LECTURER CADRE CHEMISTRY SYLLABUS

Physical Chemistry

1. Basic principles of chemistry:- Importance of chemistry, Nature of Matter, Properties of Matter and their measurement, Uncertainty in measurements, Laws of chemical combinations, Dalton's Atomic Theory, Atomic and Molecular Masses, Mole concept and molar masses Percentage Composition, Stoichiometry and Stoichiometric Calculations

2 Atomic structure:- Sub atomic Particles, Atomic models, Developments Leading to the Bohr's model of atom, Bohr's Model for hydrogen atom, towards Quantum Mechanical model of the Atom, Quantum mechanical model of Atom, Nature of electromagnetic radiation, photoelectric effect limitations of Bohr's model, Dual nature of matter, de-Broglie's relationship, Heisnberg uncertaintiy principle, various quantum numbers(principle, angular momentum , magnetic and spin quantum numbers) and their significance, shapes of s,p and d - orbitals, electron spin quantum number, Rules for filling electrons in orbitals-aufbau principle Paulli's exclusion principle and Hund's rule, electronic configuration of elements, extra stability of half- filled and completely filled orbitals.

3 Chemical Bonding and Molecular Structure:-Kossel - Lewis approach to chemical bond formation, concept of ionic and covalent bonds, Ionic Bonding, Formation of Ionic bonds, factors affecting the formation of ionic bonds, calculation of lattice enthalpy, Covalent Bonding, Concept of electronegativity, Fajan's rule, dipole moment, Valence Shell Electron Pair Repulsion(VSEPR) theory and shapes of simple molecules, Quantum mechanical approach to covalent bonding , Valence bond theory - its important features, concept of hybridization involving s,p and d orbitals, Resonance, Molecular Orbital Theory ,LCAOs , types of molecular orbitals (bonding, antibonding), sigma and pi-bonds, molecular orbitals electronic configurations of homonuclear diatomic molecules, concept of bond order, bond length and bond energy, Elementary idea of metallic bonding, Hydrogen bonding and its applications.

4. States of Matter:-Intermolecular Forces, Thermal Energy, Intermolecular forces vs thermal interactions, The Gaseous state, The Gas laws, Ideal gas equation, Kinetic Molecular theory of Gases, Liquification of Gases, Liquid state

5. Thermodynamics:- Fundamental of thermodynamics, System and surroundings, extensive and intensive properties, state functions, types of processes, First law of thermodynamics ,concept of work, heat internal energy and enthalpy, heat capacity, molar heat capacity, Hess's law of constant heat summation, Enthalpies of bond dissociation, combustion ,formation, atomization, sublimation , phase transition, hydration, ionisation and solution. Second law of thermodynamics, Spontaneity of processes, AS of the universe and ΔG of the s system as criteria for spontaneity, ΔG° (standard Gibbs energy change) and equilibrium constant.

6. Equilibrium:- Meaning of equilibrium, concept of dynamic equilibrium. Equilibria involving physical processes: Solid - liquid, liquid - gas and solid - gas equilibria, Henry's law, general characterics of equilibrium involving physical processes. Equilibria involving chemical process: Law of chemical equilibrium, equilibrium constants (K_p and K_c) and their significance, significance of ΔG and ΔG° in chemical equilibria, factors affecting equilibrium concentration, pressure, temperature, effect of catalyst; Le Chatelier's principle. Ionic equilibrium: Weak and strong electrolytes, ionization of electrolytes, various concepts of acids and bases (Arrhenius Bronsted - Lowry and Lewis) and their ionization, acid - base equilibria (including multistage ionization) and ionization constants, ionization of water, pH scale, common ion effect, hydrolysis of salts and pH of their solutions, solubility of sparingly soluble salts and solubility

products, buffer solutions.

7. Redox Reactions and Electrochemistry:- Electronic concept of oxidation and reduction, redox reactions, oxidation number, rules for assigning oxidation number balancing of redox reactions. Electrolytic and metallic conduction, conductance in electrolytic solutions, specific

and molar conductivities and their variation with concentration: Kohlrausch's law and its applications. Electrochemical cells - Electrolytic and Galvanic cells, different types of electrodes, electrode potentials including standard electrode potential, half-cell and cell reactions, emf of a Galvanic cell and its measurement; Nernst equation and its applications; Relationship between cell potential and Gibbs' energy change, Dry cell and lead accumulator; Fuel cells. Corrosion, its types and method of preventions.

8. Chemical Kinetics:- Rate of a chemical reactions, factors affecting the rate of reactions: concentration, temperature, pressure and catalyst; elementary and complex reactions, order and molecularity of reactions, rate law, constant and its units, differential and integral forms of zero and first order reactions, their characteristics and half-lives, effect of temperature on rate of reactions - Arrhenius theory, activation energy and its calculation, collision theory of bimolecular gaseous reactions.

Concepts of catalysis:- Homogenous and heterogeneous catalysis.

9. Surface chemistry:- Adsorption - Physisorption and chemisorptions and their characteristics, factors affecting adsorption of gases on solids - Freundlich and Langmuir adsorption isotherms, adsorption from solutions, Colliodal state-distinction among true solutions, colloids and suspensions, classification of colloids- lyophilic, lyophobic; multi molecular, macromolecular and associated colloids (micelles), preparation and properties of colloids - Tyndall effect, Brownian movement, electrophoresis, dialysis, coagulation and flocculation; Emulsions and their characteristics.

10. Solid States-: General Characteristics of solid state, Amorphous and Crystalline Solids, Classification of Crystalline Solids, Crystal Lattices and Unit Cell, Close-Packed Structures, Packing Efficiency, Calculations Involving Unit Cell Dimensions, Imperfections in Solids, Electrical Properties, Magnetic Properties.

11. Solutions:- Types of Solutions, Expressing concentration of solutions, Solubility, Vapour pressure of liquid solutions, Ideal and Non-ideal solutions, Colligative Properties and collision theory of bimolecular gaseous reactions (no derivation).
Determination of Molar Mass, Abnormal Molar Masses.

12. Photochemistry: Interaction of Radiation with Matter, Difference between Thermal and Photochemical Processes. Laws of Photochemistry: Grothus – Drapper Law, Stark – Einstein Law, Jablonski Diagram depicting various processes occurring in the Excited State, Qualitative Description of Fluorescence, Phosphorescence, Non Radiative Processes (Internal Conversion, Intersystem Crossing), Quantum Yield, Photosensitized Reactions – Energy Transfer Processes (simple examples).

13.QUANTUM CHEMISTRY

Fundamental Aspects of Quantum Chemistry

Fundamental Background: Postulates of Quantum mechanics, Commutators of operators, Unitary, linear and Hermitian operators, Operators for the dynamic variables of a system such as position,

linear momentum, angular momentum and total energy, Concept of Normalization and Orthogonality, Schrödinger wave equation: time independent and time dependent wave equation.

Applied Aspects of Quantum Chemistry

- Application of Quantum Chemistry in Translation motion: Particle in one dimension, two- and three-dimensional box: Differential equation and its solution, Normalization and orthogonality of wave functions, Graphical representation of wave functions and probability densities, Energy level diagram.
- Application of Quantum Chemistry in other model systems: Harmonic oscillator and Rigid rotator: Classical and Quantum mechanical treatment, Hermite polynomial, sketches of wave functions and probability densities, and energy levels.
- Application of Quantum Chemistry in Atomic system: Solution of Schrodinger equation for hydrogen and hydrogen-like atoms, Physical representation of s and p orbitals, Radial and Angular plots.

Approximate Methods

- Variation principle and Perturbation theory: first order and non-degenerate. Applications of variation method and perturbation theory to the Helium atom.
- Angular Momentum
- Ordinary angular momentum and Quantum mechanical operators for angular momentum. Eigen function and Eigen values of angular momentum using ladder operators, Addition of angular momentum.

Molecular Orbital Theory

Huckel Theory of conjugated systems, bond order and charge density calculation, Applications of Huckel molecular orbital theory to Ethylene, Butadiene, Cyclopropenyl radical, Cyclobutadiene systems. Introduction to extended Huckel theory.

14. Basic principles and applications of spectroscopy:- Rotational, vibrational, electronic, Raman, ESR, NMR.

Spectroscopy and their types

- General Introduction to Spectroscopy: Nature of radiation energies corresponding to various kinds of radiations, atomic and molecular transitions, selection rules & chemical processes effecting the natural line width of a spectral line, general applications; determinations of concentration, isosbestic points, finger printing, Job's method of Isomolar solutions.
- Electronic Absorption Spectroscopy: Vibrational and electronic energy levels in a diatomic molecule, relationship of Potential energy curves to electronic spectra. Nomenclature, Assignment of transitions, Spin-orbit couplet criteria to aid in Bond assignment, Intensity of Electronic Transition i) Oscillator Strengths, Transition moment Integrate Derivation of some selection rules, spectrum of formaldehyde, Spin-Orbit &vibronic coupling contribution to Intensity mixing of d & p orbital's in certain summitries, higher state mixing, Oscillator strengths, Intensity of electronic transitions, charge transfer transitions, polarized absorption spectra. Applications, finger printing, molecular addition compounds in Iodine, effect of solvent polarity on charge transfer.
- Mass Spectrometry: Instrument operation and presentation of spectral processes that can occur when a molecule and a high energy electron combine, finger print applications.

Interpretation of mass spectra, effect of isotope on appearance of mass spectrum, Molecular weight determination.

Electron Spin Resonance Spectroscopy

- History, Theory & Instrumentation, Block diagram of ESR spectrometer.
- ESR of organic radicals, hyperfine lines and mechanism of interactions.
- Mc-Connell relationship of electron delocalization and numericals.
- Zero field splitting with examples. Kramer's degeneracy with examples.
- Predicting number of lines in radicals and Coordination Compounds, factors affecting the 'g' value.
- Applications of ESR spectroscopy including biological applications.

Nuclear Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance Spectroscopy

- Introduction, History, Theory, Instrumentation, Characteristics of magnetic nuclei, concept of magnetic energy states.
- Larmor theorem, selection rules for the transition between magnetic states, spacing between two consecutive magnetic levels, nuclear population in different states & numerical.
- Nuclear Resonance, nuclear precession, chemical shift and factors affecting chemical shift, equivalence & non-equivalence protons, spin-spin coupling and coupling constant, deuterium exchange, 'H NMR spectrum of absolute ethyl alcohol and normal ethyl alcohol.
- AX, AB, ABX, ABC nuclear systems with examples.
- Karplus equation & numerical, interpretation of 1H-NMR spectra of representative compounds like hydrocarbons, hydroxyl compounds, aldehydes, ketones, carboxylic acids, ethers, amides, amines.
- Applications of NMR spectroscopy including MRI.

Vibration & Rotation Spectroscopy

This section covers the fundamental principles of how molecules interact with radiation through movement.

- Vibration & Rotation: Covers harmonic and anharmonic oscillators, selection rules (the "rules" for whether a transition can happen), force constants (bond strength), and how polyatomic molecules vibrate differently than simple diatomic ones.
- Raman Spectroscopy: Focuses on light scattering rather than absorption. Key topics include polarized/depolarized lines and determining if a molecule is "IR active" or "Raman active" based on its symmetry.
- Complex Effects: Includes Fermi Resonance (interaction between vibrational states) and Microwave Spectroscopy, which is used specifically to measure precise bond lengths and angles.

Application of Electronic Absorption and IR Spectroscopy

- Inorganic Complexes: Specifically mentions calculating Dq (crystal field splitting energy) and (nephelauxetic ratio) for octahedral Ni(II) complexes.
- Fingerprinting: Using IR and Raman spectroscopy as a "fingerprint" to identify unknown substances.
- Structural Determination: Using selection rules to figure out the shapes of inorganic structures and studying hydrogen bonding systems.
- Coordination Changes: Analyzing how the spectrum of a "donor" molecule (ligand) changes when it binds to a metal center, which often changes the molecule's symmetry.

Inorganic Chemistry

1.Chemical periodicity:- Modern periodic law and present form of the periodic tables, s, P, d and f block elements, periodic trends in properties of elements atomic and ionic radi, ionization enthalpy, electron gain enthalpy, valence, oxidation states and chemical reactivity.

2 General principles & process of isolation of metals:- Modes of occurrence of elements in nature, minerals, ores; Steps involved in the extraction of metals - concentration, reduction (chemical and electrolytic methods) and refining with special reference to the extraction of Al, Cu, Zn and Fe; Thermodynamic and electrochemical principles involved in the extraction of metals.

3.Hydrogen:- Position of hydrogen in periodic table, isotopes, preparation, properties and uses of hydrogen; Physical and chemical properties of water and heavy water, Structure preparation, reactions and uses of hydrogen peroxide; Hydrogen as a fuel.

4. S-Block elements:- Group-1 and 2 elements introduction, electronic configuration and general trends in physical and chemical properties of elements, anomalous properties of the first element of each group, diagonal relationships. Preparation and properties of some important compounds - sodium carbonate and sodium hydroxide; Industrial uses of lime, limestone Plaster of Paris and cement; Biological significance of Na, K, Mg and Ca.

5. P-Block elements:- Group 13 to Group 18 elements, Electronic configuration general trends in physical and chemical properties of elements across the periods and down the group; unique behavior of the first element in each group. Preparation, properties and uses of boron and aluminium; properties of boric acid, diboron, boron trifluride, aluminium chloride and alums, Allotropes of carbon, catenation; Structure & properties of silicates and zeolites. Properties and uses of nitrogen and phosphorus; Allotrophic forms, structure and uses of ammonia, nitric acid, and PCl_3, PCl_5; Structures of oxides of phosphorus. Preparation, properties, structures and uses of ozone; Allotropic forms of sulphur, sulphuric acid and structures of oxoacids of sulphur.

6. d-&f Block elements:- Position in periodic table, electronic configurations of d-block elements, general properties of the transition elements (d-Block), some important compounds of transition elements, the lanthanoids, the actinoids, some application of d- and f-Block elements. Preparation, properties and uses of $K_2Cr_2O_7$ and $KMnO_4$.

7. Co-ordination compounds & Organometallic compounds:- Introduction to co-ordination compounds, Werner's theory: ligands, co-ordination number, denticity, chelation; IUPAC nomenclature of mononuclear co-ordination compounds, isomerism; Bonding - Valence bond approach and basic ideas of Crystal field theory, colour and magnetic properties; Importance of co-ordination compounds (in qualitative analysis, extraction of metals and in biological systems), Organometallic compounds-synthesis, bonding and structure, and reactivity. Organometallics in homogenous catalysis. Cages and metal clusters.

8. Environmental Chemistry:- Environmental pollution - Atmospheric, water and soil, Atmospheric pollution - Tropospheric and Stratospheric Tropospheric pollutants - Gaseous pollutants : Oxides of carbon, nitrogen and sulphur, hydrocarbons; their sources, harmful effects and prevention; Green house effect and Global warming; Acid rain; Particulate pollutants: Smoke, dust, smog, fumes, mist; their sources, harmful effects and prevention. Stratospheric pollution - Formation and breakdown of ozone, depletion of Ozone layer - its mechanism and effects. Water Pollution - Major pollutants such as, pathogens, organic wastes and chemical pollutants; their harmful effects and prevention.

Soil pollution Major pollutants such as: Pesticides (insecticides, herbicides and fungicidies), their harmful effects and prevention. Strategies to control environmental pollution.

9. (i)Nuclear Chemistry:- Nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

(ii)Analytical chemistry :separation techniques, spectroscopic electro and thermoanalytical methods.

10. Bioinorganic Chemistry:- Photosystems, porphyrines, metalloenzymes, Oxygen transport, electron transfer reactions, nitrogen fixation.

11. Physical characterization of inorganic compounds by IR, Raman, NMR, EPR, Mossbauer, UV-, NQR, MS, electron spectroscopy and microscopic techniques.

12. Symmetry and Group Theory

Symmetry elements and symmetry operations, indistinguishable configuration, point groups for simple molecules, determination of point groups, properties of point groups, order, classes of group, representation of a group, isomorphic group, abelian group, characteristics of matrix representation,

classification of representation, reducible and irreducible representations, great orthogonality theorem, Applications of GOT, C2v, C3v, Da, Td. Oh, character tables, symmetry, the method of finding the number of irreducible representation in a reducible representation.

Applications of Group Theory

Separation of d orbitals under the influence of octahedral, tetrahedral, square planar and trigonal bipyramidal symmetry, the method of descending symmetry for d^2 configuration, symmetry of hybrid orbital, determination of symmetry of vibrational mode, symmetry consideration regarding selection rules and spectral intensities, vibronic coupling, non-centrosymmetric complexes C3v, Td polarization of electronically allowed transitions, selection rules for electronic transitions, fundamentals, overtones, combinations tones and fermi resonance in vibrational spectroscopy - the symmetry symbols for normal modes of vibrations. IR and Raman activity of vibrational mode, mutual exclusive principle and nature of vibrations in terms of change in internal coordinates in simple molecules like trans-N_2,F_2, SF_6.

Organic Chemistry

1. Purification & Characterisation of organic compounds:- Purification Crystallization, sublimation, distillation, differential extraction and chromatography principles and their applications. Qualitative analysis - Detection of nitrogen, sulphur, phosphorus and halogens. Quantitaive analysis- Estimation of carbon, hydrogen, nitrogen, halogens, sulphur, phosphorus. Calculations of empirical formulae and molecular formulae: numerical problems in organic quantitative analysis.

2. Some basic principles of organic chemistry:- Tetravalency of carbon - Shapes of simple molecules- hybridization (s and p); Classification of organic compounds based on functional groups - C = C -, -Carbon Carbon triple bond and those containing halogens, Oxygen, nitrogen and sulphur, Homologus series; Isomerism -structural and stereoisomerism. Nomenclature (Trivial and IUPAC) Covalent bond Homolytic and heterolytic : free radicals, carbocations and carbanions; stability of carbocations and free radicals, eleectrophiles and nucleophiles. Electronic displacement in a covalent bond - Inductive effect, electromeric effect, resonance and hyperconjugation.

3. Chemistry of Hydrocarbon:- Classification, Isomersim IUPAC nomenclature, general methods of preparation, properties and reactions. Alkanes - Conformations : Sawhorse and Newman projections (of ethane); Mechanism of halogenations of alkanes. Alkenes Geometrical isomerism; Mechanism of electrophilic addition: addition of hydrogen, molecular formulae; Numerical problems in organic quantitative analysis. halogens, water hydrogen halides (Markownikofff's and peroxide effect); Ozonolysis and polymerization. Alkynes - Acidic character, Addition of hydrogen, halogens, water and hydrogen halides; Polymerization. Aromatic hydrocarbons – Nomenclature, benzene -structure and aromaticity: Mechanism of

electrophillic substitution: halogenations, nitration, Friedel - Craft's alkylation and acylation, directive influence of functional group in mono - substituted benzene.

4. Organic compounds - containing Halogens;- General methods of preparation, properties and reactions; Nature of C -X bond; Mechanisms of substitution reactions, Uses; Environmental effects of chloroform & iodoform.

5. Organic compounds- containing Oxygen:- General methods of preparation, properties, reactions and uses. Alcohols, Phenols and Ethers Alcohols: Identification of primary, secondary and tertiary alcoholos; mechanism of dehydration. Phenols: Acidic nature, electrophillic substitution reactions : halogenations, nitration and sulphonation, Reimer - Tiemann reaction. Ethers : Structure. Aldehyde and ketones : Nature of carbonyl group ; Nucleophilic addition to >C=0 group, relative reactivities of aldehydes and ketones: Important reactions such as - Nucleophilic addition reactions (addition of HCN, NH_3 and its derivatives), Grignard reagent; oxidation; reduction (Wolff Kishner and Clemmensen); acidity of hydrogen, aldol condensation, Cannizzaro reaction, Haloform reaction; Chemical tests to distinguish between aldehydes and Ketones. Methods of preparation properties, reactions and uses of carboxylic acids, acidic strength and factors affecting it.

6.Organic compounds - containing Nitrogen:-general method of preparation, properties, reaction and uses. Amines: nomenclature, classification, structure ,basic character and identification of primary, secondary and tertiary amines and their basic character .diazonium salts: importance in synthetic organic chemistry

7. Polymers:- General introduction and classification of polymers, general methods of polymerization - addition and condensation, copolymerization; Natural and synthetic rubber and vulcanization; some important polymers with emphasis on their monomers and uses - polythene, nylon, polyester and bakelite.

8. Biomolecules: -General introduction and importance of biomolecules. Carbohydrates- Classification : aldoses and ketoses; monosaccharides and constituent monosaccharides of oligosaccharides, starch. Proteins - primary, secondary, tertiary and quaternary structure (qualitative ides only), denaturation of proteins, enzymes. Vitamins Classification and functions. Nucleic Acids – Chemical constitution of DNA and RNA. Biological functions of nucleic acids.

9. Chemistry in Everyday Life:- Chemical in medicines - Analgesics, tranquilizers, antiseptics, disinfectants, antimicrobials, antifertility drugs, antibiotics, antacids, antihistamines – their meaning and common examples. Chemical in food - Preservatives, artificial sweetening agents - common examples. Cleansing agents Soaps and detergents, cleansing action.

10. Common reagents (organic, inorganic and organometallic) in organic synthesis. Selective organic transformations chemoselectivity, regioselectivity, stereoselectivity. enatioselectivity. Protecting groups.

11. Physical characterization of organic compounds by IR, UV, MS and NMR.

12. Principles related to Practical Chemistry: Practical chemistry principles , laboratory techniques for analyzing and creating chemical substances. include qualitative analysis (identifying elements/ions), quantitative analysis (volumetric analysis/titration), functional group detection in organic compounds, and preparation of inorganic/organic compounds and Essential techniques .