

The following candidates have been shortlisted to attend the written test/interview for admission to the PhD Programme in the department of **Chemistry**.

Date of the written test : 29<sup>th</sup> May 2023

Date of interview: 29<sup>th</sup> and 30<sup>th</sup> May 2023

IITT/Ph.D/July 2023/0044	IITT/Ph.D/July 2023/0061	IITT/Ph.D/July 2023/0076
IITT/Ph.D/July 2023/0078	IITT/Ph.D/July 2023/0083	IITT/Ph.D/July 2023/0116
IITT/Ph.D/July 2023/0119	IITT/Ph.D/July 2023/0127	IITT/Ph.D/July 2023/0136
IITT/Ph.D/July 2023/0143	IITT/Ph.D/July 2023/0145	IITT/Ph.D/July 2023/0161
IITT/Ph.D/July 2023/0162	IITT/Ph.D/July 2023/0172	IITT/Ph.D/July 2023/0195
IITT/Ph.D/July 2023/0219	IITT/Ph.D/July 2023/0231	IITT/Ph.D/July 2023/0245
IITT/Ph.D/July 2023/0246	IITT/Ph.D/July 2023/0255	IITT/Ph.D/July 2023/0260
IITT/Ph.D/July 2023/0267	IITT/Ph.D/July 2023/0277	IITT/Ph.D/July 2023/0296
IITT/Ph.D/July 2023/0323	IITT/Ph.D/July 2023/0324	IITT/Ph.D/July 2023/0330
IITT/Ph.D/July 2023/0333	IITT/Ph.D/July 2023/0334	IITT/Ph.D/July 2023/0356
IITT/Ph.D/July 2023/0363	IITT/Ph.D/July 2023/0377	IITT/Ph.D/July 2023/0391
IITT/Ph.D/July 2023/0399	IITT/Ph.D/July 2023/0408	IITT/Ph.D/July 2023/0409
IITT/Ph.D/July 2023/0428	IITT/Ph.D/July 2023/0440	IITT/Ph.D/July 2023/0457
IITT/Ph.D/July 2023/0468	IITT/Ph.D/July 2023/0488	IITT/Ph.D/July 2023/0503
IITT/Ph.D/July 2023/0512	IITT/Ph.D/July 2023/0546	IITT/Ph.D/July 2023/0552
IITT/Ph.D/July 2023/0553	IITT/Ph.D/July 2023/0567	IITT/Ph.D/July 2023/0585
IITT/Ph.D/July 2023/0586	IITT/Ph.D/July 2023/0608	IITT/Ph.D/July 2023/0616
IITT/Ph.D/July 2023/0626	IITT/Ph.D/July 2023/0629	IITT/Ph.D/July 2023/0630
IITT/Ph.D/July 2023/0637	IITT/Ph.D/July 2023/0643	IITT/Ph.D/July 2023/0644
IITT/Ph.D/July 2023/0646	IITT/Ph.D/July 2023/0675	IITT/Ph.D/July 2023/0691
IITT/Ph.D/July 2023/0701	IITT/Ph.D/July 2023/0705	IITT/Ph.D/July 2023/0717
IITT/Ph.D/July 2023/0721	IITT/Ph.D/July 2023/0723	IITT/Ph.D/July 2023/0735
IITT/Ph.D/July 2023/0751	IITT/Ph.D/July 2023/0769	IITT/Ph.D/July 2023/0770
IITT/Ph.D/July 2023/0777	IITT/Ph.D/July 2023/0778	IITT/Ph.D/July 2023/0783
IITT/Ph.D/July 2023/0784	IITT/Ph.D/July 2023/0785	IITT/Ph.D/July 2023/0800
IITT/Ph.D/July 2023/0824	IITT/Ph.D/July 2023/0834	IITT/Ph.D/July 2023/0845
IITT/Ph.D/July 2023/0891	IITT/Ph.D/July 2023/0907	IITT/Ph.D/July 2023/0919
IITT/Ph.D/July 2023/0935	IITT/Ph.D/July 2023/0940	IITT/Ph.D/July 2023/0952
IITT/Ph.D/July 2023/0957	IITT/Ph.D/July 2023/0961	IITT/Ph.D/July 2023/0968
IITT/Ph.D/July 2023/1005	IITT/Ph.D/July 2023/1148	IITT/Ph.D/July 2023/1170
IITT/Ph.D/July 2023/1193	IITT/Ph.D/July 2023/1197	IITT/Ph.D/July 2023/1200
IITT/Ph.D/July 2023/1211	IITT/Ph.D/July 2023/1214	IITT/Ph.D/July 2023/1231
IITT/Ph.D/July 2023/1235	IITT/Ph.D/July 2023/1249	

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**Syllabus for PhD Admission Written Test/Interview (Chemistry):**

**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, benzyne 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. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.
8. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
9. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.
10. Pericyclic reactions – electrocycloaddition, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
11. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O,N,S).
12. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.
13. Structure determination of organic compounds by IR, UV-Vis,  $^1\text{H}$  &  $^{13}\text{C}$  NMR and Mass spectroscopic techniques

**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. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
7. Organometallic compounds: synthesis, bonding and structure, and reactivity, Organometallics in homogeneous catalysis.

**8.** Cages and metal clusters.

**9.** Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.

**10.** Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.

**11.** Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.

**12.** Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

### **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  $\pi$ -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; Debye-Huckel 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.** Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.