UNIVERSITY OF LUCKNOW
LUCKNOW
M.Sc. Chemistry Semester II (Core)
Inorganic Chemistry Syllabus
Paper I CH 201

Unit I

Metal ligand equilibria in solution:

Stepwise and overall formation constant, tends in stepwise constant, factor affecting the stability if metal complex with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin.

Metal Clusters:

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyls and halide clusters. Compounds with metal-metal multiple bonds

Unit II

Reaction mechanism of transition metal complexes:

Energy profile of reaction, reactivity of metal complexes, inert and labile complexes, kinetics of octahedral substitution, substitution of square planar complexes, the trans effect, mechanism of the substitution reaction, redox reaction, electron transfer reaction, outer sphere type reactions, cross reaction and Marcus-Hush theory, inner sphere type reaction

Unit III

Organometallic Chemistry:

Organoberyllium and silicon compounds: preparation stability and important reaction of transition metal alkyl and aryls. Metal carbonylsï reactions, structure and bonding, vibrational spectra of metal carbonyls for structural elucidation.

Unit IV

Infrared spectroscopy:

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, vibration of polyatomic molecules, selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factor affecting the band position and intensities, Far IR region metal ligand vibrations, normal coordinate analysis.

Raman spectroscopy:

Classical theories of Raman effect. Pure vibrational, vibrational-rotational Raman spectra, selection rule, mutual exclusion principle. Resonance Raman spectroscopy, Coherent Anti Stocks Raman spectroscopy (CARS).

Microwave spectroscopy:

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequency, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field applications.

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Unit I

Aromatic Electrophilic substitution

The arenium ion mechanism, Orientation and reactivity, energy profile diagram. The ortho / para ratio, ipso attack, orientation in other ring system, quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gatterman-Koch reaction.

Aromatic Nucleophilic substitution

The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity-effect of substrates structure, leaving group and attacking nucleophile. The Von Richter, Sommelet ï Houser and Smiles rearrangements.

Unit II

Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity.

Alicyclic halogenation (NBS), oxidation of aldehyde to carboxylic acid, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt. Sandemeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Addition to Carbon – Carbon multiple bonds

Mechanistic and stereochemical aspects of addition reaction envolving electrophiles. Nucleophiles and free radicals , regio-and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, Hydrogenation of aromatic ring. Hydroboration. Michaels reaction. Sharpless asymmetric epoxidation.

Unit III

Addition to Carbon – Hetero multiple bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, Organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Witting reaction.

Mechanism of condensation reaction involving enolates-aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Sotobbe reaction. Hydrolysis of ester and amides, ammonolysis of esters.

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Elimination Reactions

The E2, E1 and E1cB mechanism and their spectrum. Orientation of double bond. Reactivity-effects of substrates structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Unit IV

A. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant ó Jô Classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton- ^{13}C, ^{19}F and ^{31}P, FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

B. Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramers degeneracy, factor affecting the ñgò value. Isotopic and anisotopic hyperfine coupling constant, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

C. Nuclear quadrupole resonance spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient , coupling constant, splitting.

Molecular Spectroscopy

Energy level, molecular orbital, vibronic transition, vibrational progressions and geometry of the exited states, Franck-Condon principle, electronic spectra of the polyatomic molecules. Emission spectra, radiativ and nonradiativ decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

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Physical Chemistry Syllabus
Paper II CH 203

Unit I

Introduction to exact quantum Mechanical Results:

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solution of the Schrodinger equation to the some model system viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate methods:

The variation theorem, linear variation principle. Perturbation theory (first order and non- degenerate). Simple application of variation method and perturbation theory.

Molecular Orbital Theory:

Huckel theory of conjugated system, bond order and charge density calculation. Application to ethylene, butadiene etc. Introduction to extended Huckel theory.

Unit II

Angular Momentum:

Ordinary angular momentum, eigenfuctions for angular momentum, eigenvalues of angular momentum.

Electronic structure of atom:

Electronic configuration, Russell-Saunders term and coupling schemes, Slater-Condon parameter, term separation energy of p^n configuration, term separation energy for the d^n configuration, magnetic effects: spin-orbit coupling and Zeeman splitting.

Unifying Principal:

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral line, born-Oppenheimer approximation, rotational, vibrational and electronic energy level.

Unit III

Classical Thermodynamics:

Brief resume of concepts of low of thermodynamics, free energy, chemical potential and entropy. Partial molar quantities and their physical significance. Concepts of fugacity and determination of fugacity. Application of phase rule to three component system, second order phase transition.

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Non Equilibrium Thermodynamics:

Thermodynamic criteria for non ï equillibrium stat, etropy production and entropy flow, entropy balance equation for different irreversible processes (e.g. heat flow, chemical reaction etc.) transformation of generalized fluxed and forces, non equilibrium stationary states, phenomenological equation, microscopic reversibility and Onagerôs reciprocity relation, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological system, coupled reaction .

Unit IV

Statistical Thermodynamics:

Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution law (using Lgrangòs methods of undetermined multipliers.)

Partition functions- translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in the term of partition function. Application of partition function. Heat capacity behavior of solid- chemical equilibrium and equilibrium constant in the term of partition function.