

**SYLLABUS
FOR THE
Ph.D. COURSE WORK
IN
CHEMISTRY**

(with effect from 2020-2021 session)



**DEPARTMENT OF CHEMISTRY
UTKAL UNIVERSITY
Bhubaneswar 751 004, Odisha**

PREAMBLE

Every student admitted to the Ph.D. programme in the Department of Chemistry has to undertake course work and as per the UGC/University guidelines, a student can formally register for the Ph.D. programme, only on satisfactory completion of the coursework requirements.

PROGRAM OBJECTIVES

1. To gain knowledge on importance of research with systematic approach to pursue a research problem.
2. To acquire advanced knowledge and skill in modern research methods and techniques.
3. To provide hands-on training and generate expertise in modern instrumentation techniques.
4. To generate independent researchers that will be suitable for both industry and academia.
5. To create a pool of students with enhanced research competency and skill to undertake research in chemical sciences.

OUTCOMES

On successful completion of the programme the student will:

1. Gain the knowledge of types of research, research tools and methodology as well as have the ability to frame a research problem independently.
2. Acquire the basic computational techniques of data analysis.
3. Have enough basic knowledge in modernized and specialized fields of Chemistry.
4. Hand on training on different equipment, interpretation of the results and their use while pursuing research.
5. Learn the art of systematic writing of research papers, dissertation, bibliography and presentation of results in different forms.

STRUCTURE OF Ph.D. COURSE WORK IN CHEMISTRY

- (a) The duration of the Ph.D. course work shall be of ONE Semester (6 months).
- (b) The credit assigned to the Ph.D. course work, consisting of 4 (four) courses, is 18 credits and distributed as follows:

Paper code	Course title	Marks	Credit
CH-701	Research methodology	100	4
CH-702	Techniques in Chemical Research-I	100	4
CH-703	Techniques in Chemical Research-II	100	4
CH-704	Dissertation and Seminar	100	6
	Total	400	18

The written examination of papers CH-701, CH-702 and CH-703 shall be held at the end of the course. For paper CH-704, the students are required to submit a review based on work in a particular area for evaluation prior to theory examination and present the same after the theory examination.

The pass mark for the examination is 40% in aggregate as per University rules.

CH-701 RESEARCH METHODOLOGY

Credit – 4

Marks- 100

Course objectives:

1. To train the on different aspects of research methodology such as formulation of research aims and objectives; research ethics and plagiarism, systematic literature survey and use of online scientific databases, writing of scientific papers, patent, theses etc.
2. It will facilitate the students in understanding the tools and techniques of presenting the research findings in different forms and forum.
3. To inculcate knowledge of scientific methodology in analysing research data.
4. To acquaint the students with chemistry related software and their use.

Course Outcomes:

On completion of this course the students will be able to:

1. Understand the aims and objectives research and formulate a research work plan in a scientific manner.
2. Design appropriate experiments, collect and interpret the data to validate their experiments.
3. Obtain and evaluate information from a variety of databases.
4. Analyse the data using basic computer software.
5. Communicate effectively in a variety of forms like research publications, patents, etc. and presentation of research findings.

UNIT- I

Introduction to research, Objective of research, types of research, significance of research, Research methods vs. methodology, research processes, formulating research problem, criteria of good research, ethics in research.

Reporting practical and project work, organizing a poster display and oral presentation.

UNIT- II

Scientific writing

Writing scientific papers, justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism, writing of thesis, patent law, filing of patent.

Literature survey-I

Print resource: Primary sources (Journals and patents), Secondary resources (abstracts, CA, Beilstein, compendia and tables of information current contents, collective indexes, reviews, awareness service, general treatise, monographs on specific areas, reference books),

UNIT- III

Literature survey-II

Web resources, Journal access through web – Digitized and digital formats, E-journals, E-books, E-consortium, UGC infonet, Online and Digital libraries, Useful web links: Scifinder, Scopus, Scirus, Science Direct. Citation index, Impact factor, H-index, Internet discussion groups and communities, Blogs, Preprint servers, Sharing documents online, Online

submission system, Tracking manuscript status, End-note and SciProof, Digital object identifier (DOI), Hot articles.

UNIT- IV

General Safety Measures in Research and handling of chemicals

General safety in laboratories, Safety equipments, Responsibility for accident prevention: Personal protection, laboratory protocol. Hazardous Chemicals: classification, toxicity, safe storage and handling, flammable or explosive hazards. Compressed gas and fire safety. Medical emergency accident reporting. Safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals. Disposal of explosives, biological and radioactive wastes.

Unit-V

Computer applications in chemistry

Computer technique used in chemistry with special reference to UV-Visible spectroscopy, chromatography, mass spectroscopy, crystallography, NMR. Computer Softwares used in chemistry: ArgusLab, molden, CYLView, Discovery studio, Gaussian, Gauss View, Chem Craft and Mercury softwares.

Applications of some common computer packages (MS-Excel, Origin, Chem draw, Chem-sketch) to chemistry.

Books Recommended

1. Research Methodology – Methods & Techniques, C.R. Kothari, Wiley Eastern Ltd, New Delhi 1985.
2. Research Methodology – A Step by step Guide for Beginners 2nd edn Kumar Ranjit, Pearson Education, Singapore, 2005.
3. Introduction to Research & Research Methodology M. S. Sridhar.
4. Matthias Otto, Chemometrics – Statistics and Computer Applications in Analytical Chemistry, Wiley – VCH, 1999.
5. S.K. Pundir and A. Bansal Pragati, Computer for Chemists, S.K. Pundir and A. Bansal Pragati Prakashan 2008.
6. G.Grant and W. Richards, Computational Chemistry, Oxford University press.
7. Combined Quantum Mechanical and Molecular Mechanical Methods, J. Gao and M. A. Thompson, ACS Symposium Series 1997.

CH 702 TECHNIQUES IN CHEMICAL RESEARCH-I

Credit – 4

Marks- 100

Objective: The primary objective of this course is to familiar the students with the conventional and updated methodologies/techniques for synthesis of coordination and organometallic compounds, organic compounds, different types of materials including nano and polymer materials.

Outcome: After completion of the course the student will

1. Learn the techniques of synthesis of different kinds of compounds (coordination, organometallic, organic compounds with greener approach) and materials/composite.
2. Adopt some of the techniques in future course research.

Unit-I

General methods of synthesis of metal complex complexes and organometallic compounds

Synthesis of transition metal complexes by substitution reactions, redox reaction, addition/dissociation, reaction of coordinated ligands, self-assembly, second sphere coordination.

Purification of metal complexes, growth and isolation of single crystal.

Synthesis of organometallic compounds

Synthesis of organometallic complexes by ligand substitution reaction, oxidative addition and reductive elimination reaction, insertion and elimination reaction, nucleophilic and electrophilic addition reaction.

Precaution / techniques in synthesis of organometallic compounds: handling moisture and air sensitive compounds, use of Schlenk technique, glove box and low temperature method.

Unit-II

Green organic synthesis

Principles of green synthesis, Green solvents for organic synthesis: ionic liquids, super critical fluid extraction. Organic synthesis using water resistant Lewis acids.

Solid phase and solvent free synthesis, synthesis by ball milling processes. Ionic liquids mediated synthesis. Microwave assisted organic synthesis: the reaction vessel, medium, advantages, limitations and application. Ultrasound in organic synthesis: Introduction, instrumentation, types of sonochemical reactions, esterification, substitution, oxidation, reduction.

Unit-III

General methods of material synthesis:

Precipitation, co-precipitation, sol-gel, hydrothermal, impregnation, solid state reaction techniques with examples.

Green synthesis techniques: Microwave and ultrasound methods with examples.

Unit-IV

Nanomaterials – General synthetic approaches and applications

Properties of materials, General methods of synthesis: Sol-gel, coprecipitation, thermal, hydrothermal etc

Nanomaterials: Basic ideas, Properties of materials, General method of synthesis: Top down processes - Milling, lithography, Bottom-up process - Vapour phase deposition methods, plasma-assisted deposition process, electrodeposition, liquid phase methods: coprecipitation, sol-gel, microemulsion methods with examples. Types of nanoparticles: Zero dimensional (0-D) 1D, 2-D, 3-D, Forms of nanomaterials (e.g powder, film/coating, composite, nanoporous, nanoclusters etc General applications of nanomaterials

Unit-V

Polymeric materials

Mechanism and kinetics of coordination and ring opening polymerization process. Solid Polymer electrolytes (SPE), Dendritic Polymers and their Potential Applications. Polymer for sensing applications, Synthesis of advanced polymers (Kevlar, PEEK, Silicone rubber) and polymer hydrogel. Polymer colloids (liquid polymers).

Composite materials

Basic idea of composites, alloys, blending, matrixes and reinforcements materials, carbon-carbon composites, biocomposites, nanocomposites, fabrication of fiber reinforced and polymer reinforced composites and their potential applications, Processing of composites, environmental effect on composites.

Books Recommended

1. Inorganic and Bioinorganic Chemistry, Vol. II, Synthesis and spectroscopy of transition metal complexes, A. Bianchi et al.
2. R.H. Crabtree, The Organometallic Chemistry of Transition Metals, Wiley International Publications.
3. Solid State Chemistry, A. R. West, Wiley
4. Understanding Solids, the chemistry of Materials, R.J. Tilley, Wiley
5. Kelsall Robert W, Ian Hamley and Mark Geoghegan, Nanoscale Science and Technology, Wiley Eastern, 2004.
6. Bharat Bhushan, "Springer Handbook of Nanotechnology", 2004.
7. Charles P Poole, Frank J Owens, "Introduction to Nanotechnology", John Wiley and Sons, 2003.
8. Principle of Nanotechnology, G. Ali Mansoori, World Scientific (2005).
9. Su WF. (2013), Principles of Polymer Design and Synthesis, vol 82. Springer, Berlin, Heidelberg.
10. J.R. MacCallum, C.A. Vincent, Polymer Electrolyte Reviews, Volume 2, Springer Science & Business Media
11. P. Ghosh, Polymer Science and Technology: Plastics, Rubbers, Blends and Composites, Tata MacGraw-Hill Publishing company limited, New Delhi.
12. Natural Fibre Reinforced Polymer Composites: From Macro to Nanoscale: edited by Sabu Thomas, Laly A. Pothan (2008), Old City Publications, Philadelphia, USA
13. Basic Organometallic Chemistry, University Press, B.D. Gupta and A.J Elaias. (2016)

CH-703 TECHNIQUES IN CHEMICAL RESEARCH-II

Credit – 4

Marks- 100

Objective:

1. To familiarize the students with different techniques of characterization of compounds and materials.
2. To help the student to understand basic/working principles, instrumentation, collection and interpretation of data of X-ray diffraction, Microscopic, spectroscopic and electroanalytical techniques.

Outcome: After completion of the course the student will be able:

1. To select the appropriate technique for characterization of compound and materials.
2. Hand on experience in some these instruments
3. To collect the data/spectra/images and analyse the results

UNIT I

X-ray techniques for materials characterization

X-ray diffraction: Properties and generation of X-rays, Principle, Crystal system, X-Ray methods, XRD pattern, peak position, peak width, effect of particle size, peak intensity
X-ray fluorescence: Principle, instrumentation and their applications.

UNIT II

Microscopic techniques

Principles, instrumentations and applications of Optical microscope, Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM). Basic principles of atomic force microscopy (AFM)

UNIT III

Spectroscopic methods-I

Principle, instrumentation and applications of UV-Visible Diffuse Reflectance (UV-Vis DRS) spectroscopy, Fluorescence spectroscopy.

Optical Rotary Dispersion and Circular Dichroism: Introduction, principles, Cotton effect, Octant rule, applications in determining the absolute configuration of metal complexes

UNIT IV

Spectroscopic methods-II

High resolution NMR: Pulse excitation, signal detection, sampling, FID and theory of FT NMR, Relaxation mechanisms-dipole-dipole, chemical shift anisotropy, spin-rotation and quadrupole relaxation..

Analysis of organic compounds by ^1H and ^{13}C -NMR, Introduction to ^{31}P and ^{19}F NMR.

Mass spectroscopy: Introduction to soft ionization techniques and illustrative examples of macromolecular and supramolecular chemistry.

Unit-V

Electroanalytical Techniques

Linear sweep voltammetry, Cyclic Voltammetry, Reversibility, Differential pulse voltammetry, Electrochemical sensors, ion-sensitive electrodes, glass-membrane electrodes, Introductory idea on gas sensors.

Books Recommended

1. Principles and Practice of Analytical Chemistry F.W. Fifield, 5th edn, Blackell Publications.
2. Elements of X-Ray Diffraction- B.D. Cilluty
3. Solid state chemistry- A.R. West
4. Basic one and two-dimensional NMR spectroscopy, Horst Friebolin, 5th Edition, Wiley-VCH, 2011.
5. High resolution NMR techniques in organic chemistr, T.D.W. Claridge, 2nd edition, Elsevier, 2009.
6. Fundamentals of Analytical Chemistry - D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch.
7. Organic Spectroscopy- W. Keemp.
8. Fundamental concepts of Inorganic Chemistry, Asim K. Das, CBC Publication (Vol 7).

CH-704 DISSERTATION AND SEMINAR

Credit – 6

Marks- 100

Objective:

1. To develop the skill to write dissertation report in a specific topic of research interest with complete follow up of research methodology.
2. Critical analysis of published results.
3. To develop communication skill in presentation.

Outcome: After completion of this course the student will:

1. Improve ability to find the research gap in a specific topic and formulate the research problem to carry out.
2. Enhance the competency level on collection of appropriate literature, reading, synthesizing the findings, for writing of a review/research article.
3. Learn to communicate the article to journal for publication.