

Syllabus for written test for Ph.D entrance Examination

Core subject (Chemical Science)

Unit-I

Inorganic Chemistry

Chemical periodicity, Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory), Chemical bonding in diatomics; elementary concepts of MO and VB theories. 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, spectral and magnetic properties, reaction mechanisms, Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications, Organometallic compounds: synthesis, bonding and structure, and reactivity, Organometallics in homogeneous catalysis, Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.

Unit-II

Physical Chemistry

Basic principles of quantum mechanics: Postulates; operator algebra; particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta, Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules. 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. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations. Chemical kinetics: Empirical rate laws and

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temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions, Solid state: Crystal structures; Bragg's law and applications; band structure of solids.

Unit-III

Organic Chemistry

IUPAC nomenclature of organic molecules including regio- and stereoisomers, Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction, Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions, Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes, Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species, Determination of reaction pathways, Common named reactions and rearrangements – applications in organic synthesis, 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, Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S), Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acid and alkaloids.

Unit-IV

Spectroscopy

Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance, Structure determination of organic compounds by IR, UV-Vis, ^1H & ^{13}C NMR and Mass spectroscopic techniques, Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.

References:

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- 10) Stereochemistry of carbon compounds - E. L. Eliel.
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Research Methodology (Chemical Science)

Unit-I

Scope, meaning, purpose and importance of research, Research process, Qualities of a good researcher, Principal elements of research, Characteristic features of research, Classifications of research, types of research, Fundamental/pure research, Application oriented research, applied research, product development, Ethics in Research, Research establishments, Research funding agencies, National and International Research awards..

Unit-II

Introduction to research problem, Components of research problem, Sources of selecting a suitable research problem, Concepts of project definition, Planning, Scope, Project progress and project status, Project management, Experimentation, Validation of results, Error identification & reduction /elimination. Type-I and Type-II errors, Standard deviation.

Unit-III

Primary and Secondary data, Sources, Advantages and Disadvantages of Secondary data, Importance of publications, Reputed Research journals of international and national level, Literature review: Concepts, Importance, Sources of literature survey, Theoretical modeling and comparison of theory and experiments, Schedule, Descriptive analysis; Tabulation, Cross-tabulation.

Unit-IV

Basics of computers, General awareness of computer Hardware i.e. CPU and other peripheral devices (input/output and auxiliary storage devices). Basic knowledge of softwares related to chemical and life science experiments and programming languages, General awareness of popular commercial software packages and other scientific application packages.

Unit-V

Publications, Quality of research work and papers –indexing, impact factor, H-Index, citation index, Meaning and principles of plagiarism, methods of plagiarism check, plagiarism checking software. Principles of intellectual property rights, patents, copyrights, trademarks and their importance, Writing PhD research proposal, Literature review, objectives, work plan, Generation of results, analysis of results.

Dr. Anshu

References

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