JGI JAIN DEEMED-TO-BE UNIVERSITY | FACULTY OF ENGINEERING AND TECHNOLOGY

Ph.D. Entrance Examination Syllabus - August 2022

Chemistry

Module I:

Crystal structure: Crystallization and fusion process, crystallography, crystal systems, properties of crystals, crystal lattice and unit cell, crystal structure analysis by X ray, The Laue's method and Bragg's method, X-ray analysis of NaCl crystal system, calculation of d and λ for a crystal system.

Electrochemical cells: Reversible and irreversible cells, EMF and its measurements, standard cells, cell reaction and EMF, single electrode potential and its calculation, calculation of cell EMF, thermodynamics of cell EMF, types of electrodes, classification of electrochemical cells with and without transference, applications of EMF measurement i) Solubility product of sparingly soluble salt, ii) Determination of pH, iii) Potentiometric titration.

Photochemistry: Introduction, thermal reactions and photochemical reactions, laws of photochemistry, quantum yield, measurement of quantum yield, types of photochemical reactions, photosynthesis, photolysis, photo catalysis, photosensitization, photophysical process, fluorescence, phosphorescence, quenching, Chemiluminescence.

Module II:

Molecular Orbital Theory: Limitations of Valence Bond theory (VBT), need of Molecular Orbital Theory (MOT), features of MOT, formation of molecular orbitals (MO's) by LCAO principle, rules of LCAO combination, different types of combination of Atomic orbital (AO's): σ, π and δ MOs, Non-bonding combination of orbitals (formation of NBMO), M.O. energy level diagram for homonuclear diatomic molecules, bond order and existence of molecule from bond order.

Ionic Solids: Crystalline and amorphous solids, crystal structures, simple cubic, body centered cubic and face centered cubic, properties of ionic solids, packing arrangements of anions in an ionic solids, voids in crystal structure, tetrahedral and octahedral, ionic radius, Pauling's univalent and crystal radii, conversion of univalent radii to crystal radii, problems based on conversion of radii, radius ratio effect, Lattice energy, Born-Lande equation, Born Haber cycle and its applications, Schottky and Frenkel defect.

Module III:

Reactions of unsaturated hydrocarbons and carbon oxygen double bond: Mechanism of electrophilic addition to C=C bond, orientation & reactivity, rearrangements, (support for formation of carbocation), addition of hydrohalogen, Anti Markownikoff's addition (peroxide effect) with mechanism, addition of halogens (dl pairs and meso isomers), hypohalous acids

(HOX), hydroxylation (mechanism of cis and trans 1,2-diols), hydroboration- oxidation (formation of alcohol), hydrogenation (formation of alkane), ozonolysis (formation of aldehydes & ketones).

Carbanions and their reactions: Reactions involving carbanions and their mechanisms: Aldol, Claisen, Dieckmann and Perkin condensations. Synthesis and Synthetic applications of Malonic ester, Acetoacetic ester and Wittig reagent.

Retrosynthetic analysis and applications: Retrosynthesis and synthesis of target molecules: Acetophenone, Crotonaldehyde, Cyclohexene, Benzylbenzoate, and Benzyl diethyl malonate.

Rearrangement reactions: Mechanism of rearrangement reaction involving carbocation, nitriene and oxonium ion intermediate. Beckmann, Bayer-Villiger, Pinacol-pincolone, Curtis, Favorski, Claisen rearrangement.

Module IV:

Electromagnetic radiation: its interaction with matter - Einstein coefficients - time dependent perturbation theory - transition probability - transition dipole moments - energy levels in atoms and molecules – Born-Oppenheimer approximation - selection rules - intensity and width of spectral lines.

Rotational spectra: Diatomic and polyatomic molecules - selection rules, rotational Raman spectra - vibrational spectra of diatomic molecules - rotational character of vibration spectra - morse potential of real molecules - selection rules - overtones and combination - Fermi resonance.

Vibrational spectra: Polyatomic molecules - harmonic and anharmonic oscillators - Morse potential - selection rules - normal modes of vibrations of polyatomic molecules - selection rules - Fourier transformation in IR spectroscopy - Raman spectroscopy – fundamentals - rotational Raman - vibrational Raman spectra - IR/ Raman instrumentation.

NMR spectroscopy: Basic principles of proton magnetic resonance - Chemical shift, Shielding and deshielding of protons, Analysis of NMR spectrum of Ethanol – spin coupling. Application of NMR in identification of simple organic molecules and basic principles of Instrumentation.

Separation techniques: Solvent extraction, chromatography - thin layer chromatography, ion exchange chromatography and size exclusion chromatography, HPLC, Gas chromatography.

Module V:

Introduction to **Nano science and Nano materials**, Nano scale and its significance-size dependent properties. Synthesis of Nanomaterials: Top down and bottom up approaches, Synthesis by Sol-gel, precipitation and chemical vapor deposition. Carbon Nanotube –

discovery, structure of carbon Nano tube – single walled Carbon Nano tube and multi walled Carbon Nano tube. Synthesis of carbon Nano tubes by Arc- Evaporation method, Laser Ablation process and purification of carbon Nanotubes. Futuristic applications of Nano materials in current, medium and long terms.

Introduction to polymers, monomer, functionality of monomers, types of polymerization – addition, condensation, cationic and anionic polymerization. Structure of monomeric units and partial structures of polymers. Plastic- preparation uses of- polythene (LDPE and HDPE) and PVC. Fibres- rayon, polyamide – Nylon 6, 6 Nylon 6, Nylon 6, 10. Urea – formaldehyde and Phenol – formaldehyde resins, polyester, rubber and elastomers- Preparation and uses of natural and synthetic rubber.