Course Title: Basic Chemistry I **Full Marks:** 100
Course No.: CHE 101 (major/minor) **Pass Marks:** 35
Nature of the Course: Theory **Year:** I

Course Objectives:

- To stimulate, create and sustain their interest in the study of chemistry.
- To provide a body of chemical knowledge appropriate for higher studies.
- To make aware the importance of scientific method of accurate experimental work.
- To provide mechanistic approaches of organic reactions.

Group A: Inorganic Chemistry

Atomic structure:- Bohr's theory and refinements, wave mechanical model of the atom, matter waves, de Broglie's equation, Heisenberg's uncertainty principle, Schrödinger's wave equation (time independent), physical significance of wave function, probability density pattern for hydrogen atom, radial and angular wave functions, radial distribution curves, shapes of s, p, d orbital ; charge cloud diagrams and boundary surface diagrams, nodal planes, quantum numbers and their significance, energy level diagram. **9 hrs**

Multi-electron system:- Pauli exclusion principle, Hund's rule of maximum multiplicity, energy level diagrams across d-block elements, stability of completely filled, half filled and empty orbital. **3 hrs**

Nuclear Chemistry:- Composition of nucleus, nuclear stability, binding energy, radioactivity, half life determination and nuclear reactions, group displacement law and radioactivity series, application of nuclear chemistry. **4 hrs**

Periodic classification of elements and physical properties: Long form of periodic table (significance and limitation), IUPAC classification of periodic table and its merits and demerits, periodicity of elements, s, p, d and f blocks, long form of periodic table, discussion of properties like atomic, ionic and covalent radii, ionization potential, screening or shielding effect, electro negativity, different scales of electro negativity measurements (Pauling, Mulliken and Allred and Rochow), electron affinity (Periodic variation, experimental determination of electron affinity).

7 hrs

Chemical bonding : Ionic bond: packing of ions in crystal, radius ratio, lattice energy, Born equation, Born-Haber cycle, covalent character in ionic compounds, polarizing power and polarizability (Fajan's rule), bond moment and dipole moments, percentage ionic character from dipole moments and electro negativity differences, characteristics of ionic compounds, structure of ionic solids, ionic compounds of type AX (NaCl, CsCl, ZnS), AX_2 (CaF_2, TiO_2), layer structures, stoichometric and non- stoichometric defects. **8 hrs**

Covalent Bond: General characteristics of coordinate-covalent bond, valence bond approach, directional characteristics of covalent bond, resonance energy, hybridization, the extent of orbital participation in molecular bonding, (sp, sp^2, sp^3, d^2sp^3, dsp^2, sd^3, dsp^2, dsp^3), multiple bonding, three electron bond, two electron three centered bond, sigma-and pi-bonds, bond length and bond order, bond strength, valence shell electron pair repulsion theory (VSEPR), theory of directed valence, shapes of simple inorganic molecules and ions containing bonds and lone pairs, hydrogen bond (theories of hydrogen bonding, valence bond treatment), metallic bond (Free electron theory and band theory), conductors, insulators and semiconductors, elementary idea of L.C.A.O. and concept of united atoms in molecular orbital theory, bonding, antibonding, and non-bonding orbitals, M.O. configurations of simple diatomic molecules (H_2, He_2, N_2, O_2, F_2, CO, NO, HCl and related species) and molecular ions (O_2^-, O_2^{--}, NO^+, CO^+). σ and π bonds and delocalized π-bonds in inorganic species (CO_2, SO_2, SO_3^{--}, CO_3^{--}, NO_3^-, N_3^- etc). **10 hrs**

Acids and Bases: Lewis acid-base concept, hard and soft acids and bases (HSAB), application of HSAB principle, relative strengths of acids and bases and the effect of substituents and solvents on them. **4 hrs**

Principles of qualitative and quantitative Analysis: Solubility product, common ion effect, their application in group separation, principles of gravimetric and volumetric analysis. **5 hrs**

Group B: Organic Chemistry

Structure and Properties: Atomic orbitals, molecular orbitals, hybrid orbitals, polarity of bonds, melting point, acids and bases, dipole-dipole interaction, hydrogen bonding, inductive effect, electromeric effect, resonance, mesomeric effect or conjugative effect, hyperconjugation effect, steric effect, IUPAC nomenclature. **4 hrs**

Alkanes: Energy of activation, progress of reaction, energy profile diagram, exothermic and endothermic reaction, Fischer projection formulas, Andiron formulas, Newman projection formula, free rotation about the C-C single bond, conformation of n-butane, physical properties, industrial source, industrial source vs. laboratory preparation, Grignard reagent, coupling of alkyl halide with organometallic compounds, reactions: halogenations (substitution reaction), mechanism of halogenations, orientation of halogenations, relative reactivity of alkanes toward halogenations, ease of abstraction of hydrogen, homolytic bond dissociation energies and relative stability of free halogenations, orientation, reactivity and selectivity, non-rearrangement of free radicals, combustion, pyrolysis. **10 hrs**

radicals, ease of formation of free radicals, structure of free radicals, transition state for

Stereochemistry: Introduction, structural isomers and stereoisomer, stereoisomerism, optical activity, polarimeter, specific rotation, enantiomerism and optical activity, chirality, chiral centre, enantiomers, racemic modification, resolution of racemic modification, configuration, absolute configuration (R and S), sequence rules, diastereomers, meso compound, reaction involving stereoisomers, generation of a chiral centre (only one chiral centre), geometrical isomerism.

7 hrs

Alkyl Halide (Nucleophilic Substitution): Homolytic and heterolytic fission, structure (the functional group), classification and nomenclature of alkyl halides, physical properties, preparation, nucleophilic aliphatic substitution reactions, nucleophiles and leaving groups, rate of reaction (effect of concentration), the S_N2 reaction (mechanism and kinetics), the S_N2 reaction (stereochemistry, inversion of configuration), the S_N1 reaction (mechanism and kinetics), carbocations (structure and relative stability), S_N1 reaction (stereochemistry), rearrangement of carbocations, S_N1 vs. S_N2 reaction, factors affecting S_N mechanism (effect of substrate, nucleophile, solvent, and leaving group). **10 hrs**

Alcohols and Ethers: Introduction, nomenclature, structure, physical properties, industrial source, fermentation, fuel from carbohydrate, ethanol, preparation, reactions, alcohols as acids, bases, reaction of alcohols with hydrogen halides, formation of alkyl sulphonates, oxidation of alcohols, industrial source of ethers, preparation of ethers, Williamson synthesis, reactions of ethers (PCl_5, HX), role of solvent, solubility (ionic solutes, protic and aprotic solvents, ionic pair).

6 hrs

Alkenes: Physical properties, industrial source, preparation, dehydrohalogenation of alkyl halide, kinetics of dehydrohalogenation, E2 reaction (mechanism, orientation and reactivity), E1 reaction (mechanism, orientation and reactivity), dehydration of alcohols, reaction of alkenes, reaction at the carbon-carbon double bond, (hydrogenation, addition of hydrogen halides, addition of hydrogen bromide and peroxide effect, addition of sulphuric acid, addition of water, electrophilic addition (mechanism, orientation and reactivity), addition of halogens, and mechanism, halohydrin formation, oxymercuration-demercuration, hydroboration-oxidation, (orientation and mechanism of hydroboration), free radical addition (mechanism and orientation), hydroxylation, ozonolysis, analysis of alkenes, application of alkenes to prepare polymers (polypropelene and polyethylene).

9 hrs

Alkynes: Structure of acetylene, physical properties, industrial source of acetylene, preparation of alkynes, reactions of alkynes, reduction to alkenes, electrophilic addition to alkynes, hydration of alkynes, acidity of alkynes, reactions of metal acetylides, analysis of alkyne. **4 hrs**

Group C: Physical Chemistry

Gaseous State: Review on kinetic theory of gases, derivation of kinetic gas equation, average velocity, most probable velocity, average kinetic energy of gas molecules, molecular interpretation of temperature, gas laws (Boyle's, Charles's, Graham's, Avogadro's & Dalton's laws) and root mean square velocity of gas molecules derived from kinetic gas equation, related numericals

Maxwell-Boltzmann distribution law for molecular velocities, distribution of velocities, different types of velocities (most probable, average & root mean square) of gas molecules and their derivation from Maxwell's equation, collision properties: collision diameter, collision frequency, mean free path, related numericals

Deviation of real gas from ideal behavior, van der Waals equation (derivation and explanation of volume and pressure corrections), Boyle's temperature and van der Waals constants, compressibility factors and its uses, critical phenomenon, relation between van der Waals constants and critical constants, related numericals.

Liquefaction of gases: Faraday method, Linde's and Claude's principles of liquefaction of air.

12 hrs

Liquid and Solid States: Properties of liquids, surface tension and its determination by drop weight & capillary rise methods, viscosity and fluidity, effect of temperature on viscosity & surface tension, determination of viscosity by Ostwald's viscometer, applications of surface tension and viscosity measurements, numericals.

Properties of crystalline & amorphous; ionic, covalent, metallic & molecular solids, crystal structure and unit cells, crystal systems and Bravais lattices, cubic crystals (simple, body centered and face centered cubic), laws of crystallography, Miller indices, numericals. **8 hrs**

Chemical and Ionic Equilibriums: Applications of law of mass action to homogeneous equilibrium, effect of temperature, pressure, concentration and inert gases on chemical equilibrium, numerical problems on chemical equilibrium

Quantitative treatments on hydrolysis of salts and related numerical problems, common ion effects in ionic equilibrium, buffer solution, buffer capacity and buffer range, numerical problems in pH and buffer, pH change in acid base titration (weak and strong), theory of acid base indicator: Ostwald's theory, quinonoid theory, selection of acid base indicators in titrations.

8 hrs

Colligative Properties: Raoult's law and determination of vapor pressure lowering, laws of elevation of boiling point and depression of freezing point, osmotic pressure and determination of molecular weight from colligative properties, van't Hoff factor, abnormalities in solution due to association and dissociation, numerical problems. **6 hrs**

Chemical Kinetics**:** Review on the rate of a chemical reaction, pseudo order reaction, rate equations (differential and integrated form) for zero and second order reaction, half life of reaction, determination of order of a reaction, effect of temperature on the reaction rate: Arrhenius equation and activation energy, related numerical, kinetic study of some reaction mechanism (reaction between O_2 and HBr, I_2 and propanone in acidic medium) **8 hrs**

Thermodynamics and Thermo-chemistry: Review on (some thermodynamic terms, Hess law & bond energy), isothermal but not reversible expansion of an ideal gas, isothermal reversible expansion of an ideal gas, experimental determination of $\triangle E$ using bomb calorimeter, (H) enthalpy, experimental determination of $\triangle H$, enthalpy of physical changes (enthalpy of fusion, vaporization, sublimation), molar heat capacity at constant pressure and volume, relation between C_p and C_v, variation of heat of reaction with temperature (Kirchoff's equation), calorific value of fuel and food, numerical problems. **8 hrs**