations for zeroth, first and second order reactions. Half–life of a reaction and its dependence on initial concentration for different orders. Methods for determination of the order from the half-life for single-reactant systems. Temperature dependence of the reaction rate, Arrhenius equation. Concept of pre-exponential factor, activation energy and their calculation.

Qualitative ideas of the Collision theory and Activated Complex theory of bimolecular reactions.

Unit 2: Catalysis (5 lectures)

Types of catalysis – homogeneous and heterogeneous. Cause of catalytic effect on reaction rate. Introductory ideas of acid-base catalysis. Mechanism of catalysed reactions at solid surface, effect of particle size. Enzyme catalysis, its characteristics, Michaelis-Menten mechanism. Specificity and selectivity in enzyme catalysis.

Unit 3: Stereochemistry (7 Lectures)

(a) Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations.
(b) Conformations with respect to ethane, butane and cyclohexane.
(c) Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; *cis–trans* nomenclature; CIP Rules: R/ S and E / Z Nomenclature

Unit 4: Chemistry of Aliphatic Hydrocarbons (8 Lectures)

Alkanes:

(a) *Preparation:* Catalytic hydrogenation, Wurtz Reaction, Wurtz-Fittig Reaction, Kolbe reaction

(b) *Reactions*: Combustion reaction, Cracking, Free radical substitutions: Halogenation - relative reactivity and selectivity.

Alkenes:

(a) *Preparation*: Elimination reactions: Dehydration of alkenes anddehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction).
(b) *Reactions*: cis-addition (alk. $KMnO_4$)and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Unit 5: Chemical Bonding (10 lectures)

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Born-Landé equation with derivation. Madelung constant, Born-Haber cycle and its application, Solvation energy.

Covalent bond: Lewis structure, Valence Shell Electron Pair Repulsion Theory (VSEPR), Shapes of simple molecules and ions containing lone-and bond-pairs of electrons multiple bonding, sigma and pi-bond approach, Valence Bond theory (Heitler-London approach). Hybridization containing s, p and s, p, d atomic orbitals, shapes of hybrid orbitals, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of simple homonuclear and heteronuclear diatomic molecules, e.g., N_2, O_2, C_2, B_2, F_2, CO, NO (idea of s-p mixing and orbital interaction to be given).

Unit 6: Acid Base and Redox Chemistry (5 lectures)

Arrhenius, Brönsted and Lewis theories of acids and bases, Strength of Brönsted acids and bases in water, Strength of Lewis acids and bases. Hard and soft acid-base (HSAB) concept and its applications.

Redox equations, Standard electrode potential and its application to inorganic reactions.

Recommended Textbooks/ References:

1. P. W. Atkins and J. De Paula. Physical Chemistry (10th Ed.), Oxford University Press, 2014.
2. G.W. Castellan. Physical Chemistry, 4th Ed., Narosa, 2004.
3. T. Engel and P. Reid. P. Physical Chemistry, 3rd Edition, Prentice-Hall, 2012.
4. D.W. Ball. Physical Chemistry, Cengage India, 2012.
5. R. G. Mortimer. Physical Chemistry 3rd Ed., Elsevier: NOIDA (UP), 2009.
6. I. N. Levine. Physical Chemistry 6th Ed., Tata McGraw-Hill, 2011.
7. C. R. Metz. Physical Chemistry 2nd Ed., Tata McGraw-Hill, 2009.

8. E. L. Eliel & S. H. Wilen Stereochemistry of Organic Compounds, Wiley: London, 1994.
9. D. Nasipuri, Stereochemistry of Organic Compounds Principle of Application. New Age International Private Limited; 4th edition (2020).
10. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
11. S. Sengupta, Basic Stereochemistry of Organic Molecules, Oxford Univ. Press; 2nd Ed., 2018.
12. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007 John Wiley & Sons, Inc.
13. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
14. S. Sengupta, Organic Chemistry, Oxford University Press; First Edition, 2014.
15. J. D. Lee: A new Concise Inorganic Chemistry, E. L. B. S.
16. Huheey, J.E., Keiter, E. L., Keiter, R. L. and Medhi, O. K. Inorganic Chemistry: Principles of Strucutre and Reactivity, Prentice Hall, 4th ed.
17. Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd Ed., 2020.
18. Cotton, F. A., Wilkinson, G., Gaus, P. L. Basic Inorganic Chemistry, Wiley, 2021.
19. Sarkar, R. P. General and Inorganic Chemistry (Part I & II), New Central Book Agency, 2012.
20. Douglas, B.E., McDaniel, D.H., Alexander J.J., Concepts & Models of Inorganic Chemistry, (3rd Ed.) John Wiley & Sons, 1999.
21. Rodger, G. E. Inorganic and Solid-State Chemistry, Cengage Learning, 2002.

Lab Experiments for Chemistry Minor – II:

Physical Chemistry Lab

1. Study of the iodine clock reaction to judge the slowing down of the reaction rate with the passage of time.
2. To gauge the effect of added manganous ion catalyst to the initial rate of the titration process between oxalic acid solution versus permanganate ion in strong acidic medium done at room temperature.

Inorganic Chemistry Lab

1. Titrimetric Analysis
(i) Calibration and use of apparatus.
(ii) Preparation of solutions of different molarity/normality of titrants.
(iii) Use of primary and secondary standard solutions.

2. Acid-Base Titrations
(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.

3. Oxidation-Reduction Titrimetry

(i) Estimation of Fe(II) using standardized $KMnO_4$ solution involving oxalic acid solution.
(ii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine/ anthranilic acid) and external indicator.
(iii) Estimation of Fe(III) using standardized $KMnO_4$ solution.

Recommended Books/References:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand, New Delhi, 2011.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, Eighth Edition, McGraw-Hill (2003).
3. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry, Third Edition, W, H. Freeman(2003).
4. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis Sixth Edition, Pearson, 2009.
5. Svehla G. and Sivasankar I. B, Vogel's Qualitative Inorganic Analysis, Pearson, India, 2012.
6. Gulati, S., Sharma J. L. and Manocha, S. Practical Inorganic Chemistry, CBS publishers and Distributors Pvt. Ltd. India, 2017.
7. Barua, S., A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016
8. Mukherjee, G. N., Handbook of Inorganic Analysis, U. N. Dhur and Sons Pvt. Ltd., 1st ed., 2014.
9. Raj, G. Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd., 2013

Course Outcomes:

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

1. Know about and perform calculations on the rate laws for simple reactions of various orders and on temperature dependence of the reaction rate.
2. To learn about determination of the progress of a reaction and to experimentally perform such a determination.
3. To have an introductory understanding of the collision theory and the activated complex theory of chemical reactions.
4. Understand the types of catalysed reactions and the cause behind the catalytic effect, and the mechanisms of such reactions at solid surfaces, enzyme environments and acid-base mediums.
5. Understand the effect of spatial arrangements of atoms in organic molecules on their properties and reactivities.
6. Interpret reactions and properties of aliphatic hydrocarbons.
7. Have introductory idea about chemical bonding.
8. Calculate relevant bonding parameters, interpret trends, predict and draw molecular structures using various bonding theories.
9. Apply acid-base and redox concepts to inorganic compounds and reactions.
10. They will also have hands-on experience at learning titrimetric techniques.

Semester III

Paper: Chemistry Minor – III **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. To know about the s- and p- block elements, their physicochemical properties and their compounds.
2. To appreciate the reactivity of alkynes.
3. To understand reaction mechanism of reactions involving aromatic and aliphatic compounds.

4. Understanding different concepts involved in chemical thermodynamics and chemical equilibrium.
5. To obtain some hands-on experience on experimental thermochemistry.

Unit 1: The s- and p- Block Elements (15 Lectures)

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy. Allotropy in C, S, and P. Oxidation states with reference to elements in unusual and rare oxidation states like in carbides and nitrides, inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

Compounds of s- and p- Block Elements: Hydrides and their classification (ionic, covalent and interstitial), structure and properties with respect to stability of hydrides of p-block elements.

Unit 2: Alkynes (4 Lectures)

Reactions of alkynes:
(a) Addition reaction: Reduction, hydration, addition of hydrogen halide and halogen.
(b) Acidity of alkyns.
(c) Alkylation of terminal alkynes, introduction to multistep organic synthesis.

Unit 3: Aromatic Compounds (6 Lectures)

Electrophilic aromatic substitution reactions of benzene, substituted benzene:
(a) Mechanism of Nitration, Halogenation, Friedel-Crafts alkylation and acylation, sulphonation.
(b) Regioselectivity in electrophilic aromatic substitution reaction.
(c) Kolbe-Schmitt reaction, Reimer-Tiemann reaction, Gattermann reaction.

Nucleophilic aromatic substitution reactions of aryl halides:
(a) Nucleophilic aromatic substitution: S_NAr (addition-elimation mechanism), Influence of EWG, relative rates of different halides.
(b) Benzyne mechanism: Structure, stability and isolation of benzyne intermediate, regioselectivity.

Unit 4: Alkyl halides and alcohols – Nucleophilic substitution reactions (5 Lectures)

(a) Nucleophilic substitution reactions (S_N1, S_N2, S_Ni) of alkyl halides and alcohols.
(b) Effect of substrate, leaving group, nucleophile/base and solvent in substitution reactions.
(c) Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit 5: Chemical Thermodynamics (9 Lectures)

Important principles and definitions of thermodynamics and thermochemistry. Concepts of work (w), heat (q), internal energy (U), enthalpy (H) and heat capacities (C_p and C_v). Concept of standard state and standard enthalpies of formation, bond energy, bond dissociation energy and resonance energy. Kirchhoff's equation. The second law of thermodynamics and the concept of entropy and of spontaneity. Gibbs and Helmholtz energy functions and their use in discussing spontaneity of processes.

Unit 6: Chemical Equilibrium: (6 Lectures)

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. The concept of reaction quotient (Q). Distinction between ΔG and $\Delta G°$, Le Chatelier's principle. Relationships among K_p, and K_c for reactions involving ideal gases.

Lab Experiments for Chemistry Minor – III:

A. Organic Chemistry:

1. Tests for aliphatic and aromatic compounds
2. Test for saturation and unsaturation
3. Detection of extra elements (N, S, Cl, Br, I)
4. Functional group test for COOH, Phenolic OH, carbonyl group, amine, nitro, and amide groups.

B. Physical Chemistry:

1. Determination of heat capacity of a calorimeter by using hot and room-temperature water.
2. Determination of heat capacity of the calorimeter and enthalpy of neutralisation of a strong acid (HCl) with a strong base (NaOH).
3. Determination of heat capacity of the calorimeter and enthalpy of neutralisation of a weak acid (CH_3COOH) with a strong base (NaOH).

Recommended Text Books / References:

• J. D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
• F.A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
• D. F. Shriver and P. W. Atkins: Inorganic Chemistry, Oxford University Press.
• Puri, B. R., Sharma, L. R. and Kalia, K. C. Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
• Morrison, R. N. & Boyd, R. N. Organic Chemistry, 6th Edn., Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
• Pine, S. H. Organic Chemistry, Fifth Edition, McGraw Hill, (2007)
• Clayden J., N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., (2012), Oxford University Press.
• Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
• Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

• G. M. Barrow: Physical Chemistry, Tata McGraw Hill, 2007.
• G. W. Castellan: Physical Chemistry 4th Ed., Narosa Publishing House, 2004
• J. C. Kotz, P. M. Treichel, J. R. Townsend, General Chemistry, Cengage Learning India Pvt. Ltd., New Delhi, 2009.
• B. H. Mahan: University Chemistry, 3rd Ed., Narosa Publishing House, 1998.
• H. Petrucci, General Chemistry, 5th Ed., Macmillan Publishing Co., New York, 1985.
• B. D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.

Course Outcomes:

On completion of the course, the students will be able to:

1. Understand the trends in physico-chemical properties of s- and p- block elements.
2. Gain insight into the structure and properties of compounds formed by s- and p-block elements.
3. Describe general reactivity of alkynes.
4. Understand basic aspects of organic reaction mechanism and apply them in organic transformations.
5. The students will know fundamentals of physical chemistry viz., principles of thermodynamics, thermochemistry, and chemical equillibria.
6. They will also have an opportunity to verify some of these concepts hands-on in the laboratory.

Semester IV

Paper: Chemistry Minor – IV   Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To realise the structure, bonding, chemical properties and applications of some important compounds of p- block elements.
2. To know about the general principles of metallurgy.
3. To know about various elimination and substitution reactions of aliphatic compounds and organometallic reagent.
4. To follow various reactions involving preparation of ether, epoxides, their reactions, acidity of phenols, and oxidation of alcohols and glycols
5. To acquire skills about the conventional methods for the qualitative analysis of various organic compounds including detection of elements (N, S, Cl, Br, I).
6. To know thermodynamic properties and behaviour of solutions and immiscible/partially miscible liquid mixtures.
7. To visualise phase equilibrium in pure substances and binary mixtures, and about ionic equilibrium in aqueous solutions.
8. To learn about qualitative techniques for analyses of inorganic salt mixtures.

Unit 1: Chemistry of p-Block Elements (8 Lectures)

Concept of multicentre bonding (diborane).
Structure, bonding and important properties like oxidation/reduction and acidic/basic nature of the following compounds, and their applications in industrial, organic and environmental chemistry:
Hydrides of nitrogen (NH_3, N_2H_4, N_3H, NH_2OH); Oxoacids of P, S and Cl;
Halides and oxohalides: PCl_3, PCl_5, $SOCl_2$ and SO_2Cl_2

Unit 2: General Principles of Metallurgy (7 Lectures)

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent.
Hydrometallurgy, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond's process.

Unit 3: Alkyl halides and alcohols: Elimination reactions (7 Lectures)

(a) Elimination reactions (E1, E2, E1cB) of alkyl halides and alcohols.

(b) Elimination vs substitution.
(c) Organometallic compounds: Grignard's reagent, Gilman's reagent and organo Li reagents and their synthetic utility.

Unit 4: Alcohols, Phenols, Ethers and Epoxides (8 Lectures)

(a) Oxidation reactions of alcohols: Oxidation by PCC, PDC, $KMnO_4$, CrO_3, Jone's reagent, Swern oxidation.
(b) Preparation, properties and reactions of glycols: Oxidation by periodic acid and lead tetraacetate.
(c) Acidity of phenol and factors affecting it.
(d) Williamson ether synthesis, reaction of ethers with acids.
(e) Preparation of epoxides, ring opening reactions (nucleophilic and acid catalyzed) of epoxides.

Unit 5: Solutions (6 Lectures)

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, non-ideal solutions and their deviations from Raoult's law. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes.
Partial miscibility of liquids: Critical solution temperature, effect of impurity on partial miscibility of liquids. Immiscibility of liquids and the principle of steam distillation.

Unit 6: Phase Equilibrium (4 Lectures)

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs phase rule and its thermodynamic derivation. Clausius–Clapeyron equation and its importance. Phase diagrams of one-component and two component systems.

Unit 7: Ionic Equilibrium (5 Lectures)

Strong and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis - hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Lab Experiments for Minor Chemistry – II:

A. Inorganic Chemistry:

Semi-micro qualitative analysis of inorganic salt mixtures containing not more than four ionic species (two anions and two cations, and excluding insoluble salts) out of the following:

Cations: NH_4^+, K^+, Pb^{2+}, Ag^+, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Anions: CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}
(Spot tests should be carried out wherever feasible.)

B. Physical Chemistry:

1. To determine the solubility of a salt in water at room temperature and hence its solubility product.
2. To find the degree of ionization and ionization constant of acetic acid (a weak acid) by conductivity measurements.

Recommended Text Books / References:

• J. D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
• F. A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
• B. R. Puri, L. R. Sharma, and K. C. Kalia: Principles of Inorganic Chemistry, Vishal Publishing Co., India, 33rd ed., 2020.
• D. F. Shriver and P. W. Atkins: Inorganic Chemistry, Oxford University Press.
• R. P. Sarkar: General and Inorganic Chemistry (Parts I & II), New Central Book Agency, 2012.
• Morrison, R. N. & Boyd, R. N. Organic Chemistry, 6th Edn., Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
• Pine S. H. Organic Chemistry, Fifth Edition, McGraw Hill, (2007)
• Clayden J., N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., (2012), Oxford University Press.
• G. M. Barrow: Physical Chemistry, Tata McGraw Hill, 2007.
• G. W. Castellan: Physical Chemistry 4th Ed., Narosa Publishing House, 2004
• J. C. Kotz, P. M. Treichel, J. R. Townsend, General Chemistry, Cengage Learning India Pvt. Ltd., New Delhi, 2009.
• B. H. Mahan: University Chemistry, 3rd Ed., Narosa Publishing House, 1998.
• H. Petrucci, General Chemistry, 5th Ed., Macmillan Publishing Co.: New York, 1985.
• B. D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
• S. Barua: A Textbook of Practical Chemistry, Kalyani Publishers, 2nd ed., 2016.

Course Outcomes:

On completion of the course, the students will:

1. Understand the structure and bonding aspects of certain important compounds formed by p-block elements, and follow the correlation between their bonding aspects, chemical properties and applications.
2. Appreciate the basic chemistry underlying metallurgical processes.
3. Understand basic aspects of elimination and substitution reactions.
4. Interpret oxidation reactions involving different reagents for alcohols, glycols and epoxidation.
5. Recognise various reactions involved in qualitative analysis of organic compounds.

6. Appreciate the various important aspects of physical chemistry, such as ideal and non-ideal solutions and their thermodynamics properties, and the thermodynamics of phase equilibrium and the fundamental concepts of ionic equilibrium.
7. Explore some of these concepts, such as ionic equilibrium and solubility etc., on a hands-on basis in the laboratory.

Semester V

Paper: Chemistry Minor – V Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To understand the different aspects of chemical bonding and intermolecular forces and to know their importance in physical and chemical properties.
2. To know the preparation, properties, and reactions of functional groups like carbonyl compounds, carboxylic acids, and their derivatives.
3. To have introductory knowledge about electrochemical conduction,
4. To get introduced to colloids and micelles.

Unit 1: Chemical Bonding – II (15 lectures)

Ionic Bonding: Polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.
Metallic Bond: Qualitative idea of free electron model, Band Theory, Conductors, Semiconductors, Insulators.
Weak Chemical Forces: van der Waals, ion-dipole, dipole-dipole, induced dipole dipole-induced
dipole interactions, hydrogen bond, effects of hydrogen bonding on melting points, boiling points and solubility.

Unit 2: Carbonyl Compounds (8 Lectures)

Preparation: from acid chlorides and from nitriles.
Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_3 and its derivatives.
Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation.
Reduction reactions: Clemmensen reduction and Wolff Kishner reduction, Meerwein-Ponndorf-Verley reduction, reduction using hydride transfer reactions: $LiAlH_4$, $NaBH_4$, DIBAL.

Unit 3: Carboxylic Acids and their Derivatives (7 Lectures)

Carboxylic acids (aliphatic and aromatic): Preparation: Acidic and Alkaline hydrolysis of esters, reaction of Grignard reagent with solid CO_2
Acidity of carboxylic acids.
Preparation of Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion.
Nucleophilic substitution reactions at acyl group, Reformatsky Reaction, Perkin condensation, Hell-Vohlard-Zelinsky Reaction.

Unit 4: Electrochemical Conduction **(8 Lectures)**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Determination of solubility and solubility products of sparingly soluble salts by conductance measurements. Kohlrausch law of independent migration of ions. Concept of drift velocity, ionic mobility and transference number. Conductometric titrations (only acid-base).

Unit 5: Colloids **(7 Lectures)**

Definition of colloids, sols and lyophilic colloids; structure and stability of colloids. Electrical double layer and electrokinetic phenomena – electrophoresis and electro-osmosis.

Surface-active agents (surfactants) and their cleansing action, micelle formation, critical micelle concentration (CMC).

Lab Experiments (Physical Chemistry):

At least four of the following experiments:

1. Conductometric determination of solubility of a sparingly soluble salt such as $CaSO_4$

2. Conductometric titration of an oxalic acid solution with NaOH solution to find the alkali strength

3. Potentiometric titration of an oxalic acid solution with NaOH solution using cell EMF measurements (employing mV function of pH meter).

4. Construction of a salt bridge and its use in Daniel cell.

5. Preparation of a lyophilic sol (starch or gum)

6. Preparation of a lyophobic sol (ferric hydroxide/ aluminium hydroxide).

7. Determination of coefficient of viscosity of starch sol in varying dilutions using Ostwald viscometer to judge its change with dilution.

Recommended Books:

1. Atkins P. W. and De Paula J., Physical Chemistry, (10th Ed.) Oxford University Press, 2014.
2. J. C. Kotz, P. M. Treichel, J. R. Townsend, General Chemistry, Cengage Learning India, New Delhi, 2009
3. Castellan, G. W. Physical Chemistry, 4th Ed., Narosa, 2004.

4. B. H. Mahan: University Chemistry, 3rd Ed., Narosa Publishing House, 1998.
5. Morrison, R. N. and Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. McMurry, J. E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
7. Clayden, J., Greeves, N. and Warren, S. Organic Chemistry, 2nd Ed. (2012), Oxford University Press.
8. S. Sengupta. Organic Chemistry, Oxford University Press; First Edition, 2014.
9. D. R. Klein. Organic Chemistry, John Wiley & Sons Inc; 4th edition (Dec. 2020).
10. P. S. Kalsi. Organic Reactions and Their Mechanisms, New Age International Pvt. Ltd. Fifth Edition.
11. B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.
12. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra, New Central Book Agency
13. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry, 8th Ed.; McGraw-Hill: New York (2003).
14. B.R. Puri, L.R. Sharma & K.C. Kalia Principles of Inorganic Chemistry.
15. R.P. Sarkar, General and Inorganic Chemistry.
16. J.D. Lee Concise Inorganic Chemistry, ELBS, 1991.
17. B.E. Douglas, D.H. Mc Daniel & J.J. Alexander Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
18. P.W. Atkins & D.N. Shriver Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
19. J.E. Huheey Inorganic Chemistry, Prentice Hall, 1993.

Course Outcomes:

On completion of the course, the students will be able to:

1. Relate the chemical and physical properties of substances to chemical bonding present.
2. Describe the preparation and various reactions of aldehydes, ketones and carboxylic acid derivatives.
3. Apply the knowledge of various organic reactions in the preparation of organic compounds in the laboratory, thus helping in developing laboratory skills.
4. Formulate organic preparations involving simple organic transformations.
5. Appreciate the phenomenon of electrochemical conduction and the class of substances called colloids, including micelles.

Semester VI

Paper: Chemistry Minor – VI Credits: 3 + 0 + 1 = 4

Learning Objectives:

1. To recognise different aspects of coordination chemistry.
2. To appreciate the preparation, properties and reactions of amines and diazonium salts.
3. To know about the chemistry of sulphur-containing compounds.
4. To understand and know about Galvanic cells and adsorption phenomena.

Unit 1: Coordination Chemistry: (15 lectures)

Werner's theory, valence bond theory (inner and outer orbital complexes), Electroneutrality principle. IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with the coordination number 4 and 6. Chelate effect.

Crystal field theory, measurement of 10 Dq (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δ_o, Δ_t). Octahedral vs. tetrahedral coordination, Qualitative aspects of Ligand Field and MO Theory.

Unit 2: Amines and Diazonium Salts (8 Lectures)

***Amines (Aliphatic and Aromatic)*:**
Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hoffmann Bromamide reaction.
Reactions: Hoffmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2, Schotten – Baumann Reaction. Electrophilic substitution of aromatic amine: nitration, bromination, sulphonation.

Diazonium salts:
Preparation: from aromatic amines.
Reactions: conversion to benzene, phenol, dyes.

Unit 3: Sulphur Containing Compounds (7 Lectures)
Preparation and reactions of thiols.
Acidity and nucleophilicity of thiols.
Disulfide formation and biological relevance of it.
Umpolung of carbonyl compounds using dithiane and synthetic utility
Desulfurization reaction

Unit 4: Galvanic Cells **(10 Lectures)**

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data. Calculation of equilibrium constant from EMF data. Concept of concentration cells, liquid junction potential and salt bridge. Determination of pH using glass electrode – working principle of common pH meters. Potentiometric titrations – qualitative treatment (acid-base and oxidation-reduction only).

Unit 5: Surface Chemistry **(5 Lectures)**

Physical adsorption and chemisorption; Concept of monolayer and multilayer adsorption; Adsorption isotherms – Freundlich and Langmuir; Adsorption in solution.

Lab Experiments (Inorganic Chemistry):

Inorganic Preparations (at least two)**:**

(i) Tetraamminecopper(II)sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

(ii) Tetraamminecarbonatocobalt(III) ion

(iii) Potassium tris(oxalato)ferrate(III)

Chromatography of metal ions:

Principles involved in chromatographic separations.

Paper chromatographic separation of the following metal ions (at least one pair):

i. Ni(II) and Co(II)

ii. Fe(III) and Al(III)

Inorganic Quantitative Analyses (at least two):

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).

ii. Estimation of water of crystallization in Mohr's salt by titrating with $KMnO_4$.

iii. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.

Recommended Textbooks/References:

1. Atkins P. W. and De Paula J., Physical Chemistry, (10th Ed.) Oxford University Press, 2014.
2. J. C. Kotz, P. M. Treichel, J. R. Townsend, General Chemistry, Cengage Learning India, New Delhi, 2009

3. Castellan, G. W. Physical Chemistry, 4th Ed., Narosa, 2004.
4. B. H. Mahan: University Chemistry, 3rd Ed., Narosa Publishing House, 1998.
5. Morrison, R. N. and Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. McMurry, J. E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
7. Clayden, J., Greeves, N. and Warren, S. Organic Chemistry, 2nd Ed. (2012), Oxford University Press.
8. S. Sengupta. Organic Chemistry, Oxford University Press; First Edition, 2014.
9. D. R. Klein. Organic Chemistry, John Wiley & Sons Inc; 4th edition (Dec. 2020).
10. P. S. Kalsi. Organic Reactions and Their Mechanisms, New Age International Pvt. Ltd. Fifth Edition.
11. Inorganic Chemistry by Meisler and Tarr, Pearson Education.
12. B.R. Puri, L.R. Sharma & K.C. Kalia Principles of Inorganic Chemistry.
13. R.P. Sarkar, General and Inorganic Chemistry.
14. J.D. Lee Concise Inorganic Chemistry, ELBS, 1991.
15. B.E. Douglas, D.H. Mc Daniel & J.J. Alexander Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
16. P.W. Atkins & D.N. Shriver Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
17. J.E. Huheey Inorganic Chemistry, Prentice Hall, 1993.
18. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
19. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
20. Vogel, A.I. A textbook of Quantitative Analysis, ELBS 1986.
21. Advanced Practical Inorganic Chemistry by Gurdeep Raj.
22. Barua, S. A Text Book of Practical Chemistry, 2nd Ed, Kalyani Publishers, 2016.

Course Outcomes:

On completion of the course, the students will be able to:

1. Interpret the structural aspects of coordination complexes and their stability.
2. Describe the methods of preparation of amines and their derivatives and discuss the synthetic utilities of such compounds in day-to-day life.
3. Outline the preparation and reactions of thiols and related sulphur compounds and relate their applications in biology and organic synthesis.
4. Appreciate the working of Galvanic cells and predict their EMV and thermodynamic properties.
5. Analyse the phenomenon of adsorption and quantify it in terms of isotherms.

Semester VII

Paper: Chemistry Minor – VII **Credits: 3 + 0 + 1 = 4**

Learning Objectives:

1. To appreciate how complex chemical reactions and chain reactions take place.
2. To be knowledgeable about the basics of polymer science, and about the various kinds of inorganic polymers.
3. To be aware of the different aspects of noble gases and their compounds.
4. To know the various structural forms of carbohydrates and reactions of carbohydrates
5. To recognise the different types of nucleic acids and their functions, components of nucleic acids such as the nucleobases, DNA replication and biosynthesis of proteins.
6. To learn techniques of separation and isolation of biomolecules and analyses of oils and fats.

Unit 1: Reaction Dynamics **(5 Lectures)**

Consecutive, concurrent and opposing reactions. Steady state treatment – kinetics of decomposition of N_2O_5. Kinetics of chain reactions – H_2+Br_2 reaction, branching and non-branching chain reaction, concept of explosion limits.

Unit 2: Introduction to Polymers **(10 Lectures)**

Monomers, repeat units, degree of polymerization, concepts of linear, branched and network polymers with examples. Classifications of polymers as fibres, elastomers and plastics. Introductory concepts of free-radical and coordination chain polymerisations. Dispersity and average molecular weight concept. Number, weight and viscosity average molecular weights – numerical calculations, dispersity index. Determination of viscosity average molecular weight by using Ostwald viscometer.

Unit 3: Inorganic Polymers **(8 lectures)**

Types of inorganic polymers, comparison with organic polymers, silicates, zeolites, silicones and siloxanes. Borazines, and phosphazenes.

Unit 4: Noble Gases **(7 lectures)**

Occurrence and uses, Inertness of noble gases, preparation and properties of XeF_2, XeF_4 and XeF_6. Structure and bonding in noble gas compounds (VBT, VSEPR theory).

Unit 5: Carbohydrates: **(6 Lectures)**

Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), D,L and R,S configuration of Glucose and Fructose, Mutarotation, oxidation with Br_2 water and concentrated HNO_3 and stereochemical outcome of the oxidation reactions, Structure of disacharrides (sucrose and lactose) and polysacharrides (starch and cellulose).

Unit 6: Lipids **(4 Lectures)**

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

Unit 7: Nucleic Acids **(5 Lectures)**

Components of nucleic acids, Nucleosides and nucleotides.
Structure of polynucleotides, complimentary base, genetic codes and degeneracy of genetic codes. RNA and protein biosynthesis: transcription and translation

Lab Experiments (Organic Chemistry):
A. Preparations (mechanism of reactions involved to be discussed) of the following (any two):
(a) Oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone
(b) Bromination of Phenol/Aniline/Acetanilide
(c) Benzoylation of amines/phenols
Recrystallisation, determination of melting point and calculation of quantitative yields be done.

B. Other Organic Chemistry Experiments (any three of the following):
1. Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
2. Identify and separate the sugars present in the given mixture by paper chromatography.
3. Determination of saponification value of an oil/fat.
4. Determination of iodine value of an oil/fat.
5. Determination of concentration of Glycine solution by formylation method.
6. Extraction of DNA from onion/cauliflower.

Recommended Books:

1. Atkins P. W. and De Paula J., Physical Chemistry, (10th Ed.) Oxford University Press, 2014.
2. Castellan, G. W. Physical Chemistry, 4th Ed., Narosa, 2004.
3. B. H. Mahan: University Chemistry, 3rd Ed., Narosa Publishing House, 1998.
4. Engel, T. & Reid, P. Physical Chemistry Third Edition, Prentice-Hall, 2012.

5. V.R. Gowariker, N.V. Viswanathan and J. Sreedhar. Polymer Science. (New Age International), New Delhi
6. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. 4th Edition. W.H. Freeman and Co.
7. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. 28th Edition. Lange Medical Books/ McGraw-Hill.
8. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. 6th Edition. W.H. Freeman and Co.
9. Voet, D., Pratt, C. W. and Voet, J. G. (2012) Principles of Biochemistry. 4th Edition. Wiley.
10. A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
11. F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
12. B.R. Puri, L.R. Sharma & K.C. Kalia Principles of Inorganic Chemistry.
13. R.P. Sarkar, General and Inorganic Chemistry.
14. J.D. Lee Concise Inorganic Chemistry, ELBS, 1991.
15. B.E. Douglas, D.H. Mc Daniel & J.J. Alexander Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
16. P.W. Atkins & D.N. Shriver Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
17. J.E. Huheey Inorganic Chemistry, Prentice Hall, 1993.
18. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
19. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.

Course Outcomes:

On completion of the course, the students will be able to:

1. Recognise how complex chemical reactions and chain reactions take place.
2. Appreciate the basics of polymer science, and outline various kinds of inorganic polymers.
3. Recognise the different aspects of noble gases and their compounds.
4. Delineate the various structural forms of carbohydrates and reactions of carbohydrates.
5. Appreciate the chemistry and biochemistry of lipids and nucleic acids.

Semester VIII

Paper: Chemistry Minor – VIII   Credits: 4 + 0 + 0 = 4

Learning Objectives:

1. To appreciate the role of metal ions and metal-containing complexes in biological systems.
2. To know about the structural properties of amino acids and proteins, synthesis of amino acids and peptides.
3. To perceive the mechanism of enzyme action, factors that affect enzyme activity and enzyme inhibition.
4. To know about the structure identification and determination techniques through molecular spectroscopy.

Unit 1: Bioinorganic Chemistry **(20 lectures)**

Metal ions present in biological systems. Classification of elements according to their biological activity. Sodium/Potassium pump. Myoglobin and Haemoglobin – Structure, Functions, Oxygen binding, Cooperativity, Bohr effect.

Diseases caused by excess and deficiency of Cu/Fe. Toxicity of metal ions (Hg, Pb, Cd and As), chelating agents in medicine.

Unit 2: Amino Acids, Peptides and Proteins: **(12 Lectures)**

Preparation of Amino Acids: Strecker synthesis and Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: ester of –COOH group, acetylation of $–NH_2$ group, complexation with Cu^{2+} ions, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C–terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) and C-activating groups and Merrifield solid-phase synthesis.

Unit 3: Enzymes **(10 Lectures)**

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action, factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition).

Unit 4: Introduction to Molecular Spectroscopy (18 Lectures)

Basic Ideas: Concept of electromagnetic radiation and its absorption and emission by matter. Regions of electromagnetic radiation for specific transitions. Concept of selection rules, width and intensity of spectral lines.

Infrared Spectroscopy**:** Selection rules; Stretching and bending vibrations; Modes of vibration and degrees of freedom in linear and nonlinear molecules (CO_2 and H_2O); Characteristic group vibration and fingerprint region.

Electronic Spectroscopy: Beer-Lambert law and colourimetric estimation of concentration. Singlet and triplet states, Jablonski diagram and concept of fluorescence and phosphorescence.

Recommended Books

1. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. 4th Edition. W.H. Freeman and Co.
2. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. 28th Edition. Lange Medical Books/ McGraw-Hill.
3. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. 6th Edition. W.H. Freeman and Co.
4. Voet, D., Pratt, C. W. and Voet, J. G. (2012) Principles of Biochemistry. 4th Edition. Wiley.
5. Introduction to Spectroscopy by Pavia, Cengage India Private Limited; 5th edition.
6. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
7. B.R. Puri, L.R. Sharma & K.C. Kalia Principles of Inorganic Chemistry.
8. R.P. Sarkar, General and Inorganic Chemistry.
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10. P.W. Atkins & D.N. Shriver Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
11. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry. Panima Publishing Company 1994.
12. Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.

Course Outcomes:

On completion of the course, the students will be able to:

Appreciate the role of metal ions and metal-containing complexes in biological systems.

1. Describe the proteins, their composition, synthesis and structural aspects.
2. Summarise the mechanism of enzyme action, factors affecting enzyme activity and enzyme inhibition.
3. Perceive the basic concepts of molecular spectroscopy in general and vibrational and molecular spectroscopy in particular.
4. Interpret the role of spectroscopy in molecular structure identification.

Cotton University: Department of Chemistry

NEP UG Syllabus: MDE (Multi-Disciplinary Elective) Courses

Semester – I

MDE (Multi-Disciplinary Elective) Chemistry – 1 **Credits: 3 + 0 + 0 = 3**

Paper Title: **Molecular Basis of Matter**

Learning Objectives:

1. To illustrate the meaning and significance of chemistry.
2. To explain the classification of matter and its atomic and molecular constitution, along with quantitative aspects of their masses and numbers.
3. To interpret the structure of atoms and molecules.
4. To describe the polymer structure and classification, with examples about common polymers.

Unit 1: Fundamentals of Chemistry **(15 Lectures)**

Definition and importance of chemistry. Definition and classification of matter (pure substances and mixtures, homogeneous mixtures and heterogeneous mixtures). Definition of atoms and molecules, Atomic structure, Simple electronic configuration of elements (without quantum number specification). Structure of atoms (electrons, protons and neutrons) – example of H, C, N and O atom. Atomic and molecular masses, actual masses of atoms and molecules, Mole concept, calculation of amount (number of moles) and number of atoms and molecules in a sample.

Unit 2: Chemicals and Chemical Structures **(18 Lectures)**

Elements and compounds, symbols and molecular formula. Covalent bonds between atoms in a molecule – examples of H_2, CO_2, H_2O, HCl. Ionic bond in ionic compounds such as the salts – continuity of ionic bonds in crystalline salts such as NaCl (each Na^+ bound to six Cl^-, every Cl^- bound to six Na^+). Types of intermolecular forces among molecules (dispersion or

London force, dipole-dipole force, hydrogen bonding). Octet rule, Lewis dot structures of simple molecules – H_2O and CH_4.

Meanings of a chemical equation. Combustion reactions of H_2, CO and CH_4. Names and structure of organic molecules – C-1 to C-4 alkanes, ethylene and acetylene. Structures of some selected compounds (ethanol, acetic acid, benzene and phenol).

Unit 3: Macromolecules and Polymers (12 Lectures)

Definition and classification of polymers (fibres, elastomers and plastics), structures and application of polymers – polyethene, polyethylene terephthalate (PET), polyvinyl chloride, polystyrene (polystyrene foam), teflon, linear polypeptide proteins, natural rubber, introduction to biodegradable polymers: examples.

Course Outcomes:

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

1. Summarize the significance of chemistry, classification of matter and its atomic and molecular organization, and will be able to calculate the masses and numbers of atoms/molecules.
2. Interpret the structure of atoms and molecules (especially organic molecules)
3. Explain polymer structure and know their classification along with examples of several common polymers.

Semester - II

MDE (Multi-Disciplinary Elective) Chemistry – 2 **Credits: 3 + 0 + 0 = 3**

Paper Title: **Fuels and Pollutants**

Learning Objectives:

1. To categorize the types of hydrocarbons in petroleum fuels, about the issue of petrol quality, and about chemical processes for obtaining good quality petroleum fuels.
2. To articulate about chemical aspects of the varieties of coal and coal products and their uses.
3. To illustrate various issues of environmental pollution along with the efforts for mitigation, from sources such as fossil fuel combustion, industrial emission of heavy metals, use of fertilizers and pesticides, use of chlorofluorocarbons in air conditioning, etc.
4. To describe the concept of green energy and its various sources.

Unit 1: Chemistry of Fossil Fuels **(15 Lectures)**

Definition of hydrocarbons, simple molecular structure of hydrocarbons, classification of hydrocarbons in petroleum – paraffins, naphthenes and aromatics. Chemical compositions of natural gas, LPG, petrol and diesel. Quality of petrol: definition of flash point, knocking and octane number. Catalytic cracking and reforming processes. Elementary idea about power alcohol. Coal – chemical constitution of coal, various common types of coal. Elementary idea about production and use of coal gas, synthesis gas (water gas) and coke.

Unit 2: Chemistry of Environmental Pollution **(18 Lectures)**

Idea of environmental pollution, Production of pollutant gases in combustion and their chemical composition, harmful effects of such pollutant gases: exhaust hydrocarbons, CO, NO_x and SO_x. Control of pollution from automobile exhaust gases – role of catalytic converters. Toxic effects of some heavy metals and their sources – Pb, Hg and Cd. Effects of chemical fertilizers, detergents and pesticides on the environment. Greenhouse gases: effects of CO_2 and CH_4 in atmosphere, efforts for their mitigation. Chlorofluorocarbons and ozone layer depletion, efforts and recent success in preventing ozone layer depletion.

Unit 3: Chemistry of Clean Energy **(12 Lectures)**

Basic idea of hydrogen fuel, hydrogen gas production from natural gas, elementary idea of fuel cell and secondary cell with examples, concept of compressed natural gas (CNG), its composition and application.

Course Outcomes:

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

1. Correlate the type and quality of hydrocarbons in petroleum fuel with their utility.
2. Correlate the types of coal and coal products from chemical viewpoint, along with their uses.
3. Summarize various issues for mitigation of environmental pollution from fossil fuel combustion, industrial emission of heavy metals, use of fertilizers and pesticides, use of chlorofluorocarbons, etc.
4. Recognise various types of green energy sources and their utilisation.

Semester - III

MDE (Multi-Disciplinary Elective) Chemistry – 3 **Credits: 3 + 0 + 0 = 3**

Paper Title: Chemistry in Daily Life

Learning Objectives:

1. To explain general ideas about the various classes of medicines with examples.
2. To understand the importance of the nutrient of our food from a chemical viewpoint for human health.
3. To define common chemicals used in life and also realise the concept of catalysis.

Unit 1: Elementary Medicinal Chemistry **(15 Lectures)**

Definition of drugs and medicines. Idea of classes of drugs: analgesics, antacids, antiparasitics, antibiotics, antiseptics and disinfectants. Examples of each of these classes (chemical structures of the examples not required). Concept of brand name and chemical name. Generic drugs. Concept of expiry date.

Unit 2: Human Nutrition **(15 Lectures)**

Elementary idea of carbohydrate, protein, fat, fibre, essential fatty acids and their types (omega-3 and omega-6) with examples (linoleic acid, DHA, alpha-linolenic acid, etc.), the vitamins and the essential minerals necessary for human nutrition and health, concept of hydrogenation and trans-fat problem, food nutritional values of food classes – fruits, vegetables, cereals, legumes, dairy, meat/fish/egg etc., concept of balanced diet including calorie, protein, various minerals, various vitamin etc.

Unit 3: Common Chemicals Around Us **(15 Lectures)**

Acids and bases in daily life, Cleansing action of surfactants, Use of ion-exchange resin, Cosmetic chemistry- Sunscreen and moisturizer, Importance of nanochemistry in daily life, Brief idea about water purification process- RO, SDS, TDS, UV-protection etc. Elementary idea of catalysis, enzyme-catalysed reactions (production of ethanol from molasses)

Course Outcomes:

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

1. Categorise various classes of medicines with examples.
2. Relate about the nutrients of food necessary for human health.

3. Have knowledge about various chemicals used in day-to-day life.
4. Describe basic ideas about catalysis, especially enzyme catalysis with examples.

Cotton University: Department of Chemistry
NEP UG Syllabus: SECs (Skill Enhancement Courses)

Semester – I

SEC - 1 (Chemical Analysis for Everyday Life) Credits: 2+0+1 = 3

Learning Objectives

1. To learn about the ideas of qualitative and quantitative chemical analysis, and to correct various possible errors in such analysis.

2. To know about the nutritional components of food and also the preservatives, colouring matters and adulterants that get added to it; and to be able to identify via chemical analysis such components and additives.

3. To know about the characteristic constitution of potable water and agriculturally useful soil, and to be able to perform some elementary analysis and to suggest corrective measures for samples that deviate from desirable norm.

Unit 1: Basic Ideas in Analysis (6 Lectures)

Qualitative and quantitative analysis. Accuracy, precision and sources of errors in quantitative measurements: Instrumental and reagent errors, personal and operational errors, errors of method. Brief idea about procedures for correction of aforesaid errors.

Unit 2: Analysis of Food Materials (12 Lectures)

Nutritional components of food – carbohydrates, fats, proteins, minerals and vitamins. Basic qualitative tests for identification of starch, reducing sugars, fats and proteins. Principle of quantitative titrimetric determination of calcium in foodstuff. Concept of food processing; preservatives, colouring matters and adulterants. Identification of some adulterants in some common food items such as starch in milk, detergent in milk, chalk powder in sugar, added colour in food grains. [as in: *vikaspedia.in/health/health-campaigns/beware-of-adulteration*]

Unit 3: Analysis of Water and Soil (12 Lectures)

Concept of potable water, treatments to obtain potable water, minerals present and dissolved oxygen in potable water. Concept of pH, acidity and alkalinity of water; determination of pH and of alkalinity. Determination of dissolved oxygen. Composition of soil, procedure for pH measurement of soil, correction of undesirable acidity or alkalinity of soil, estimation of calcium and magnesium ions in soil by complexometric titration.

Lab Experiments for SEC- 1

1. To measure, in triplicate set of measurements, the marked volume of a 25 mL size pipette in terms of a burette.
2. To do qualitative tests for identification of starch, reducing sugars, fats and proteins in four food materials containing these four items.
3. Identification of colouring matter in food grains.
4. Identification of some common adulterants: Starch in milk, detergent in milk, chalk powder in sugar.
5. Determination of pH of a water sample and a soil sample.

Course Outcome: Students would be able to correct for common errors in chemical analysis, and to follow as well as perform some common chemical analysis on food, water and soil.

Semester II

SEC - 2 (Tools in Computational Chemistry) Credits: 2+0+1 = 3

Learning Objectives

1. To learn about and create 2-D printable/web-publishable drawing of chemical structures and reactions in computers using specialised computer software.

2. To learn about and create/edit 3-D molecular models in computers using specialised computer software, and to view and interpret their textual contents.

3. Downloading and opening macromolecular structural data as PDB files from online resource, and interpreting those in terms of chains, ligands and water present.

4. To know about computational chemistry approaches such as molecular mechanics (MM), *ab initio* and semi-empirical quantum mechanics (QM), molecular dynamics (MD) and docking for performing computations on molecular and macromolecular systems.

Unit 1: Computer Models of Molecules and Macromolecules (16 Lectures)

Introduction to two-dimensional molecular drawings and three-dimensional molecular models. Sketching two-dimensional drawings using BIOVIA Draw/ ChemDraw/ BKChem. Building three-dimensional molecular models using Avogadro/ GaussView/ ArgusLab – constructing the raw backbone, selecting and changing an atom, adding and hiding the hydrogen atoms, cleaning (refining) molecular geometry, saving in various formats. Computer storage of the molecular model in the XYZ (.xyz) file format – the content pattern of the XYZ files, use of Angstrom unit of length, absence of bond connectivity data therein. The z-matrix specification of the molecular geometry, illustration with a suitable file format such as Fenske-Hall format, use of degree unit for angles. Downloading, storing and opening macromolecular structural data as PDB files, interpreting PDB files in terms of chains, ligands, water molecules, etc. using Chimera/ PMV etc.

Unit 2: Computational Approaches about Intermolecular Interactions (14 Lectures)

Introduction to Molecular Mechanics (MM) approach – all-atom and united-atom approaches, potential energy as sum of various covalent and non-covalent interactions, idea of force fields, examples of common force fields in MM. Introduction to Molecular Dynamics (MD) using Tinker. Introduction to semi-empirical methods – commonly used methods. Use of MM and semi-empirical methods for molecular geometry optimisation in ArgusLab/ Avogadro etc. Concept of docking of a drug molecule with a protein macromolecule. Quantum Mechanics (QM) approach, commonly used level of theory and basis sets for QM calculations, use of charge and spin multiplicity parameters – example of a QM calculation about a simple molecule using Gaussian or Firefly (i.e., PCGAMESS) etc.

Lab Experiments for SEC- 2

1. Drawing a 2-D diagram of salicylic acid using BIOVIA Draw/ ChemDraw/ BKChem
2. Draw the reaction for synthesis of aspirin using BIOVIA Draw/ ChemDraw/ BKChem
3. Construct a 3-D molecular model of 2-hydroxy butanoic acid using Avogadro/ GaussView, save it as an XYZ file and optimize its geometry
4. View the contents of an XYZ file using Notepad/gedit, and convert it to the Fenske-Hall z-matrix format using a web-based molecular model converter such as WebQC.
5. Search and download the PDB structure of human pepsin 3b enzyme (PDB ID 3UTL) from the RCSB PDB online resource, and view the structure in UCSF Chimera software and locate the water molecules present in it.
6. Taking a XYZ molecular model already created, run a geometry optimisation using the MM (Molecular Mechanics) UFF force-field option.
7. Using a downloaded ligand-bound receptor protein structure such as 5TGZ or 5XR8, perform the pre-docking macromolecule preparation steps of removing ligand and water species, and adding the missing hydrogen atoms using PMV or UCSF Chimera.

Course Outcomes:

1. Students would be able to create 2-D drawing of chemical structures and reactions, and create/edit 3-D molecular models in computers using specialised computer software, and to obtain and interpret their textual contents.

2. They would be able to download and open macromolecular structural PDB files from online resource, and interpreting those in terms of chains, ligands and water present.

3. They would know about molecular mechanics (MM), *ab initio* and semi-empirical quantum mechanics (QM), molecular dynamics (MD) and docking for performing computations on molecular and macromolecular systems.

Semester III

SEC- 3 (Chemistry Tools for Pollution Studies) Credits: 2+0+1 = 3

Learning Objectives

The objective of this course is to make the students aware of environmental pollution and understand the role of chemistry in mitigating it.

Unit 1: Chemistry of Air Pollution (14 Lectures)

Parameters of air quality and their permissible limits. Contaminants and Pollutants. Primary air pollutants and formation of secondary air pollutants, smog formation. Automobile vehicles as a source of air pollution and its control using catalytic converters. Increasing level of CO_2 in air and green house effect, measures (such as shifting to greener energy sources, afforestation, preventing deforestation, etc.) to control CO_2 pollution. CFCs as pollutants, ozone layer depletion and measures for its mitigation.

Unit 2: Chemistry of Soil and Water Pollution (16 Lectures)

Parameters of water and soil, their permissible limits. Soil and water pollution due to anthropogenic sources: changes in pH in both cases, reclamation of problem soil, adverse effects of petroleum exploration and processing on soil and water, concept of BOD and COD of water, increase of BOD in water, decrease of dissolved oxygen in water, effect of industrial effluents and thermal pollution on aquatic life, pesticides in soil and water, its trophic level biomagnification. Groundwater pollution by pesticides and heavy metals. Fertilizers, detergents and sewage as water pollutants, eutrophication of water bodies.

Lab Experiments for SEC- 3

1. Determination of dissolved oxygen in a water sample.
2. Determination of COD in a water sample.
3. Indicating presence of soaps and detergents in water sample by surface tension measurements with distilled water as the reference liquid.
4. Determination of lead in ground water by complexometric titration.

Course Outcomes:

Students will acquire adequate knowledge about the chemicals and chemical phenomena related to environmental pollution. This will enable them to move towards greener aspects.

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