



## Ph.D Entrance Test Syllabus Session: 2024-25 Chemistry

## Part A: Research Methodology

**Part B : Chemistry** 

### Part-A

### **Research Methodology**

**Unit – I:** Research Methodology: Research: Objectives and motivation; Research types Approaches, Methodology and Process of Rsearch : Steps involved, Data collection, Data processing ; Qualitative and Quantitative analytical / statistical methods involved in research. Research Ethics - Ethical issues and Environmental impact aspects, Commercialising research – Copy right , Intellectual property rights and patent law .

**Unit – II:** Structure and components of scientific reports - Types, Steps, Layout and structure; Illustrations and tables - Bibliography, referencing and footnotes – Reproduction of published material – Plagiarism - Citation and acknowledgement - Reproducibility and accountability. General idea about Citation, Citation Index, Impact factors of journals etc. General idea about: Seminars; Symposia; Workshops; Conferences. Making deliberations (Oral presentation) – Planning – Preparation and Making presentation – Use of visual aids - Importance of effective communication –.

**Unit** – **III:** Quantitative approaches in research methodology: Statistical tools and approaches accuracy and precision, testing confidence limits, Linear, non-linear, multiple variable correlations, idea of matrix and its analysis, drawing of good fit lines, slopes, correlation coefficients and their significance.

**Unit** –**IV:** Basic Instrumentation: Detectors: sensor and transducers, types – pressure, optical, flow meter, acclrometers and inclinometers, temperature sensors, chemical sensors etc; sensor networking, Instruments- conventional, microprocessor based systems and Computer Aided (CAA) instruments – brief introduction of packages, tailoring of plots.

**Unit** – V: Using Computers: Using Excel and Origin for graphical representations and statistical analysis, idea of SPSS (and/or Matlab). Basics of Molecular modelling and molecular force fields, brief introduction to QSAR, Applications of SAR and in Combinatorial Spectral analysis, Searching scientific atricles using internet and search engines, url, (making use of Power-point / Flash / Video (moviemaker) for making deliberations)



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# Part-B Chemistry

#### **Unit – I Organic Chemistry**

1. IUPAC nomenclature of organic molecules.

2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic

compounds.

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.

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.

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.



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### Unit –II: 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.

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.

### Unit –III: 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.

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 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; conduct metric 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