

Department of Studies and Research in Chemistry
Karnataka State Open University
Mukthagangothri, Mysore-6

Course: Ph.D.

Subject: Chemistry

Syllabus for Ph.D. Course work and Entrance exam

Paper-I

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.

References

- 1) Booth W. C. Colomb and G.G Williams. (2005) The Craft of Research, Chicago University Press.
- 2) William M. K and Trochim. (2003) Research Methods, 2nd Ed, Biztantra Publications.
- 3) Jonathan Grix. (2004) The Foundation of Research, Palgrave Study Guides.
- 4) Wisker Gina. (2001) The Post Graduate Research Handbook, Palgrave
- 5) Rugg G. and Petre M. (2004) The Unwritten Rules of Ph.D research, Open University Press.
- 6) Bruce M Cooper (1979) Writing Technical report. Penguin Books.
- 7) Judith F Olson, Writing Skills Success. Goodwill Skill Builders Series, Goodwill Publishing House, New Delhi.
- 8) Craig Harkins & Daniel L Plung, Eds. (1982) A Guide for Writing Better Technical Papers. IEEE Press.
- 9) Robert A. Day (1998) How to Write and Publish a Scientific Paper. Oryx Press.
- 10) Kothari C.K. (2004) 2/e, Research Methodology – Methods and Techniques (New Age International, New Delhi)
- 11) S.K. Verma and M. Afzal Wani (Eds.) Legal Research and Methodology, ILI Publication 2nd Ed 2001 (2015 Reprint)
- 12) Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
- 13) Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
- 14) Anthony M Graziano and Michael L Rau, Research Methods: A Process of Inquiry, Prentice Hall, 2006.
- 15) Peter C Jurs, Computer Software Applications in Chemistry, 2nd Ed., John Wiley & Sons, New York, 1996

Paper-II

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

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 & ¹³C 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:

- 1) Comprehensive Inorganic chemistry, J. C. Bailar, H. J. Emeleus, Sir R. Nyholm, R. F. Tortman- Dickenson (Pergamon Press, 1973) Volume 1 to 5.
- 2) Physical methods for chemists R.S. Drago (Saunders Co. 1992).
- 3) Inorganic Material Chemistry, M. T. Weller (Oxford, 1994).

- 4) Catalysis : Principles & Applications, B. Vishvanathan, S. Sivasankar and A.V. Ramaswamy (Narosa Publication House, New Delhi 2004).
- 5) Advanced Organic Chemistry, Fourth Edition, Part A and B F.A.Carey and R.J.Sundberg.
- 6) Organic Chemistry, Clayden, Greeves,Warren and Wothers.
- 7) Advanced organic chemistry by J. March, 6th Ed.
- 8) Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
- 9) Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons.
- 10) Stereochemistry of carbon compounds - E. L. Eliel.
- 11) Organic synthesis – M. B. Smith.
- 12) Quantum Chemistry by Ira. N.Levine; Prentice Hall; 7th Ed 2013.
- 13) Quantum Chemistry by John. P. Lowe, Kirk. Peterson; Academic Press; 3rd Ed. 2005.
- 14) Chemical Kinetics and Reaction Dynamics by Paul L Houston, Dover Publications 2006.
- 15) Physical Chemistry by G. M. Barrow, McGraw Hill, New York, 1996.
- 16) Fundamentals of Physical Chemistry by Maron and Lando.
- 17) Physical Chemistry by P. W. Atkins, ELBS, London, 4th Ed, 1990.
- 18) A Text Book of Physical Chemistry by Samuel Glasstone, McMillan, London.