



Course Structure & Syllabus of Ph.D. Course Work



Effective from
Academic Session 2025-26

Department Of Applied Sciences & Humanities (Chemistry)
Faculty of Engineering & Technology

Khwaja Moinuddin Chishti Language University
Sitapur-Hardoi Bypass, IIM Road, Lucknow - 226013



STRUCTURE OF Ph. D. Chemistry COURSE WORK

| S. No | Course Code | Course Name | Credit |
|-------|------------------|--|-----------|
| 1. | PHDCHM 101 | Research and Publication Ethics (Common for all the departments) | 2 |
| 2. | PHDCHM 102 | Computer Applications and IPR in Chemistry | 2 |
| 3. | PHDCHM 103 | Research Methodology | 4 |
| 4. | PHDCHM 104A-104D | Subject Specific Course * | 4 |
| | | Total Credits | 12 |

Evaluation Scheme:

| Course Code | Course Name | L | T | C | IA | ESE | Tot. |
|------------------|--|---|---|-----------|----|-----|------------|
| PHDCHM 101 | Research and Publication Ethics | 2 | | 2 | 30 | 70 | 100 |
| PHDCHM 102 | Computer Applications and IPR in Chemistry | 2 | | 2 | 30 | 70 | 100 |
| PHDCHM 103 | Research Methodology | 3 | 1 | 4 | 30 | 70 | 100 |
| PHDCHM 104A-104D | Subject Specific Course* | 3 | 1 | 4 | 30 | 70 | 100 |
| | Total Marks | | | 12 | | | 400 |

* Select one course from the available Subject Specific Course (Elective courses: **PHDCHM 104A-104D**).

L: Lecture, T: Tutorial, C: Credit, IA: Internal Assessment, ESE: End Semester Examination.

Subject Specific Course:

It will be an optional course and each student is required to select one course from the available Subject Specific Courses (electives courses) (recommended by department) as per the advice of supervisors. Concern supervisors will be the overall evaluation in-charge of his/her course.

- PHDCHM 104A**- Advances in Medicinal & Organic Chemistry
- PHDCHM 104B**- Biosynthesis of Natural Products and Contemporary Heterocyclic Systems
- PHDCHM 104C**- Advanced Physical Chemistry
- PHDCHM 104D**- Advanced functional materials
- Any Swayam/NPTEL/MOOC Courses (Optional)- Available at the commencement of the Course Work.



Ph.D Chemistry Coursework Syllabus w.e.f. (2025-2026)

PHDCHM 101: RESEARCH AND PUBLICATION ETHICS (AS ANNEXURE-1)

PHDCHM 102: COMPUTER APPLICATION

**Maximum Marks:100
Credit: 02, IA Marks: 30, ESE Marks: 70**

Course Objectives:

1. To equip students with a foundational understanding of computer systems
2. To understand the operating systems, and essential software applications.
3. to gain practical skills in using Microsoft Word and Excel.
4. To understand basic concepts of data communication, networking, and internet technologies.

Unit-I

Computer Basics and Application Introduction to basic software

computer, Input/Output devices, Characteristics of Computers, Applications of Computer, Types of computers, Mini Computer, Micro Computer, Mainframe Computer, Basics computer applications understanding: MS, Microsoft Power Point, Microsoft Excel, Microsoft Access, Primary and secondary memory, Hardware and software, Overview of windows, Unix etc., File management, Different File formats, Introduction to Chemistry related software: Gaussian, Gaussview, ChemDraw, TopSpin etc.

UNIT-II

Intellectual Property Rights (IPR) in Chemical Sciences:

Introduction to IPR: concepts, importance, and categories. Patents: criteria of patentability, novelty, inventive step, industrial applicability, Patent specification drafting basics for chemical inventions, Patent databases. Copyrights, trademarks, trade secrets relevant to scientific research.

UNIT-III

MS Word: Tabulation, insertion, deletion of tables, images, and equations of chemical compounds, Saving and opening existing documents, references etc., Microsoft Power Point: designing presentation, scientific reports, poster, mail merge etc., Microsoft Excel: Data entry, tabulation, and basic formulas, Graphs: Bar, Pie-chart etc., trendlines, and statistical functions (Sum, mean, SD, regression etc), Microsoft Access

UNIT-IV

Introduction to Networking, LAN, MAN, WAN, WWW: Internet vs Intranet, Multimedia and Types of media, Browser, URL, Web page, Email, Usage of Webs as a tool for scientific literature survey.

Recommended Books:

1. Fundamental of Computers – By V.Rajaraman B.P.B. Publications
2. Fundamental of Computers – By E. Balagurusamy, McGraw Hill Education.
3. Introduction to Computers and C Programming – By D.S. Yadav & S.K. Bajpai, New Age Publication.
4. Fundamental of Computers – By P.K. Sinha
5. Computer Concepts – By Vikas Gupta, Dreamtech Press



Ph.D Chemistry Coursework Syllabus w.e.f. (2025-2026)

PHDCHM 103: RESEARCH METHODOLOGY

Maximum Marks: 100

Credit: 04, IA Marks: 30, ESE Marks: 70

Course Objectives

1. **Understand laboratory safety and chemical hazards** – Gain awareness of the toxicity, explosive nature, and harmful effects of chemicals commonly used in research laboratories, and apply appropriate safety precautions and handling procedures.
2. **Develop academic integrity** – Understand plagiarism guidelines, learn methods to prevent plagiarism, and uphold ethical practices in academic and research work.
3. **Apply purification and separation**
4. **Analyze and interpret experimental data**
5. **Prepare scientific research reports** – Understand the proper format, structure, and style of writing research reports, and learn the correct methods for citation, referencing, and preparing bibliographies.

Unit-I

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedures, personal protective equipment's, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous and pyrophoric chemicals, flammable or explosive hazards, procedures for working with cryogens, Good Laboratory Practices, Storage and disposal of chemical wastes (aqueous, organic and radioactive wastes), incineration and transportation of hazardous chemicals.

Unit-II

Purification Techniques:

A brief knowledge about various techniques such as, reaction monitoring and work ups, distillation, fractional distillation, crystallization, fractional crystallization.

Chromatography:

- Column
- TLC
- Paper
- Gas Chromatography
- Ion Exchange
- HPLC

- Gel permeation

Unit-III

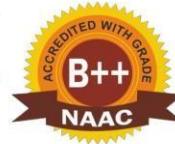
Literature Survey: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples. Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Search engines, Scirus, Google Scholar, Chem-Industry, Wiki- Databases, Chem-Spider, Science Direct, Sci-Finder, Scopus.

Unit - IV

Scientific Writing: Scientific Document; Organization and writing of research paper, short communications, review articles, monographs, technical and survey reports, authored books, and edited books and dissertation. Writing ethics. Avoiding plagiarism, references and bibliography.

Recommended Books:

1. C. R. Kothari, Research Methodology: Methods and Techniques, New Age International, New Delhi, 2004.
2. Justin Zobel, Writing for computer Science, Third Edition, Springer, 2014.
3. Kumar R. Research Methodology: A Step by Step Guide for Beginners, 3rd ed., Pearson Education, 2010.
4. Ranjit Kumar, “Research Methodology: A Step by Step Guide for Beginners”, 2/e, Pearson India, 2005.
5. Michael P. Marder, Research Methods for Science, Cambridge University Press, 2011.
6. P. Oliver, Writing Your Thesis, New Delhi: Vistaar Publications, 2004.
7. Gregory, Ethics in Research, Continuum, 2005.
8. C. Radhakrishna Rao, Statistics and Truth, CSIR, 1989.
9. Sheldon M Ross, Introduction to Probability and Statistics for Engineers and Scientists, Elsevier, 2010.
10. RA Day, How To Write and Publish a Scientific Paper, Cambridge University Press, London, 1992.
11. B. Latour, Woolgar., Laboratory Life: The Construction of Scientific Facts, 2nd Edition, Princeton: Princeton University Press, 1986.
12. S.K. Yadav, “Elements of Research Writing”, UDH Publishers & Distributors, Pvt. Ltd. New Delhi, 2015.
13. Douglas C. Montgomery and George C. Runger, “Applied Statistics & Probability for Engineers”, 3rd ed, Wiley India, 2007.
14. Bernard P. Zeigher, Herbert Praehofer, Tag Gon Kim, “Theory of modeling and simulation integration discrete event and continuous complex dynamic systems”, Academic, 2000.



Ph.D Chemistry Coursework Syllabus w.e.f. (2025-2025)

SUBJECT SPECIFIC COURSES (CHOOSE ONE)

PHDCHM104A- Advances in Medicinal & Organic Chemistry

Maximum Marks:100

Credit: 04, IA Marks: 30, ESE Marks: 70

Unit I

Introduction to Medicinal Chemistry

Role of Medicinal Chemists, Medicines, Drug targets: Enzyme, Receptors, Carrier proteins, Structural proteins, Nucleic acids, Lipids, Carbohydrates. Pharmacokinetics of Drug: Absorption, distribution, metabolism, excretion, administration, dosing of drug. Biological testing, Current trends in Drug discovery: The lead compound, Natural and Synthetic sources of lead compounds.

Unit II

Computer Aided Drug Design

Molecular and Quantum Mechanics in drug design, Energy Minimization Methods, Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra precision docking. Definition of structure-activity relationships (SAR), Binding interaction, The pharmacophore. Quantitative Structure Activity Relationships (QSAR). Physicochemical parameters and methods to calculate physicochemical parameters.

Unit-III:

Modern Synthetic Methodologies

Transition-metal catalysis: Pd, Ni, Cu catalyzed C–C and C–X bond formations, C–H activation and functionalization strategies, Skeletal editing: C–C, C–N, C–O bond reorganization approaches, Asymmetric catalysis: organocatalysis, biocatalysis, chiral transition-metal catalysts and radical-mediated organic transformations, Multicomponent reactions (MCRs) and cascade/one-pot methodologies

Unit-IV

Sustainable Organic Synthesis and Spectroscopic Technique

Introduction to Principles and concepts of green chemistry. Approaches for green: synthesis/reaction: Green starting materials, Green solvents: Aqueous medium, Ionic liquids, Solvent free reactions. Green metrics: atom economy, E-factor, process mass intensity (PMI), Recent advances in Electrochemical & photocatalytic synthesis and mechanochemistry.

Interpretation of spectra of compounds based on UV-Visible, IR, Mass and NMR spectroscopy

Recommended Books:

1. Fundamentals in medicinal chemistry- G. Thomas. 2nd edition
2. Introduction to medical Chemistry, G. L. Patrick
3. Medicinal Chemistry & Drug discovery- Burger (Volume 1-6)
4. Organic chemistry (McGraw-Hill series in chemistry) 4th Edition-by Stanley H. Pine
5. Organic Chemistry-by Jonathan Clayden, Nick Greeves, Stuart Warren, Peter Wothers. (Oxford)



PHDCHM104B

Biosynthesis of Natural Products and Contemporary Heterocyclic Systems

Maximum Marks:100

Credit: 04, IA Marks: 30, ESE Marks: 70

Unit-I

Biosynthesis of Natural Products Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of biosynthetic precursors,

Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin) and carotenoids, steroids – cholesterol

Unit-II

Nonaromatic Heterocyclics & Aromaticity

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and thietanes Aromaticity: Introduction, Aromatic and antiaromatic compounds. Criteria for aromaticity. Huckel's $4n+2\pi$ electron rule for benzene and non benzenoid aromatic compounds. E.g. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

Unit-III

Synthesis, Reactivity, Aromatic character and Importance of Heterocyclic Compounds

Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole. OC (CB1) 19:

Unit-IV

Heterocyclic compounds with more than two Hetero Atoms

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3- triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

Recommended Books :

1. I. L. Finar: Organic Chemistry (Vol. I & II), E. L. B. S.
2. R. T. Morrison & R. N. Boyd: Organic Chemistry, Pearson Education.
3. Arun Bahl and B. S. Bahl : Advanced Organic Chemistry, S.Chand
4. Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.



PHDCHM104C- Advanced Physical Chemistry

Maximum Marks:100

Credit: 04, IA Marks: 30, ESE Marks: 70

Unit-I

Advanced Surface Chemistry

Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film of liquids (electro-kinetic phenomenon), catalytic activity at surfaces and their mechanism, Various adsorption isotherms models including two, three, four, and five parameters. Giles classification of Adsorption isotherms shapes. Activated carbon properties, adsorption capacity, iodine number, molasses number, product density, mesh size ash content, IUPAC classification of macro-meso-and micro-porous materials (pore size distribution), and industrial applications of adsorption.

Unit-II

Colloids and Surface Phenomenon

Surface active agents, Classification of Surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Kraft temperature, factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellezation, mass action method and phase separation model of micellezation, solubilization, micro emulsion, reverse micelles, surface films. Surface characterization: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XRD, SEM etc.

Unit-III

Advance Electrochemistry

Debye - Huckel theory of strong electrolytes- Debye Huckel-Onsagar (DHO) equation-validity of DHO equation. Activity coefficients of electrolytes- ionic strength, Debye-Huckel limit in law, modifications of DHALL, qualitative test and verification of DHLL, activity coefficient, solubility measurements. The electrical double layer at the electrode- electrolyte interface, Electro kinetic phenomena, electrical double layer and its structure, Lippmann Equation, electrode kinetics.

Unit-IV

Ultrasonics Sonochemistry

Fundamental aspects of sonochemistry, ultrasonics, cavitation, sonication, sonoprocessing, food processing, sonocrystallisation, environmental remediation, sonoelectrochemistry, Cavitation-the origin of sonochemical effects, Introduction to power ultrasound in chemistry, Bubble dynamics and observations, Acoustic bubbles, Acoustic streaming, and Cavitation microstreaming, The growth of bubbles in an acoustic field by rectified diffusion, Importance of sonication and solution conditions on the acoustic cavitation activity, Acoustic bubbles and Sonoluminescence , Experimental observation of an acoustic field, Ultrasonic atomization, Sonochemical synthesis and characterization of materials. Ultrasound assisted reactions: Types of sonochemical reactions, Homogenous, Heterogeneous liquid-liquid and liquid-solid reactions.

Recommended Books

1. Physical Chemistry- S. Glasstones, D. Van Nostrand, 1965
2. Principles of Electrochemistry-S. Glasstones, D. Van Nostrand, 1965
3. Modern Electrochemistry-K.N. Reddy
4. Chemical Kinetics-K.J. Laidler, Pearson Education, 2004
5. Physical Chemistry- P.W. Atkins
6. Physical Chemistry (Part IV) -K.L. Kapoor
7. Physical Chemistry-Br. Puri, Lr. Sharma, Madan S. Pathania
8. Physical Chemistry-G.K. Vemulapalli
9. Physical Chemistry-K.J. Laidler, Pearson Education, 2004
10. Basics Chemical Kinetics- G.L. Agrawal, Tata-Mc Graw Hill
11. Fundamentals of Molecular Spectroscopy- Colin N. Banwell
12. Surface Chemistry– A Goel
13. Introduction to Surface Chemistry & Catalysis– Gabor A. Somorjai
14. Electrochemistry– Philip H. Rieger
15. Chemical Kinetics and Catalysis– Richard Mishel
16. Chemical Kinetics– Keith J Laidler
17. Handbook of Ultrasonics and Sonochemistry- Muthupandian Ashokkumar, Springer Nature
18. Practical Sonochemistry: Power Ultrasound Uses and Applications- T J Mason, D Peters
19. Micelle-Yoshikiyo Mori
20. Sonochemistry-Kenneth S. Suslick



PHDCHM104D- Advanced functional materials

Maximum Marks:100

Credit: 04, IA Marks: 30, ESE Marks: 70

Unit I

Introduction to nanomaterials

Nanomaterials, role of size in nanomaterials, nanoparticles, semiconducting nanoparticles, nanostructures, nanowires, nanoclusters. Physico-Chemical and biological routes for the synthesis of nanomaterials, Optical, electronic, magnetic and electrical properties; band-gap, catalysis, and electronic devices.

Unit II

Characterization Techniques:

X-ray diffraction, electron (SEM & TEM) and optical microscope, UV-VIS-IR spectrophotometers, thermal, magnetic and electrical measurements. Lithographic techniques: AFM, E-beam and SEM.

Unit III

Polymers and carbon based nanostructures

Preparation and characterization of block copolymer based nanocomposites, nanoparticles polymer ensembles, Fullerenes, CNTs, graphenes; Properties: mechanical, optical and electrical, nanomaterials in drug-delivery.

Unit IV

Modified Biopolymers: Definition of biopolymers, classification, mechanism of action, influence of various factors on the function of biopolymers, **Modified Biopolymers:** methods for biopolymer modifications, Applications of biopolymers

Recommended Books:

1. “Electron Microscopy and Analysis” – Peter J. Goodhew, John Humphreys, Richard Beanland (Taylor & Francis)
2. “Nanomaterials for Drug Delivery and Therapy” – Alexandru Mihai Grumezescu (Elsevier)
3. “Handbook of Biopolymers and Biodegradable Plastics” – Sabu Thomas, Nandakumar Kalarikkal, Ann Rose Abraham (Elsevier)

ANNEXURE 1

Course Title:

- **Research and Publication Ethics (RPE)**-Course for awareness about the publication ethics and publication misconducts.

Course Level:

- 2 Credit course (30 hrs.)

Eligibility:

- M.Phil., Ph.D. students and interested faculty members (It will be made available to post graduate students at later date)

Fees:

- As per University Rules

Faculty:

- Interdisciplinary Studies

Qualifications of faculty members of the course:

- Ph.D. in relevant subject areas having more than 10 years' of teaching experience

About the course

Course Code: CPE- RPE

Overview

- This course has total 6 units focusing on basics of philosophy of science and ethics, research integrity, publication ethics. Hands-on-sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy:

- Class room teaching, guest lectures, group discussions, and practical sessions.

Evaluation

- Continuous assessment will be done through tutorials, assignments, quizzes, and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Course structure

- The course comprises of six modules listed in table below. Each module has 4-5 units.

| Modules | Unit title | Teaching hours |
|-----------------|--------------------------------|----------------|
| Theory | | |
| RPE 01 | Philosophy and Ethics | 4 |
| RPE 02 | Scientific Conduct | 4 |
| RPE 03 | Publication Ethics | 7 |
| Practice | | |
| RPE 04 | Open Access Publishing | 4 |
| RPE 05 | Publication Misconduct | 4 |
| RPE 06 | Databases and Research Metrics | 7 |
| | Total | 30 |

Syllabus in detail

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 hrs.)**
 1. Introduction to philosophy: definition, nature and scope, concept, branches
 2. Ethics: definition, moral philosophy, nature of moral judgements and reactions
- **RPE 02: SCIENTIFIC CONDUCT (5 hrs.)**
 1. Ethics with respect to science and research
 2. Intellectual honesty and research integrity
 3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
 4. Redundant publications: duplicate and overlapping publications, salami slicing
 5. Selective reporting and misrepresentation of data
- **RPE 03: PUBLICATION ETHICS (7 hrs.)**
 1. Publication ethics: definition, introduction and importance
 2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
 3. Conflicts of interest
 4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
 5. Violation of publication ethics, authorship and contributorship
 6. Identification of publication misconduct, complaints and appeals
 7. Predatory publishers and journals

PRACTICE

- **RPE 04: OPEN ACCESS PUBLISHING(4 hrs.)**

1. Open access publications and initiatives
2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

- **RPE 05: PUBLICATION MISCONDUCT (4hrs.)**

- A. Group Discussions (2 hrs.)**

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

- B. Software tools (2 hrs.)**

Use of plagiarism software like Turnitin, Urkund and other open source software tools

- **RPE 06: DATABASES AND RESEARCH METRICS (7hrs.)**

- A. Databases (4 hrs.)**

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

- B. Research Metrics (3 hrs.)**

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, i10 index, altmetrics

References

Bird, A. (2006). *Philosophy of Science*. Routledge.

MacIntyre, Alasdair (1967) *A Short History of Ethics*. London.

P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865

National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition*. National Academies Press.

Resnik, D. B. (2011). What is ethics in research & why is it important. *National Institute of Environmental Health Sciences*, 1–10. Retrieved from <https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm>

Beall, J. (2012). Predatory publishers are corrupting open access. *Nature*, 489(7415), 179–179. <https://doi.org/10.1038/489179a>

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