FACULTY OF SCIENCES

SYLLABUS

FOR

Ph. D. Chemistry Entrance Exam

November 2022

DEPARTMENT OF CHEMISTRY

SARDAR PATEL UNIVERSITY MANDI- 175001

HIMACHAL PRADESH

Group theory: The concept of group, Symmetry elements and symmetry operations, Assignment of point groups to Inorganic molecules, some general rules for multiplications of symmetry operations, Multiplication tables for water and ammonia, Representations (matrices, matrix representations for C_2V and C_3V point groups irreducible representations), Character and character tables for C_2V and C_3V point groups. Applications of group theory to chemical bonding (hybrid orbitals for σ-bonding in different geometries and hybrid orbitals for π-bonding. Symmetries of molecular orbitals in BF_3, C_2H_4 and B_2H_6.

Non-Aqueous Solvents: Factors justifying the need of Non-Aqueous solution Chemistry and failure of water as a Solvent. Solution chemistry of Sulphuric acid: Physical properties, Ionic self-dehydration in H_2SO_4, high electrical conductance in spite of high viscosity, Chemistry of H_2SO_4 as an acid, as a dehydrating agent, as an oxidizing agent, as a medium to carry out acid-base neutralization reaction and as a differentiating solvent. Liquid BrF_3: Physical properties, solubilities in BrF_3, self-ionization, acid base neutralization reactions, solvolytic reactions and formation of transition metal fluorides.

Inorganic Hydrides: Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wade's Rules, preparation, structure and bonding in boron hydrides (boranes) and carboranes.

Organic Reagents in Inorganic Chemistry: Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of the following reagents in analysis:

(a) Dimethylglyoxime
(b) EDTA
(c) 8-Hydroxyquinoline
(d) 1,10-Phenanthroline
(e) Thiosemicarbazones
(f) Dithiazone

Metal-Ligand Bonding: Recapitulation of Crystal Field Theory including splitting of *d*-orbitals in different environments, Factors affecting the magnitude of crystal field splitting, structural effects (ionic radii, Jahn-Teller effect), Thermodynamic effects of crystal field theory (ligation, hydration and lattice energy), Limitations of crystal field theory, Adjusted Crystal Field Theory (ACFT), Evidences for Metal-Ligand overlap in complexes, *Molecular Orbital Theory* for octahedral, tetrahedral and square planar complexes (excluding mathematical treatment)

Atomic Spectroscopy: Energy levels in an atom, coupling of orbital angular momenta, coupling of spin angular momenta, spin orbit coupling, spin orbit coupling *p2* case, Determining the Ground State Terms-Hund's Rule, Hole formulation (derivation of the Term Symbol for a closed sub-shell, derivation of the terms for a d^2 configuration), Calculation of the number of the microstates.

Electronic Spectra: Splitting of spectroscopic terms (S,P,D,F and G,H,I), d^{11}-d^9 systems in weak fields (excluding mathematics), strong field configurations, transitions from weak to strong crystal fields. Correlation diagrams (d^{11}-d^9) in Oh and Td environments, spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B, C and β parameters. Electronic spectra of complex ions: Selection rules (Laporte, orbital and spin selection rules), band intensities, band widths, spectra in solids, spectra of aqueous solutions of d^1-d^9 ions in Oh and Td environments, Evaluation of 10 Dq, Spectrochemical and Nephelauxetic series, charge- transfer spectra.

Photoelectron Spectroscopy: Basic principle, photoionization process, ionization energies, Koopman's theorem, ESCA, photoelectron spectra of simple molecules, (N_2, O_2) Photoelectron spectra for the isoelectronic sequence Ne, HF, H_2O, NH_3 and CH_4, chemical information from ESCA, Auger electron spectroscopy – basic idea.

Magnetochemistry: Origin of Magnetic moment, Magnetic susceptibility (diamagnetic, paramagnetic), spin only moment, Russell Saunder's coupling, quenching of orbital angular moment, orbital contribution to a magnetic moment, magnetic moments from magnetic susceptibilities, temperature dependence of magnetic susceptibility, Factors determining paramagnetism, application of magnetochemistry in co-ordination chemistry in spin free and spin paired octahedral and tetrahedral complexes, Van Vlecks formula for magnetic susceptibility.

Metal π Complexes Preparation, reactions, structures and bonding in carbonyl, nitrosyl and phosphine complexes, structural evidences from vibrational spectra. Structure and bonding in metal cyanides, stabilization of unusual oxidation states of transition metals.

Introductory Analytical Chemistry: *Data Analysis*– Types and sources of errors, propagation of errors, detection and minimization of various types of errors. Accuracy and precision, average and standard deviation, variance, its analysis and confidence interval, tests of significance (*F*-test, *t*-test and paired t-test), criteria for the rejection of analytical data (4d rule, 2.5d rule, Q-test, average deviation and standard deviation), least-square analysis.

Lanthanides and Actinides: Spectral and magnetic properties, comparison of Inner transition and transition metals, Transuranium elements (formation and colour of ions in aqueous solution), uses of lanthanide compounds as shift reagents, periodicity of translawrencium elements.

Nuclear Chemistry: Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, Q-value. Natural and artificial radioactivity, radioactive decay and equilibrium, Nuclear fission, fission product and fission yields, Nuclear fusion.

Inorganic Photochemistry: Basic principles, absorption, excitation, kasha rule, electronically excited state, its life-time and energy dissipation process. Photochemical behaviour of transition metal complexes, charge transfer spectra of crystalline and gasous alkali halides. Photochemistry of chromium(III) octahedral complexes, $[Cr(H_2O)_6]^{3+}$ and $[Cr(NH_3)_6]^{3+}$. Photochemistry of cobalt(III) complexes, $[Co(NH_3)_5X]^{2+}$ and $[Co(en)_3]^{3+}$.

Inorganic Reactions and Mechanism: Substitution reactions in octahedral complexes, acid hydrolysis reactions, base hydrolysis and anation reactions, substitution reaction, reactions occurring without rupture of metal-ligand bond. Substitution reactions of square planar complexes. Theories of trans-effect, labile and inert complexes. Mechanism of redox reactions.

Polymeric Inorganic Compounds: General chemical aspects (synthesis, properties and structure) of phosphazenes, borazines, silicones, sulphur- nitrogen cyclic compounds and condensed phosphates.

Stability of Coordination Compounds: Stability constants, stepwise formation constants, overall formation constants, relationship between stepwise and overall formation constants, factors affecting the stability constants (with special reference to metal and ligand ions), Difference between thermodynamic and kinetic stability.

Homogeneous Transition metal catalysis: General considerations, Reason for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), basic concept of catalysis (molecular activation by coordination and addition), proximity interaction (insertion/inter-ligand migration and elimination, rearrangement). Phase transfer catalysis. Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones). Asymmetric hydrogenation (Olefins).

Some important homogeneous catalytic reactions:- Ziegler Natta polymerization of ethylene and propylene, oligomerisation of alkenes by aluminumalkyl, Wackers acetaldehyde synthesis, hydroformylation of unsaturated compounds using cobalt and rhodium complexes, Monsanto acetic acid synthesis, carbonylation of alkenes and alkynes using nickel carbonyl and palladium complexes.

Metalloporphyrins: Porphyrins and their salient features, chlorophyll (structure and its role in photosynthesis). Transport of Iron in microorganisms (siderophores), types of siderophores (catecholate and Hydroxamato siderophores).

Metalloenzymes: Structure and functions of Carboxy peptidases and Carbonic anhydrase.

Oxygen Carriers: Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutzmachanism), Cyanide poisoning and its remedy. Non-heme protiens (Hemerythrin & Hemocyanin).

Transport and storage of metals: The transport mechanism, transport of alkali and alkaline earth metals, ionophores, transport by neutral macrocycles and anionic carriers, sodium/potassium pump, transport and storage of Iron (Transferrin & Ferritin).

Inorganic compounds as therapeutic Agents: Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health.

Supramolecular Chemistry: Introduction, Bonding other than covalent bond. Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxenes and their applications.

Stereochemistry: Introduction to Basic Concepts of Stereochemistry: Isomers and their properties, Threo and Erythro isomers, Chirality, Optical isomerism, Geometrical isomerism, Conventions for configurations- D,L and R,S systems, Racemic mixture and Racimization, Resolution of Racemic mixtures, Measurement of optical activity, optical purity, Streoselective and Streospecific reactions, epimerization, epimers, anomers and mutarotation, Axial Chirality (Allenes and Biphenyls), Planar chirality, Helicity, Chirality involving atoms other than carbon atoms, Prochirality: prostreoisomerism and Asymmetric synthesis. Conformational and Streoisomerism of acylic and cylic systems, cyclohexane, decalins, effect of conformation on reactivity in acylic and cyclohexane systems.

Reaction Mechanism: Structure and Reactivity: Thermodynamic and kinetic requirements, Kinetic and Thermodynamic control, Hammonds postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Effect of structure on reactivity: resonance and field effects, steric effect. Quantitative treatment: Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation. Methods of determining Reaction mechanisms.

Aliphatic Nucleophilic Substitution: Reactivity effect of substrate structure, leaving group and nucleophile. The SN_2, SN_1, mixed SN_1 and SN_2, SET mechanisms & SNi mechanism. The neighboring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance. Non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements-Wagner-Meerwein, Pinacol-Pinacolone and Demjanov ring expansion and ring contraction. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Esterification of carboxylic acid, transesterification, Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.

Aliphatic Electrophilic substitution: Bimolecular mechanisms- SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts, halogenation of aldehydes, ketones, acids and acyl halides. Effect of substrates, leaving group and the solvent system on reactivity. Aliphatic diazonium coupling, Acylation at aliphatic carbon, alkylation of alkanes, Stork-enamine reactions

Free radical reactions: Geometry of free radicals, Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate neighboring group assistance, Reactivity in aliphatic and aromatic substrates at a bridgehead and attacking radicals. Effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts (Gomberg Bachmann reaction), Hoffmann -Loffler- Freytag reaction, Hunsdiecker reaction.

Aromatic Electrophilic Substitution: Arenium ion mechanism, orientation and reactivity, ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir - Haack reaction, Scholl reaction, Amination reaction, Fries rearrangement, Hofmann-Martius Reaction, Reversal of Friedel Craft alkylation.

Aromatic Nucleophilic Substitution: SNAr, SN1, benzyne and SRN1 mechanism. Reactivity, effect of substrate structure, leaving group and attacking nucleophile, Von Richter, Sommelet-Hauser, and Smiles rearrangements, Ullman reaction, Ziegler alkylation, Schiemann reaction.

Common Organic Reactions and Their Mechanisms: Perkin condensation, Michael reaction, Robinson annulation, Diekmann reaction, Stobbe condensation, Mannich reaction, Knoevenagel condensation, Benzoin condensation, Witting reaction, Hydroboration, Hydrocarboxylation, Ester hydrolysis, Epoxidation.

Reagents in Organic Synthesis: Synthesis and applications of BF_3, NBS, Diazomethane, Lead tetra-acetate, Osmium tetraoxide, Woodward Prevorst hydroxylation reagent, $LiAlH_4$, Grignard reagent, organozinc and organolithium reagent.

Elimination Reactions: Discussion of E_1, E_2, E_1cB and E_2C Mechanisms and orientation, Reactivity: Effects of substrate structures, attacking base, leaving group and medium. Mechanism and Orientation in Pyrolytic eliminations, Cis elimination, elimination in cyclic systems, eclipsing effects, cleavage of quaternary ammonium hydroxides, Shapiro reaction, Conversion of Ketoxime to nitriles.

Pericyclic Reaction: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5 hexatrienes and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions: conrotatory and disrotatory motions, 4n and 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements-Suprafacial and Antarafacial shifts of H, sigmatropic shifts involving carbon moieties, Claisen, Cope and aza-Cope rearrangements, Ene reaction.

Ultra Violet and Visible Spectroscopy: Electronic transitions (185-800 nm), Beer- Lambert Law, Effect of solvent on electronic transitions, Ultra Violet bands of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Steric effect in biphenyls, Fieser- Woodward rules for conjugated dienes and carbonyl compounds, ultra violet spectra of aromatic and heterocyclic compounds.. Applications of UV- visible spectroscopy in organic chemistry.

Infrared Spectroscopy: Principle, Instrumentation and sample handling, Characteristic vibrational frequencies of common organic compounds, Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Introduction to Raman spectroscopy. Applications of IR and Raman Spectroscopy in organic chemistry.

Nuclear Magnetic Resonance (NMR) Spectroscopy: General introduction, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus- relationship of coupling constant with dihedral angle. First and second order spectra, Simplification of complex spectra-nuclear magnetic double resonance, spin tickling, INDOR, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Introduction to resonance of other nuclei – ^{19}F, ^{31}P, ^{13}C, NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta- stable peak, McLafferty rearrangement. Nitrogen Rule. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy.

Resonance Spectroscopy: Principle and theory of Electron Spin Resonance (ESR). Hyperfine structure of ESR. Fine structure of ESR (electron-electron coupling / Zero – field splitting of ESR signal. McConnell relation. Mossbaur spectroscopy: isomer – shift, quadrupole interaction and magnetic hyperfine interaction.

Photochemistry: Introduction and Basic principles of photochemistry. Interaction of electromagnetic radiations with matter, Types of excitations, fate of excited molecules, Franck-Condon principle. Kinetics of Excimer and exciplex formation. Energy transfer from electronically excited molecules (Stern – Volmer mechanism). E- type and P- type delayed fluorescence.

Quantum yield, transfer of excitation energy, actinometry. Photochemistry of alkenes: cis-trans isomerization, dimerization of alkenes, photochemistry of conjugated olefins, photo-oxidation of alkenes and polyenes Photochemistry of Aromatic compounds: Isomerization, addition and substitution, photo-reduction of aromatic hydrocarbons.

Photochemistry of Carbonyl compounds: Norrish Type I and II, Intermolecular and Intramolecular hydrogen abstraction, Paterno -Buchi reaction, α and β- cleavage reactions of cyclic and acyclic carbonyl compounds, Formation of oxetane and cyclobutane from α,β unsaturated ketones, Photo-reduction of carbonyl compounds, Photo- rearrangement of enones, dienones, epoxyketones, Photo Fries rearrangement.

Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin. Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H), α-tocopherol (Vitamin E), Biological importance of vitamins.

Enzymes: Remarkable properties of enzymes like catalytic power, specificity and regulation, Mechanism of enzyme action: Proximity effects and molecular adaptation, Chemical and biological catalysis, Transition state theory, orientation and steric effects, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypeptidase A). Fischer's lock and key and Koshland's induced fit hypothesis, Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Coenzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, Lipoic acid, vitamin B_{12}. Mechanisms of reactions catalyzed by the above coenzymes.

Organic Reagents: Reagents in organic synthesis: Willkinson catalyst, Lithium dialkyl cuprates (Gilman's reagents), Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung) Dicyclohexylcarbobiimide (DCC), and Trimethylsilyliodide, DDQ, SeO_2, Baker yeast, Tri-n-butyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane. Grubbs Catalysts.

Oxidations: Introduction, Different oxidative process. Aromatiztion of six membered ring, dehydrogenation yielding C-C double bond, Oxidation of alcohols, Oxidation involving C-C double bond, Oxidative cleavage of ketones, aldehydes and alcohols, double bonds and aromatic rings, Ozonolysis, Oxidative decarboxylation, Bisdecarboxylation, Oxidation of methylene to carbonyl, Oxidation of olefines to aldehydes and ketones.

Reductions: Introduction, Different reductive processes. Reduction of carbonyl to methylene in aldehydes and ketones, Reduction of nitro compounds and oximes, Reductive coupling, Bimolecular reduction of aldehydes or ketones to alkenes, metal hydride reduction, Acyloin ester condensation, Cannizzaro reaction, Tishchenko reaction, Willgerodt reaction.

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, biosynthesis of the following representative molecules: Monoterpenoids: Citral, α-terpeneol, Farnesol (acyclic), zingiberene (monocyclic), abietic acid and β-carotene.

Alkaloids and Steroids: Classification, chemistry of nicotine, quinine, papaverine, morphine and reserpine. General biosynthetic studies on steroids, chemistry of Cholesterol, cortisone, progesterone, oestrone, transformations in steroid molecules.

Molecular Spectroscopy: Rotational spectra of non – rigid diatomic molecules and symmetric - top molecules. Anharmonic oscillator, overtones and hot bands. Diatomic vibrator – rotator (P, Q and R – branches). Rotational – vibrational spectra of symmetric – top molecules. Raman Spectroscopy. Rotational and vibrational Raman spectra of linear molecules, symmetric top molecules, overtones and mutual exclusion principle.

Kinetics of complex reactions: Consecutive and competitive (parallel) first order reactions. Kinetic vs. thermodynamic control reaction. Chain / free radical reactions; thermal ($H_2 – Br_2$) and photochemical $H_2 – Cl_2$) reactions. Rice – Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde as 3/2 or ½ order reactions. Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

Transition state theory and its kinetic and thermodynamic formulation. Potential energy surfaces (basic idea). Kinetics in solutions: diffusion controlled reactions, their rates and influence of the solvent. Kinetics of polymerization: free radical polymerization and Step – Growth Polymerization. Collisions and transition state theories in simple gas reactions, Lindman and Hinshelwood treatment.

Catalytic activity at surfaces: adsorption and catalysis, the Langmuir – Hinshelwood mechanism, the Eley – Rideal mechanism. Examples of catalysis: hydrogenation, oxidation and cracking and reforming (qualitative treatment only).

Thermodynamics: Laws of thermodynamics, Gibb's and Helmholtz free energy functions and their significance. Partial molal quantities. Partial molal free energy and its variation with temperature and pressure. Determination of partial molar volume. Carnot cycle, Thermodynamic criteria for the feasibility of the process in terms of entropy change, internal energy change, enthalpy and free energy (Gibb's and Helmholtz) change. Gibb's and Helmholtz equation and its utility in cell reaction. Thermodynamics of ideal solutions. Fugacity and activity. Graphical method for the determination of fugacity.

Chemical potential in case of ideal gases. Chemical equilibrium constant and its temperature dependence. Law of chemical equilibrium and its application. Clausius and Clapeyron equation and its application for the determination of colligative properties (depression in freezing point, elevation in boiling point and relative lowering of vapour pressure). Determination of molecular weight of non – volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Van't Hoff equation for dilute solutions and its application.

Nernst heat theorem and third law of thermodynamics and its application. Thermodynamic derivation of phase rule and its application to two component systems. Distribution law, its thermodynamic derivation and application. Zeroth law of thermodynamics.

Corrosion: causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), passivity and its breakdown. Corrosion prevention (electrochemical, inhibitor, and coating methods).

Statistical Thermodynamics: Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, The most probable distribution: Maxwell-Boltzmann distribution, quantum statistics: The Bose-Einstein statistics and Fermi- Dirac Statistics. Thermodynamic probability (W) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions, the electronic and nuclear partition functions for monatomic, diatomic and polyatomic gases.

Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, Third law of thermodynamics and entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, Einstein theory and Debye theory of heat capacities of monatomic solids.

Quantum Chemistry: Operators in quantum mechanics. Introduction to angular momentum. Eignvalues and eignfunctions. Hermitian operator. Postulates of quantum mechanics. Time dependent and time independent Schrodinger wave equations. Some analytically soluble problems (complete solutions) of particle in a one and three dimensional box, harmonic – oscillator, the rigid rotor, the hydrogen atom and the quantum mechanical tunnelling.

Quantum Mechanical Treatments of Molecular Systems: The Born-Oppenheimer Approximation. The linear combination of atomic orbital (LCAO)-approximation. Molecular orbital and Valence –Bond treatments with respect to H_2 and H^+.

Basic concept of Density Functional Theory

Huckel Molecular Orbital Theory: Huckel Molecular Orbital Theory of conjugated electron Systems (conjugated linear and cyclic hydrocarbon systems). Application to ethylene, allyl systems (radical, cation and anion), Butadiene, cyclobutadiene and benzene and their physical representations.

Adsorption at solid – gas interface: Concept of ideal and non – ideal adsorption. Heat of adsorption. Types of adsorption isotherms. Single – layer adsorption – Langmuir adsorption isotherm and its derivation. Multilayer adsorption – B.E.T. theory and its kinetic derivation. Application of BET theory in its determination of surface area of the solid. Catalytic activities at surfaces: adsorption and catalysis.

Adsorption at solid – liquid interface: Gibbs adsorption equation. Isotherms of concentration and temperature change for the adsorption in solutions. Chromatographic adsorption: column chromatography and its theory. Theory of chromatography involving one solute and several solutes.

Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape and size. Thermodynamics of micelle formation, hydrophobic effect (a qualitative view only). Aggregation at high surfactant concentration (a qualitative aspect). Surface tension and detergent, Practical application of surfactants.

Electrochemistry: Quantitative treatment of Debye - Hückel and Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution their limitations and modifications. Pair-wise association of ions (Bjerrum and Fuoss treatment). Determination of association constant (KA) from Debye – Huckel Limiting Law. Extended Debye – Huckel Law. Qualitative treatment of ion – solvent interactions (ion solvation).

Chemistry of nano – materials: Definition and historical perspective. Effect of nanoscience and nanotechnology in various fields. Synthesis of nanoparticles by chemical routs and their characterization techniques. Properties of nanostructured material: optical, magnetic and chemical properties. An overview of applied chemistry of nanometerials.

Bonding in crystals: Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory. Imperfections: Point defects (Schottky and Frankel defects). Thermodynamic derivation of these defects. Theories of Bonding: Free electro theory (a qualitative treatment) Zone theory; allowed energy zones, Brillioun zones, k – space, Fermi surfaces and density states.

Protein molecules: Protein sequence and structure (primary structure), secondary structure: Ramachandran plot, (α-helix, β-strand, β-sheet, turns and loops), torsion angles, tertiary structure (ion-ion, ion-dipole and dipole-dipole interactions), quaternary structure, globular and fibrous proteins, structure of heamoglobin and myoglobin and their physiological roles, Protein folding and refolding, Protein misfolding, Chaperones and chemical factors (Intra and intermolecular interactions) leading to folding/refolding/misfolding. Brain diseases associated with it, structure of virus.

Macromolecules: Introduction to Macromolecules, (classification and importance). Synthetic and natural polymer. Polymerization (condensation and addition reactions). Molecular forces and chemical bonding in macromolecules and their effects on the physical properties. Polymer solutions, criteria for polymer solubility, conformations of dissolved polymer chains. The Amorphous, Semicrystalline and Crystalline States of Polymers.