BENGALURU CITY UNIVERSITY B.Sc (CBCS) SYLLABUS(2020-21 onwards) CHEMISTRY I SEMESTER -BLOW UP

SECTION – A

26hrs.

Atomic Structure	:13 hrs
Chemical Bonding and Molecular Structure	:13 hrs

SECTION A

Atomic Structure

13 hrs.

Bohr's theory: Postulates, derivation of expressions for radius and energy for hydrogen and hydrogen like atoms, calculation of ionization potential. Hydrogen atom spectra-Explanation of the origin of spectral lines using Bohr's theory, Rydberg formula, calculation of Rydberg constant, frequency and wavenumber of spectral lines, merits and limitations of Bohr's theory. Numerical problems on all the above concepts.

Dual behaviour of matter and radiation - derivation of de Broglie's relation for calculation of wavelength, differences between matter wave and electromagnetic wave, numerical problems.

Heisenberg Uncertainty principle: Statement and mathematical expression, probability concept of the electronic cloud, orbitals.

Limitations of classical mechanics - Need of a new approach to Atomic structure.

Quantum mechanics: Postulates, explanation of the terms wave function (normal and orthogonal), operator, eigen value and eigen function taking simple examples. Derivation of Time independent Schrodinger equation in three dimensions starting from sine wave equation $\psi = A\sin(2\pi x/\lambda)$ and explanation of various terms in it and also the sinusoidal wave. Hamiltonian and Laplacian operators, Significance of ψ and ψ^2 .

Spherical co-ordinates, expressions for conversion of Cartesian to polar coordinates. Schrödinger equation for hydrogen atom in terms of polar coordinates (no derivation), separation of variables, expressions for radial and angular parts of the hydrogenic wave functions 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, principal quantum number (n), orbital angular momentum(I) and quantum numbers m_l and m_s . Shapes of s, p and d atomic orbitals, nodal planes. Discovery of spin – Stern Gerlach experiment, spin quantum number (s) and magnetic spin quantum number (m_s).

Rules for filling electrons in various orbitals: Aufbau principle, Pauli's exclusion principle, Hund's rule of maximum multiplicity, (n+l) rule – Illustration taking simple examples. Electronic configurations of the atoms- General electronic configurations for s, p, d and f block elements and electronic configurations of elements up to atomic number 54. Stability of half-filled and completely filled orbitals – explanation taking examples from d-block elements, concept of exchange energy, relative energies of atomic orbitals. Anomalous electronic configurations explanation taking examples from d-block elements.

2. Chemical Bonding and Molecular Structure

13 hrs

lonic Bonding: Illustration with an example. Conditions for formation of ionic bond. General characteristics of ionic bonding. Lattice energy and Solvation energy (definition and explanation taking examples) and their importance in the context of stability and solubility of ionic compounds (alkali metal halides and hydroxides). Statement of Born-Landé equation, numerical problems. Born-Haber cycle (for ionic solids of type MX and MO) and its applications, numerical problems.

Covalent character of ionic bond - Polarising power and polarisability – definition and explanation taking examples, effects of polarisation. Fajan's rules- rules and illustration with suitable examples.

Covalent bond: Illustration taking an example, factors favouring covalent bond, polar covalent molecules – explanation taking examples. Dipole moment – definition, SI unit, bond moment and percentage ionic character – calculation from dipole moment measurements for simple diatomic molecules such as HX.

Covalent bond - VB Approach: Postulates of valence bond theory and limitations. Shapes of some inorganic molecules and ions: (i) Hybridisation - definition, bond angle and diagram - explanation taking suitable examples of linear (BeF₂), trigonal planar (BF₃), square planar [tetraamminecopper (II) ion], tetrahedral (SiF₄), trigonal bipyramidal (PCI₅) and octahedral (SF₆) arrangements. (ii) VSEPR theory – Rules, illustration of structure of molecules taking suitable examples (NH₃, H₂O, BrF₃, ICI²⁻) Concept of resonance, Resonating structures in various inorganic and organic compounds (CO₃²⁻, O₂, CO, benzene)

Covalent bond -MO Approach: Basic principles, differences between atomic and molecular orbitals, rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals (diagrams).

Rules for filling MOs, energy level diagrams for MOs, nonbonding combination of orbitals.MO treatment of homonuclear diatomic molecules of 1^{st} and 2^{nd} periods including idea of s-p mixing-examples H₂, He₂⁺, Be₂, N₂, O₂, O₂²⁻,O₂⁺ and heteronuclear diatomic molecules such as CO, NO and NO⁺ (electronic configuration, energy level diagram, calculation of bond order, explanation of bond strength and magnetic properties).Comparison of VB and MO approaches.

Metallic bonding: Band theory – postulates, diagram indicating energy bands, illustration taking example (lithium), explanation of electrical properties of metals, semiconductors and insulators.

Semiconductors: Extrinsic, intrinsic, doping, n-type and p-type, examples and applications.

SECTION – B

26hrs.

Fundamentals of Organic Chemistry & Stereochemistry	: 8hrs.
Aliphatic Hydrocarbons	: 9hrs.
Aromatic hydrocarbons	: 9 hrs.

Fundamentals of Organic Chemistry

Bond cleavage - Homolysis and heterolysis- Explanation with examples.

Types of reagents: Electrophilic and nucleophilic reagents-definition and examples (both neutral and ionic).

Reactive intermediates - generation, structure and relative stabilities of primary, secondary and tertiary- carbocation, carbanion, carbon free radicals-explanation for relative stability and reactivity based on inductive, resonance and hyper conjugative effects. Carbenes and nitrenes -definition and examples.

Types of reactions:

i) Addition: addition of hydrogen and hydrogen halides to alkenes and alkynes,
HCN to aldehydes and Ketones

ii)Substitution: reaction of aq KOH, alc KCN with haloalkanes.

iii)Elimination-dehydration of alcohols, dehydrohalogenation of haloalkanesexamples. (examples for reactions with respect to compounds having upto four carbons shall be discussed)

Isomerism: Structural and Stereoisomerism

4 hrs.

Chain, position, functional, metamerism, tautomerism types explanation with an example.

4 hrs.

Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations of 2,3-dichlorobutane.

Conformations with respect to ethane, butane (Newmann representations) and cyclohexane (puckered rings)- energy profile diagrams.

Geometrical isomerism: conditions (examples of but-2-ene and 1,2-dimethyl cyclopropane to be given- concept of restricted rotation to be mentioned), cis trans isomers. Examples: maleic and fumaric acid, dichloroethene, but-2-enal. Optical isomerism- definition. Chiral centre, concept of chirality, examples of compounds with one chiral centre - glyceraldehyde, lactic acid.

Aliphatic hydrocarbons

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

Alkanes (up to five carbons):

i) Preparation: Corey- House reaction and Wurtz reaction - Comparison.

ii) Reactions: free radical substitution: Halogenation of alkanes-mechanism of bromination of ethane.

a) Relative rates of different classes of hydrogen atoms based on the stability of the radicals.

b) Relative reactivities of halogens in the halogenation of alkanes based on the magnitude of activation energies of the rate determining step.

Alkenes (up to five carbons):

i) Preparation: cis alkenes (partial catalytic hydrogenation) and trans alkenes (Birch reduction), Wittig reaction-stereo selectivity to be mentioned.

ii) Reactions: cis-addition (alk. KMnO₄) and trans-addition (bromine) to alkenes,

Addition of HX (Markownikoff's and anti-Markownikoff's addition)- Mechanisms.

Hydration, ozonolysis-significance, oxymercuration-demercuration,

hydroboration-oxidation reactions.

9 hrs.

Dienes: (up to four carbons) Classification- isolated, conjugated, cumulated-one example for each. Structure of allene and butadiene.

Reactions: i)1, 2-addition and 1, 4 addition reactions-explanation based on resonance structures. ii) Diels Alder reaction: 1, 3-butadiene with maleic anhydride as an example.

Alkynes (up to five carbons):

i) Preparations-from vicinal and germinal dihalides

ii) Reactions-Acidic nature of terminal alkynes: reaction with ammoniacal solutions of silver nitrate and cuprous chloride. Significance – conversion of lower terminal alkynes to higher alkynes. Oxidation with KMnO₄, ozonolysis.

Aromatic hydrocarbons

9 hrs.

Nomenclature: Mono, di and tri substituted benzene,

Aromaticity: Criteria for aromaticity and Huckel's rule. Examples: benzene

naphthalene, anthracene, phenanthrene, cyclopropenylcation, cyclopentadienyl anion, cycloheptatrienylcation (tropylium ion).

Anti-aromaticity: Features, examples: cyclobutadiene, cyclopentadiene.

Non aromatics: Features, examples: butadiene, hexa-1, 3, 5-triene.

Preparation: Benzene and Chlorobenzene from phenol, Sandmeyer reactionconversion of aniline to chloro, bromo and iodo-benzene.

Electrophilic substitutions reactions: General mechanism of electrophilic substitution reaction, evidence for the formation of phenyl carbocation- kinetic isotopic effect.

Nitration of benzene: mechanism, energy profile diagram, evidences for the formation of nitronium ion.

Orienting influence of substituents: i) Ring activating and deactivating groupsexamples ii) o-p orienting and m-orienting groups-examples Orienting influence of phenol, toluene, chlorobenzene, nitrobenzene towards electrophilic substitutions. Comparison of reactivity of these compounds with respect to benzene towards electrophilic substitutions- explanation using inductive, resonance, hyperconjugative effects.

Oxidations: Side chain oxidation of toluene to benzaldehyde (Etard's reaction) and benzoic acid(using alk KMnO₄).

Alkenyl benzenes: Styrene, preparation by Wittig reaction and from ethyl benzene by dehydrogenation. uses of styrene. cis and trans-stilbenes-structures and their preparations.