



# GANDHI INSTITUTE OF TECHNOLOGY AND MANAGEMENT (GITAM)

(Declared as Deemed to be University u/s 3 of UGC Act, 1956)

Visakhapatnam | Hyderabad | Bengaluru

Accredited by **NAAC** with **A++** Grade

Website: [www.gitam.edu](http://www.gitam.edu)

## GITAM SCHOOL OF SCIENCE

### PhD Entrance Test Syllabus

#### PhD in Science: Chemistry

##### a) Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and hetero nuclear 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 thermos analytical methods.
9. Bioinorganic chemistry: photosystems, porphyrins, metallo enzymes, 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<sub>2</sub>, A<sub>2</sub>B<sub>3</sub>, ABO<sub>3</sub> (perovskite) and AB<sub>2</sub>O<sub>4</sub> Spinels structures.
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.



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3. Atomic structure and spectroscopy; term symbols; many-electron systems and anti symmetry principle.
4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated  $\pi$ -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.



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#### Organic Chemistry

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
4. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
6. Common named reactions and rearrangements – applications in organic synthesis.
7. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).
8. Structure determination of organic compounds by IR, UV-Vis,  $^1\text{H}$  &  $^{13}\text{C}$  NMR and Mass 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