## Semester I

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### CHE-RC/HG-1016: CHEMISTRY1

**ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS**

**(Credits: Theory-04, Lab-02)**

**Theory: 60 Lectures**

***Course Objective:*** *This course may be divided into two broad parts-inorganic and organic chemistry. In inorganic chemistry part the students will be taught atomic structure, chemical bonding and molecular structure. The organic chemistry part contains fundamentals of organic chemistry, stereochemistry and aliphatic hydrocarbons.*

***Learning Outcome:*** *After completion of this course the students will learn the atomic structure through the basic concepts of quantum mechanics. They will understand the chemical bonding through VB and MO approaches. In organic part, the students are*

*expected to learn basic ideas used in organic chemistry, stereochemistry, functional groups, alkanes, alkenes, alkynes etc.*

***Section A: Inorganic Chemistry-1*** **(30 Periods)**

**Atomic Structure:** *Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de-Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.*

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of $\psi$ and $\psi^2$, Schrödinger equation for hydrogen atom. Radial and angular parts of the hydogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers $m_l$ and $m_s$. Shapes of *s*, *p* and *d* atomic orbitals, nodal planes. Discovery of spin, spin quantum number (*s*) and magnetic spin quantum number ($m_s$).

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

**(14 Lectures)**

**Chemical Bonding and Molecular Structure**

*Ionic Bonding:* General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

*Covalent bonding:* VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.
Concept of resonance and resonating structures in various inorganic and organic compounds. MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for *s-s*, *s-p* and *p-p* combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods

(including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and $NO^+$. Comparison of VB and MO approaches.

**(16 Lectures)**

***Section B: Organic Chemistry-1*** **(30 Periods)**

**Fundamentals of Organic Chemistry**

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

**(8 Lectures)**

**Stereochemistry**

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. 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 (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

**(10 Lectures)**

**Aliphatic Hydrocarbons**

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

**Alkanes:** (Upto 5 Carbons). *Preparation:* Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* Free radical Substitution: Halogenation.

**Alkenes:** (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). *Reactions:* cis-addition (alk. KMnO4) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

**Alkynes**: (Upto 5 Carbons) *Preparation:* Acetylene from $CaC_2$ and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides.

*Reactions:* formation of metal acetylides, addition of bromine and alkaline $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$.

**(12 Lectures)**

**Recommended Books:**


1. J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
2. F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
3. Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
4. James E. Huheey, *Ellen Keiter and Richard Keiter: Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
5. T. W. Graham Solomon: *Organic Chemistry, John Wiley and Sons*.
6. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry,* Orient Longman.
7. E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
8. I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
9. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
10. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand


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## LAB: CHEMISTRY1

### ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

**60 Lectures**

***Section A: Inorganic Chemistry - Volumetric Analysis***

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.

2. Estimation of oxalic acid by titrating it with $KMnO_4$.

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

4. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.

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

***Section B: Organic Chemistry***

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)

2. Separation of mixtures by Chromatography: Measure the Rf value in each case (combination of two compounds to be given)

(a) 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

(b) Identify and separate the sugars present in the given mixture by paper chromatography.

**Recommended Books:**


1. Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
2. Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
3. Textbook of Practical Organic Chemistry, A.I. Vogel , Prentice Hall, 5th edition.
4. Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.


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