GITAM SCHOOL OF SCIENCE
Department of Chemistry
PhD in Science: Chemistry
PhD Entrance Test Syllabus - 2024-2025

PhD in Science: Chemistry

a) Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).
3. Concepts of acids and bases, Hard-Soft acid base concept, non-aqueous solvents.
4. Main group elements and their compounds: Allotropy, synthesis, structure, and bonding,
   industrial importance of the compounds.
5. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.
6. Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis.
7. Cages and metal clusters.
8. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
9. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.
10. Nuclear chemistry: nuclear reactions, fission and fusion
11. Solid state Chemistry: Crystal structures - Crystallographic point groups; Description of structures – AB, AB_2, A_2B_3, ABO_3 (perovskite) and AB_2O_4Spinelsstructures.
12. Mechanisms of Inorganic Reactions: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes. Factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism. Oxidation-reduction reactions, mechanism of one electron transfer reactions, Inner sphere, outer sphere, and mixed redox reactions.

Physical Chemistry

1. Basic principles of quantum mechanics: Postulates; operator algebra; exactly- solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.

2. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.

3. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.

4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.

5. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.

6. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.

7. Chemical thermodynamics: Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.

8. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.

9. Electrochemistry: Nernst equation, redox systems, electrochemical cells; DebyeHuckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

10. Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions

11. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.

12. Solid state: Crystal structures; Bragg's law and applications; band structure of solids. 13. Polymer chemistry: Molar masses; kinetics of polymerization.

14. Symmetry and Group Theory: Symmetry elements, Group Axioms (laws), Character table.

GANDHI INSTITUTE OF TECHNOLOGY AND MANAGEMENT (GITAM)
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OrganicChemistry

1. IUPACnomenclatureoforganicmolecules includingregio-andstereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism inacyclicandcycliccompounds;stereogenicity,stereoselectivity,enantioselectivity,diastereoselectivityandasymmetric induction.
3. Aromaticity:Benzenoidandnon-benzenoidcompounds–generationandreactions.
4. Organic reactive intermediates: Generation, stability and reactivity ofcarbocations,carbanions, freeradicals,carbenes,benzynesandnitrenes.
5. Organic reaction mechanisms involving addition, elimination and substitutionreactions with electrophilic, nucleophilic or radical species. Determination ofreactionpathways.
6. Commonnamedreactionsandrearrangements–applicationsinorganicsynthesis.
7. Synthesisandreactivityofcommon heterocyclic compoundscontainingoneortwoheteroatoms (O,N, S).
8. Structuredetermination oforganiccompounds byIR, UV-Vis,^{1}H&^{13}CNMRandMass spectroscopic techniques

Analytical Chemistry

1. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient
2. Fundamental principles and Instrumentation of the following : UV Visible spectroscopy, Atomic Emission& Atomic Absorption Spectroscopy, X-ray Fluorescence spectroscopy, Voltametry , Thermogravimetry, HPLC and GC