

Department of Theoretical and Computational Chemistry
MS in Theoretical and Computational Chemistry
Syllabus for the Admission Test (3rd Batch), Session: 2018-2019
Date of the Admission Test: 06 September, 2019; Place: Curzon Hall Auditorium

Physical chemistry

- Electromagnetic radiation: wave length, wave number, frequency and their units, calculation based on $E = h\nu$.
- Thermochemistry: enthalpy of solution, neutralization, hydration, atomization, lattice enthalpy, calculations of thermochemistry, calculations of ΔH from bond energy data.
- 1st law of thermodynamics; heat, work and internal energy; Fundamental concept of entropy(S) and free energy (G).
- Equilibrium and equilibrium constant (K_c and K_p): writing expression of K_c and K_p , units of K_c and K_p , calculation of K_c and K_p .
- Equation of state: $PV = nRT$, description and calculations.

Organic Chemistry

- Organic reactions and their mechanism: inductive effect, mesomeric effect and electrometric effect;
- Hemolytic fission: free radical; Heterolytic fission: carbocation and carbanion; Electrophiles and nucleophiles.
- Isomerism: (a) Structural isomerism: chain, position, functional isomerism, metamerism and tautomerism; Stereoisomerism: geometrical and optical isomerism.
- Reactions of alkanes, alkenes, alkyl halides, alcohols, aldehydes and ketones, carboxylic acids, amines, amino acids and proteins.
- Aromatic compounds: Benzene, aromatic halogen compounds, aromatic nitro compounds, aromatic amines, aryl diazonium salts, phenols, aromatic aldehydes and ketones, aromatic carboxylic acids.

General and Inorganic chemistry

- Atomic structure; ionization potential and electron affinity.
- Chemical bonding: ionic, covalent co-ordinate (dative covalent); Hybridization; Shape of molecules.
- Intermolecular force of attraction: dipole- dipole, ion-dipole, hydrogen bonding, dispersion force (London force). Redox reactions: oxidation number, oxidizing and reducing agents, writing and balancing redox reactions.
- Acid, base, alkali, and salts; pH, pK_a and pK_b of aqueous solution, buffer solution; solubility and solubility product. Chemistry of transition metal and metal ions: definition and electron configuration, ligand and ligand exchange reaction, coordination number.

Analytical Chemistry

- Mole calculation of acid-base reactions
- Mole calculation of redox reaction
- pH, pK_a and pK_b calculation, pH calculation of buffer solution
- Calculation of solubility and solubility product.