MANAV RACHNA INTERNATIONAL INSTITUTE OF RESEARCH & STUDIES
(Deemed to be University under section 3 of the UGC Act 1956)

Ph.D ADMISSION TEST (MR-PAT)

Ph.D. in Chemistry

Module 1: Inorganic Chemistry

1.1 Chemical periodicity, Quantum numbers, atomic orbitals, electronic configuration, Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory), Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents, Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds, Transition elements and coordination compounds: structure, bonding theories, VBT, CFT, spectral and magnetic properties, redox chemistry, Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis, Cages and metal clusters.

Module 2: Organic Chemistry

2.1 IUPAC nomenclature of organic molecules, Aromaticity in benzonoid and non-benzenoid compounds, Huckel anti-aromaticity, homo-aromaticity. PMO approach for Aromaticity, Annulenes. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction, Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes, Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways, The SN1, SN2, E2, E1 and E1cB mechanisms, Name Reaction, Grignard reaction, Wittig reaction, Cannizzaro reaction, Friedel-Crafts reaction, and Diels-Alder reaction, Reimer-Tiemann reaction, Sandmeyer reaction, Etard reaction, Balz-Schiemann reaction, Kolbe's reaction, Wurtz Reaction, Clemmensen Reduction, Swarts Reaction, Rosenmund Reduction

Module 3: Physical Chemistry

3.1 Basic principles of quantum mechanics: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta, Fundamentals of thermodynamics: System and surroundings, extensive and intensive properties' state functions, types of processes. The first law of thermodynamics - Concept of work, heat internal energy and enthalpy, heat capacity, molar heat capacity; Hess's law of constant heat summation; Enthalpies of bond dissociation, combustion' formation, atomization. sublimation. phase transition, hydration. ionization. and solution. The second raw of thermodynamics **-** Spontaneity of processes: AS of the universe and AC of the system as criteria for spontaneity. Standard Gibbs energy change and equilibrium constant.

3.2 Equilibria involving physical processes: Solid-liquid, liquid - gas and solid-gas equilibria, Henry's law. General characteristics of equilibrium involving physical processes**.** Equilibrium involving chemical processes: Law of chemical equilibrium, equilibrium constants (K_p and K_c) and their significance, the significance of ΔG and ΔG° in chemical equilibrium, factors affecting equilibrium

concentration, pressure, temperature, the effect of catalyst; Le Chatelier's principle. Ionic equilibrium: weak. and strong electrolytes, ionization of electrolytes, various concepts of acids and bases (Arrhenius and Bronsted - Lowry and Lewis) and their ionization, acid-base equilibria (including multistage ionization) and ionization constants, ionization of water. PH scale, common ion effect, hydrolysis of salts and PH of their solutions, the solubility of sparingly soluble salts and solubility products, buffer solutions.

3.3 Rate of a chemical reaction, factors affecting the rate of reactions: concentration, temperature, pressure, and catalyst; elementary and complex reactions, order and molecularity of reactions, rate law, rate constants and its units, differential and integral forms of zero and first-order reactions, their characteristics and half-lives, the effect of temperature on the rate of reactions, Arrhenius theory, activation energy and its calculation, collision theory of bimolecular gaseous reactions (no derivation), Solid state chemistry, unit cells, lattices, and symmetry, X-ray diffraction techniques, Different types of bonding in solids, including ionic, covalent, metallic, and molecular, point defects, line defects, and bulk defects in crystalline materials.

Module 4: Analytical Techniques

4.1 Qualitative and Quantitative Analysis**:** Separations, chromatography, spectroscopy, Spectroscopic Analysis: UV-Vis, IR, NMR, Mass Spectrometry. Separation Techniques: Different methods for isolating and purifying substances, including chromatography, distillation, and extraction. Solution Chemistry: Understanding the properties of solutions, including concentration units, buffer solutions, and solubility.

Module 5: Applied Chemistry

5.1 Structure and function of biological molecules, enzyme kinetics, Polymer Chemistry: Structure, properties, and synthesis of polymers, Nuclear Chemistry, Water Chemistry**:** Hardness of Water, Alkalinity of Water, Wastewater Treatment, Polymer Chemistry: Corrosion Chemistry: Factors Affecting Corrosion, Types of Corrosion, Corrosion Prevention and Control. Phase rule: One and two components phase diagram, Application of phase diagram

Suggested Readings:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Comprehensive Coordination Chemistry Eds. G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
4. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
5. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
6. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
7. Structures and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
8. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
9. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackle Academic and Professional.
10. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.