

Department of Chemistry, HNB Garhwal University
Syllabus Pre-Ph.D. course (as per the UGC regulations 2016)

Paper I CHEM/Pre Ph.D.

Code SOS CHO1

MM 100

RESEARCH METHODOLOGY FOR CHEMISTRY (Credits: 4)

Unit I- Research Methodology

Research Processes Scientific research, formation of the topic. hypothesis, conceptual definitions, operational definition, gathering of data, analysis of data, revising of hypothesis. Conclusion.

Literature Survey:

Print: Sources of information: Primary and secondary; 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.

The internet and Web resources, E-journals, Journal access. TOC alerts. Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs. Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Chemdraw, Science Direct, SciFinder, Scopus.

Finding and citing published information.

Unit II- Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

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.

Unit III- Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, flammable or explosive hazards, disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives.

Unit IV- Data Analysis:

The Investigative Approach: Making and Recording Measurements. SI Units and their use Scientific method and design of experiments: Errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation, comparison of results: "T test, "f" test and "chi" square test, least squares analysis, weighted least squares analysis, regression coefficient, rejection of results, presentation of data.

Reference Books

1. Kothari, C.K. (2004) Research Methodology Methods and Techniques, New Age International, New Delhi.
2. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow
3. Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry, Oxford University Press.

4. Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.
5. Harris, D. C. Quantitative chemical analysis. 6th Ed., Freeman (2007) Chapters 35.
6. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.
7. Chemical safety matters-IUPAC-IPCS, Cambridge University Press, 1992.

Paper II CHEM/Pre Ph.D. Code SOS CH02
RESEARCH AND PUBLICATION ETHICS (Credits: 3)

MM 100

1. PHILOSOPHY AND ETHICS

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgments and reactions

2. SCIENTIFIC MISCONDUCT

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publication: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

3. PUBLICATION ETHICS

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 misconduct, complaints and appeals
6. Predatory publishers and journals

4. OPEN ACCESS PUBLISHING

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

5. PUBLICATION MISCONDUCT

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad
4. Software tools
Use of plagiarism software like Turnitin, Urkund and other open source software tools

6. DATABASES AND RESEARCH METRICS

- A. Databases
 1. Indexing databases
 2. Citation databases: Web of Science, Scopus, etc.
- B. Research Metrics
 1. Impact Factors of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
 2. Metrics: h-index, g index, i10 index, altmetrics

References

1. Bird, A. (2006). Philosophy Of Science, Routledge
2. MacIntyre, Alasdair (1967) A short history of ethics. London
3. Praveen Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN: 9789387480865
4. Beall, J. (2012) Predatory publishers are corrupting open access. Nature, 489(7415), 179-179.

Paper IIICHEM/Pre Ph.D.

Code SOS CH03

MM 100

PHYSICAL METHODS IN CHEMISTRY (credits: 4)

Unit I

Atomic Absorption Spectroscopy

Introduction and importance; atomization; flame atomization; graphite furnace atomization; instrumentation; hollow cathode lamp, detectors, monochromators; interferences - chemical & spectral; qualitative analysis; quantitative analysis; applications of atomic absorption spectroscopy.

Unit II

Atomic Emission Spectroscopy

Introduction; emission spectra; flame emission spectroscopy; evaluation methods; evaluating flame emission spectroscopy; plasma emission spectroscopy; direct current plasma; inductively coupled plasma; sample introduction; ICP instrumentation; applications; determining alkali metals by flame photometry.

Unit III

Polarography and Amperometry

Introduction; dropping mercury electrode; measurement; polarographic wave; half wave potential; maxima suppressors; quantitative analysis; qualitative analysis; inorganic applications; organic applications; cyclic voltammetry; amperometry- instrumentation, measurement; amperometric titrations.

Unit IV

Magnetic Resonance spectroscopy

High resolution NMR – chemical shift. Spin coupling – frequency lock- double resonance, applications of proton NMR, quantitative analysis, qualitative analysis. Editing techniques in ^{13}C NMR spectroscopy, 2D methods in NMR, nuclear Overhauser effect, homo- and hetero- nuclear correlations in 2D NMR and their applications.

Unit V

Mossbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Fine structure, application of the technique to the studies of (1) bonding and structure of Fe^{2+} and Fe^{3+} compounds (2) Sn^{2+} and Sn^{4+} compounds, detection of oxidation state and in equivalent MB atoms.

Reference Books

1. Vogel's Text Book of Quantitative Chemical Analysis by J. Mendham, R.C. Denney, J.D.
2. Barnes and M.J.K. Thomas, Pearson Education Pvt. Ltd., New Delhi, 2002.
3. Instrumental Methods of Analysis by Willard, Merritt, Dean and Settle CBS Publishers and Distributors, 7th Edition.
4. Fundamentals of Analytical Chemistry by Skoog, West, Holler and Crouch, 8th edition,
5. Cengage Learning Press, New Delhi, 2004.
6. Analytical Chemistry – Problems & Solutions by S.M.Khopkar, New Age International Pvt. Ltd., New Delhi, 2002.
7. Molecular Spectroscopy by W. Kemp, Macmillan Publication.

Paper IV CHEM/Pre Ph.D.

Code SOS CH04

MM 100

ART IN ORGANIC SYNTHESIS (credits: 4)

Unit I

Combinatorial synthesis

Design and synthesis of combinatorial library. Combinatorial synthesis of polypeptides, oligonucleotides and apothilones, multicomponent reaction (ugi reaction).

Unit II

Green chemistry

Principles of green chemistry, atom economy, use for microwave in synthesis, sonochemistry, aqueous phase and solid state reactions, real world cases in green chemistry.

Unit III

Asymmetric synthesis 1

Principles of asymmetric synthesis, asymmetric induction, acyclic stereocontrol, selective synthesis of enantiomers, optical purity, enantiomeric excess, chiral auxiliaries, chiral catalysts, resolution, methods using enantiomerically pure building blocks, asymmetric synthesis: addition to c-c and c-o double bonds, asymmetric- reductions, oxidation, epoxidation and dihydroxylation.

Unit IV

Asymmetric synthesis 2

Asymmetric aldol reaction, asymmetric– ammonium ylid rearrangement, – claisen rearrangement, – amino cope rearrangement, –Wittig rearrangement

Unit V

Retrosynthesis

Overview of disconnection approach, protecting groups, synthetic analysis and planning, control of stereochemistry, synthesis of juvabione and longifolene.

Reference Books

1. Advanced Organic chemistry, 4th edition part B, carey and Sundberg 2000.
2. Green chemistry: Theory and Practice, P. Anastas and J.C. Warner, Oxford University Press, Oxford UK, 1998.
3. Real world Cases in Green chemistry, Cann, Connelly, American Chemical Society, 2000.
4. Asymmetric synthesis, G. Procter, Oxford Science Publications, Oxford University Press, 1996.
5. Advance Asymmetric Synthesis, Stephenson, Springer India.
6. Stereoselectivity in Organic Synthesis, G. Procter, Oxford University Press, Oxford, 1998.
7. Art in Organic Synthesis, J.S.Anand et al., 2nd ed. Wiley interscience, New York, 1988.
8. Classics in Total Synthesis: Targets, Strategies and Methods, K.C. Nicolaou et al., VCH New York, 1996.
9. Protective Groups in Organic Synthesis-Greene (Wiley Interscience)

10. Strategic Applications and Name Reaction in Organic Chemistry Laszto Kurti, Elsevier.
11. Comprehensive Organic Synthesis - Trost and Fleming, Pergamon.

