Central Tribal University of Andhra Pradesh
Department of Chemistry

Syllabus for Research (PhD) Admission Test

PART-A: RESEARCH METHODOLOGY IN CHEMISTRY

Basic Concepts of Research

Covers the definition, scope, and objectives of research, along with the classification of research types such as descriptive versus analytical, applied versus fundamental, quantitative versus qualitative, and conceptual versus empirical. It outlines the difference between research methods and methodology, along with steps in identifying and defining a research problem. The process of conducting a literature review is discussed using both conventional and digital tools, including academic databases like Google Scholar, SciFinder, Scopus, and PubMed. It also explores various research settings including library-based, field-based, and laboratory-based investigations.

Data Collection and Documentation of Observations

Focuses on principles of experimental design and appropriate sampling techniques used in chemical research. It includes methods for accurate recording of observations in laboratory notebooks and electronic lab records. Techniques for data tabulation and graphical representation are incorporated using tools such as MS Excel, OriginLab, and GraphPad. Documentation practices also extend to scientific imaging, including the use of scale bars in microscopy and standardized methods for field photography to support observational data.

Ethics, Good Practices, and Scientific Writing

Addresses core principles of ethical research conduct, including issues of fabrication, falsification, plagiarism, and academic integrity. Guidelines related to authorship, acknowledgements, reproducibility, and ethical approval processes are outlined. Conventions of scientific writing are emphasized, including proper use of nomenclature, units, and standardized formatting. The unit includes structured instruction on preparing abstracts, full-length research papers, laboratory reports, and theses. Referencing and citation practices are explained using standard styles such as ACS, APA, and MLA, with practical exposure to tools like Zotero and Mendeley. Presentation formats such as PowerPoint slides and scientific posters are also incorporated, along with the use of plagiarism detection software.

Applications of Research in Chemistry

Highlights major research areas within chemistry including analytical, organic, inorganic, physical, environmental, pharmaceutical, and green chemistry. The interdisciplinary nature of chemistry is examined through its applications in materials science, biology, medicine, and engineering. Activities include conducting experiments based on chemical calculations, developing posters on specific research topics, and engaging in technical writing on emerging trends and innovations. Emphasis is placed on identifying different types of research encountered in everyday life and analyzing real-world chemical processes. The unit concludes with training in the composition and formatting of research proposals, including structuring objectives, methodologies, timelines, budgets, and literature integration.

PART-B: CHEMISTRY SYLLABUS

Inorganic Chemistry:

- Chemical periodicity
- 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, 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.
- Cages and metal clusters.
- Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
- Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.
- Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.
- Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

Physical Chemistry:

- 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.
- Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
- Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
- Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.
- Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
- Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.
- 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 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.
- Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.
- Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
- Polymer chemistry: Molar masses; kinetics of polymerization.
- Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

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, benzynes 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.
- Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
- 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.
- Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
- 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 acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.
- Structure determination of organic compounds by IR, UV-Vis, 1H & 13C NMR and Mass spectroscopic techniques.