CY1001: CHEMISTRY I: STRUCTURE, BONDING & REACTIVITY

Course Content:

Chemical Thermodynamics Second Law of Thermodynamics – Entropy change accompanying various processes (isothermal expansion, phase transition, heating, entropy of mixing of perfect gases); Absolute entropy and the Third Law of Thermodynamics; Statistical entropy; Spontaneity of a chemical reaction and Gibbs energy; Standard Gibbs energies of formation and reactions; Thermodynamic functions (A, G, U & H) and four fundamental equations, Maxwell relationships; variation of G with T and P, Gibbs-Helmholtz equation, Chemical potential; G versus extent of reaction ( ), Equilibrium constant through chemical potential (gas equilibria), relation between Kp & Kc; Phase equilibria, Gibbs phase rule, phase diagrams of water and carbon dioxide (supercritical H2O & CO2), Clausius-Clapeyron equation; Liquid-solid phase diagrams – two-component eutectic systems and cooling curves. Chemical Kinetics Parallel, opposing and consecutive reactions; Mechanism of complex chemical reactions; Analysing mechanisms using the steady-state approximation, Chain reactions (hydrogen-bromine reaction); Unimolecular reactions (Lindemann-Hinshelwood approach); Transition State Theory for bimolecular reactions (thermodynamic approach); Enzyme catalysis (Michaelis-Menten Mechanism). Chemisorption and Langmuir Isotherm. Basic Concepts of Quantum Chemistry Uncertainty principle; Motion of a quantum mechanical particle in one dimension; The Schrödinger wave equation for the hydrogen atom; physical meaning of a wave function, radial wave functions and probability densities, quantum numbers, wave functions and orbital shapes. Transition metal chemistry Bonding in transition metal complexes; coordination compounds; crystal field theory, octahedral, tetrahedral and square planar complexes; CFSE; Jahn-Teller theorem; Spectral, electronic and magnetic properties of coordination complexes.. Organometallic chemistry Synthesis structure and reactivity of metal carbonyls; 16 and 18 electron rules; Variety of ligands and hapticity; Type of reactions: Oxidative addition, Reductive elimination, Migratory insertion; Homogeneous catalysis, Hydrogenation, Hydroformylation, Monsanto process, Wacker process. Aromaticity Aromatic, non-aromatic and anti-aromatic compounds. Aromatic nucleophilic substitution reactions. Pericyclic reactions Definition, classifications, electrocyclic reaction of butadiene and hexatriene, photochemical [2+2] and thermal [4+2] cycloadditions, Sigmatropic rearrangements – limited to Cope and Claisen rearrangements, FMO approach – Woodward Hoffmann rules and basic stereochemistry aspects of the above reactions.

Text Books:

1. Atkin's Physical Chemistry by **PW Atkins and J de Paula**, 8th and 9th Eds., Oxford University Press.
2. Organic Chemistry by **J Clayden, N Greeves and S Warren**, 2nd Edition 2012, Oxford University Press.
3. Shriver and Atkin's Inorganic Chemistry by **P Atkins, T Overton J Rourke, M Weller and F Armstrong,** 4th Edition 2009, Oxford University Press.

Reference Books:

Nil

Prerequisite:

NIL