

Semester-I – [Chemistry]

UG0802/03 CHM-
51T-101
(4 Hrs./week)

Chemistry of s & p-block elements. Noble Gases, Nuclear
Chemistry, Fundamentals of Organic Chemistry,
Stereochemistry, Mathematical Concepts and Chemical Kinetics.

Unit-I

Periodicity of s and p-block elements:

Effective nuclear charge, Shielding or screening effect, Slater rules, Variation of effective nuclear charge in periodic table. Atomic radii (van der Waals), Ionic and crystal radii, Covalent radii (octahedral and tetrahedral). Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy. Electron gain enthalpy, Trends of electron gain enthalpy. Electronegativity, Pauling's/Mulliken's/Allred-Rochow's and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, Partial charge, Hybridization, Group electronegativity. Sanderson's electron density ratio.

Periodicity in properties of p-block elements with special reference to atomic and ionic radii, Ionization energy, Electron-affinity, Electronegativity, Diagonal relationship, Catenation.

s-Block Elements: Comparative study of properties of alkali and alkaline earth metals, Diagonal relationships, Salient features of hydrides, Solvation and complexation tendencies including their functions in biosystems, An introduction to alkyls and aryls.

Unit-II

Some Important Compounds of p-block Elements: Hydrides of boron, Diborane and higher boranes, Borazine, Borohydrides, Fullerenes, Carbides, Fluorocarbons, Silicates (structural principle), Tetrasulphurtetranitride, Basic properties of halogens, Interhalogens and polyhalides.

Chemistry of Noble Gases: Chemical properties of the noble gases, Chemistry of Xenon, Structure and bonding in Xenon compounds.

Nuclear Chemistry: Fundamental particles of nucleus (nucleons), concept of nuclides and its representation, Isotopes, Isobars and Isotones (with specific examples), forces operating between nucleons (n-n, p-p & n-p), Qualitative idea of stability of nucleus (n/p ratio).

Radiochemistry: Natural and artificial radioactivity, Radioactive disintegration series, Radioactive displacement law, Radioactivity decay rates, Half-life and average life, Nuclear binding energy, Mass defect and calculation of defect and binding energy, Nuclear reactions, Spallation, Nuclear fission and fusion. Brief discussion on atom bomb, Nuclear reactor and Hydrogen atom.

15 Lectures

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Unit-III

Fundamentals of organic chemistry: Organic Compounds: Classification and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties. Electronic Displacements: Inductive, Electromeric, Resonance and mesomeric effects, Hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength. Homolytic and Heterolytic bond fission with suitable examples. Curly arrow rules, Formal charges; Electrophiles and Nucleophiles; Nucleophilicity and basicity.

Stereochemistry of Organic Compounds: Concept of isomerism, Types of isomerism, Difference between configuration and conformation, Flying wedge and Fischer projection formulae.

Optical Isomerism: Elements of symmetry, Molecular chirality, Enantiomers, Stereogenic centre, Optical activity. Properties of enantiomers, Chiral and achiral molecules with two stereogenic centres. Diastereomers, Threo and erythro isomers, Meso compounds. Resolution of enantiomers. Inversion, Retention and racemization (with examples).

Relative and absolute configuration, Sequence rules, D/L and R/S systems of nomenclature.

Geometrical Isomerism: Determination of configuration of geometric isomers - cis/trans and E/Z systems of nomenclature. Geometrical isomerism in oximes and alicyclic compounds.

Conformational Isomerism: Newman projection and Sawhorse formulae, Conformational analysis of ethane, *n*-butane and cyclohexane.

Unit-IV

Mathematical Concepts:

Logarithmic relations, Curve sketching, Linear graphs and calculations of slopes, Differentiation of functions like: kx , e^x , x^n , $\sin x$ and $\log x$. maxima and minima, Partial differentiation and Euler's reciprocity relations, Integration of some useful/relevant functions. Permutations and combinations, Factorials, Probability, Matrices and Determinant.

Chemical Kinetics:

Chemical kinetics and its scope, Rate of a reaction, Factors influencing the rate of a reaction: concentration, temperature, pressure, solvent, light, catalyst. Concentration dependence of rates, Mathematical characteristics of simple chemical reactions - zero order, first order, second order and pseudo-order; Half-life and mean-life. Determination of the order of reaction - differential method, Method of integration, Method of half-life period and isolation method. Radioactive decay as a first order phenomenon.

Experimental methods of chemical kinetics: Conductometric, Potentiometric, Optical methods: polarimetry and spectrophotometric method. Theories of chemical kinetics. Effect of temperature on rate of reaction, Arrhenius equation, Concept of activation energy. Simple collision theory based on hard sphere model transition state theory (equilibrium hypothesis). Expression for the rate constant based on equilibrium constant and thermodynamic aspects.

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Suggested Books and References:

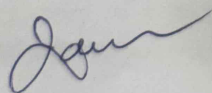
1. Concise Inorganic Chemistry by J.D. Lee, Wiley.
2. Inorganic Chemistry by Catherine E. Housecroft and Alan G. Sharpe, Pearson.
3. Selected Topics in Inorganic Chemistry by Wahid U. Malik, G. D. Tuli and R. D. Madan, S. Chand, New Delhi.
4. Advanced Inorganic Chemistry: Volume I & II by Satya Prakash, G. D. Tuli, S. K. Basu and R. D. Madan, S. Chand, New Delhi.
5. Inorganic Solids – Introduction to Concepts in Solid-state Structural Chemistry by D. M. Adams, John Wiley, London.
6. Principles of Inorganic Chemistry by Puri, Sharma & Kalia, Vishal Publishing Co.
7. Essentials of Nuclear Chemistry by H.J. Arnikar, New Age International Publishers.
8. Organic Chemistry by I. L. Finar, Pearson.
9. Organic Chemistry by R.T. Morrison, R.N. Boyd & S.K. Bhattacharjee, Pearson.
10. Stereochemistry conformation and Mechanism by P.S. Kalsi, New Age International Publishers.
11. Stereochemistry of Organic Compounds by V. K. Ahluwalia, Springer.
12. Chemical Kinetics by Keith J. Laidler, Pearson Education.
13. Principles of Physical Chemistry by B. R. Puri, L. R. Sharma & M. S. Pathania, Vishal Publishing Co.
14. Advanced Physical Chemistry by Gurdeep Raj, Goel Publishing House.
15. Physical Chemistry by W. Atkins, Oxford University Press.
16. Physical Chemistry by R. J. Silby and R. A. Alberty, John Wiley & Sons.
17. Physical Chemistry by G.M. Barrow, Tata McGraw-Hill.
18. A Textbook of Physical Chemistry: (Volume I) by K. L. Kapoor, Macmillan India Ltd.

Suggested E-resources:

All the above suggested books are available as e- books.

Online Lecture Notes and Course Materials:

All prescribed courses are available in the form of e-books, Adobe Acrobat documents (PDF), web pages etc.



II – Semester – [Chemistry]

CHM-52T-103-Chemical Bonding, Reactions Mechanism, Aromatic & Aliphatic hydrocarbons, Alkyl & Aryl Halides, States of Matter.

Unit-I

Ionic Solids: Ionic structures, Radius ratio effect and coordination number, Limitations of radius ratio rule, Lattice defects, Semiconductors, Lattice energy and Born-Haber cycle, Solvation energy and solubility of ionic solids, Polarizing power and polarisability of ions, Fajan's rule.

Covalent Bond: Valence bond theory and its limitations, Directional characteristics and shapes of simple inorganic molecules and ions. Valence shell electron pair repulsion (VSEPR) theory to NH_3 , H_3O^+ , SF_4 , ClF_3 , ICl_2 , H_2O .

Molecular Orbital Theory: Homonuclear and heteronuclear (CO and NO) diatomic molecules. Multicenter bonding in electron deficient molecules, Bond strength and bond energy, Percentage ionic character from dipole moment and electronegativity difference.

Metallic bond: Free electron, Valence bond and band theories.

Weak Interactions: Hydrogen bonding, Van der Waals forces.

15 Lecture

Unit-II

Mechanism of Organic Reactions:

Reaction intermediates: Types, shapes and relative stability; Carbocations, Carbanions, Free radicals, Carbenes, Nitrenes and Benzyne (Arenes). Types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions. Markovnikov rule, Anti-Markovnikov rule, Saytzeff's rule and Hofmann elimination. Energy considerations. Methods of determination of reaction mechanism (product analysis, intermediates, isotope effects, kinetic and stereochemical studies).

Aliphatic Hydrocarbon

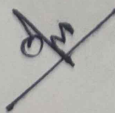
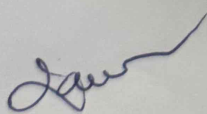
Alkanes and Cycloalkanes: Free radical halogenation of Alkanes: mechanism, orientation, reactivity and selectivity. Cycloalkanes - nomenclature, methods of formation, chemical reactions. Baeyer's strain theory and its limitations. Theory of strain-less rings.

Alkenes, Cycloalkenes, Dienes and Alkynes: Relative stabilities of alkenes. Chemical reactions of alkenes - hydroboration-oxidation, oxymercuration-reduction, epoxidation, ozonolysis and oxidation with $KMnO_4$, Polymerization of alkenes, Substitution at the allylic and vinylic positions of alkenes.

Classification and nomenclature of isolated, conjugated and cumulated dienes. Structure of allenes and butadiene. Methods of formation, properties and chemical reactions - 1,2- and 1,4-additions, Diels-Alder reaction and polymerization reactions.

Structure and bonding of alkynes, Synthetic methods, Chemical reactions - acidity of alkynes, Mechanism of electrophilic and nucleophilic addition reactions: hydroboration-oxidation, metal-ammonia reduction, oxidation and polymerization.

15 Lecture



Unit-III

Arenes and Aromaticity: Nomenclature of benzene derivatives: The aryl group, aromatic nucleus and side chain, Structure of benzene: molecular formula and kekule structure, Stability and carbon-carbon bond lengths of benzene, Resonance structure, MO diagram.

Aromaticity: Huckel's rule, aromatic ions-three to eight membered.

Aromatic electrophilic substitution: General pattern of the mechanism, role of sigma and pi complexes, Mechanism of nitration, halogenation, sulphonation, mercuration, chloromethylation and Friedel crafts reactions, Energy profile diagrams, Activating and deactivating substituents, Directive influence, orientation and ortho/para ratio. Side chain reactions of benzene derivatives, Birch reduction.

Alkyl Halides: Synthetic methods of alkyl halides, Chemical reactions, Mechanisms of nucleophilic substitution reactions of alkyl halides S_N2 and S_N1 reactions with energy profile diagrams.

Polyhalogen compounds: Chloroform, Carbon tetrachloride

Aryl Halides: Methods of formation of aryl halides, Nuclear and side chain reactions, The addition-elimination and the elimination-addition mechanisms of nucleophilic aromatic substitution reactions, Relative reactivities of alkyl, allyl, vinyl and aryl halides.

Unit-IV

States of matter

Gaseous States: Postulates of kinetic theory of gases, Deviation from ideal behavior, Van der Waals equation of state. **Critical Phenomenon:** PV isotherms of real gases, Continuity of states, the isotherms of Van der Waals equation, Relationship between critical constants and van der Waals constants, The law of corresponding states, Reduced equation of state.

Molecular Velocities: Root mean square, average and most probable velocities. Qualitative discussion of the Maxwell's distribution of molecular velocities, Collision number, Mean free path and collision diameter. Liquification of gases (based on Joule-Thomson effect.)

Liquid State: Intermolecular forces, Structure of liquids (a qualitative description). Structural differences between solids, liquids and gases. Liquid crystals: Difference between liquid crystal, solid and liquid. Classification, structure of smectic, nematic and cholesteric phases. Thermography and seven segment cells.

Solid State: Definition of space lattice, Unit cell.

Laws of crystallography- (i) Law of constancy of interfacial angles (ii) Law of rationality of indices (iii) Law of symmetry. Symmetry elements in crystals.

Basic concept of X-ray diffraction by crystals. Derivation of Bragg's equation. Determination of crystal structure of $NaCl$ and $CsCl$ (Laue's method and powder method.), Band theory of solids, Defects in solids.

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Suggested Books and References:

1. Concise Inorganic Chemistry by J.D. Lee, Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity by Ellen A. Keiter, James E. Huheey and Richard L. Keiter, Pearson.
3. Organic Chemistry by S. S. Gupta, Oxford University Press.
4. Organic Reaction Mechanisms by V. K. Ahluwalia and Rakesh Kumar Parashar, Narosa Publishing House, New Delhi.
5. Organic Chemistry – Reactions and Reagents: Covering Complete Theoretical Organic Chemistry by O. P Agarwal, Goel Publishing House, Meerut.
6. Organic Chemistry by R. T. Morrison and R. N. Boyd, Prentice Hall.
7. Organic Chemistry by I. L. Finar (Vol. I & II), ELBS.
8. Advanced Organic Chemistry by A. Bahl and B. S. Bahl, S. Chand.
9. Modern Organic Chemistry by M.K. Jain and S. C. Sharma, Vishal Publishing Co.
10. March's Advanced Organic Chemistry: Reactions,
11. Mechanisms and Structure by J. March and M. B. Smith, Wiley. Mechanism in Organic Chemistry by Peter Sykes, Pearson Education.
12. Principles of Physical Chemistry by B. R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishing Co.
13. Advanced Physical Chemistry by Gurdeep Raj, Goel Publishing House.
14. A Textbook of Physical Chemistry by K. L. Kapoor (Volume 5), Macmillan India Ltd.
15. Chemical Kinetics and Reaction Dynamics by Santosh K. Upadhyay, Springer (Anamaya Publishers, New Delhi, India).

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