

# Department of Applied Chemistry

## Ph.D. Course Work Syllabus-2023

Subject: Chemistry



M. J. P. Rohilkhand University, Bareilly



Based on Choice Based Credit System (CBCS)  
(Effective from the Session 2023-24)

## SCHEME OF PRE-Ph.D. COURSE WORK

The details of course work is given in following table:

<b>PART-A</b>		<b>PART-B</b>
Paper-I (PHDCY-701) Credits: 04	Paper-II (PHDCY-702) Credits: 04	Paper-III (PHDCY-703) Credits: 04
Research Methodology & Research Publication Ethics (as per UGC guidelines)	Subject covering Candidate's/Supervisor's/ Department's chosen research area topics	Literature Survey Report (LSR): In this course, the student has to carry out extensive literature survey in the chosen field of research and prepare a literature survey report (LSR).
Maximum Marks: 100	Maximum Marks: 100	Maximum Marks: 50

**Paper-I (PHDCY-701) Research Methodology & Research Publication Ethics Credits: 04**

1. **An overview of research methodology:** Research concept, steps involved, identification, selection and formulation of research problem, justification, hypothesis; literature collection- textual and digital resources (internet)
2. **Research design, data collection and interpretation:** Research design; sampling techniques, collection and documentation, presentation, analysis and interpretation
3. **Scientific writing:** Forms of scientific writing- Article, notes, reports, review article, monographs, dissertations, popular science articles, bibliographies,
4. **Formulation of scientific communication** - Outline preparation, drafting title, sub titles, tables, illustrations; Formatting tables- title, body footnotes; figures & graphs structure, title and legends, Impact factor, citation indices, plagiarism
5. **Computer application:** MS office, excel, power point, graphics (Origin), statistical software (SPSS), CHEMDRAW, Full Prof etc.
6. **Statistics:** Standard deviation/error; Correlation coefficient, types of correlation, regression equation, Test of significance, chi-square test, analysis of variance of data
7. **Research Publication Ethics:**
  - i. **Research Ethics and Scientific Conduct:** Introduction to Research Philosophy and Concept of Research Ethics, Ethical Aspects in Science and Research, Honesty, Research Integrity, Research Ethics and Scientific Conduct Intellectual Scientific Plagiarism), Misconducts (Falsification, Fabrication, Redundant Publications (Duplicate, Overlapping and Salami Slicing), Selective Reporting and Misrepresentation of Data.
  - ii. **Publication Ethics:** Concept of Publication Ethics and its Significance, Best Practices and Guidelines (COPE, WAME, etc.), Conflict of Interest, Publication Misconduct: Concept, Problems and Types. Violation of Publication Ethics, Authorship and Contributor-Ship. Identification of Publication, Misconduct, Complaints and Appeals.
  - iii. **Quality Parameters and Practices:** Copy Rights and Intellectual Property Rights (TPR), Plagiarism check softwares tools (TURNITIN, URKUND, etc.), Practice Databases (Indexing, Citation) and Research Metrics: *h*-index, *g*-index, *i*-10 index, Impact factor., SNIP, SJR, IPP, Cite Score etc.

**Suggested Readings:**

1. Research Methodology - Methods & Techniques, CR Kothri CR (1990), Vishva Prakashan, New Delhi.
2. Research Methodology & Statistical Techniques, S Gupta (1999) Deep & Deep Publications, New Delhi.

3. Research methodology for biological sciences, N Gurumani (2007), MJP Publishers, Chennai.
4. Introduction to Biostatistics, L Forthofer (1995), Academic Press, New York.
5. Biostatistical Analysis, JH Zar (2006), Prentice-Hall.
6. Research Design: Qualitative, Quantitative & Mixed Method Approaches. John W. Creswell (2009), Sage Publication, USA.
7. Experimental Design & Data Analysis for Biologists. PQ Gerry & JK Michael (2002), Cambridge University Press.
8. Choosing and Using Statistics: A Biologists Guide, D Calvin (2003), Blackwell Publisher
9. Kothari, C.R. (2014) Research Methodology: Methods and Techniques, 2nd ed., New Age International Publishers, New Delhi.
10. Best, J.W. and Kahn, J.V. (2006) Research in Education, 10th ed., Pearson Publication, New Delhi.
11. Koul, IL. (2019) Methodology of Educational Research, 5th ed., Vikas Publ., New Delhi (ISBN-9789353386368).
12. Garrett, H.E. (2005) Statistics in Psychology and Education, Paragon International Publishers. New Delhi.
13. Kambadur, M. Ghosh A. and Singhvi A.K. (2019) Ethics in Science Education, Research and Governance, Indian National Science Academy, New Delhi (ISBN:978-81-939482-1-7).
14. Best Practice Guidelines on Publishing Ethics (2014), A Publisher's Perspective, 2nd ed. John Wiley & Sons, Ltd.
15. Chaddah, P. (2018) Ethics in Competitive Research: Do not get Scooped; Do not get Plagiarized (ISBN-978-9387480865).
16. National Academy of Sciences, National Academy of Engineering and Institute of Medicine (2009) On Being a Scientist: A Guide to Responsible Conduct in Research, 3rd ed., National Academies Press.
17. Beall, J. (2012) Predatory Publishers Corrupting Open Access, Nature, 489 (7415):179.
18. Bird A. (2006) Philosophy of Science, Routledge.
19. Software Manual SPSS/MINITAB/MATLAB.
20. UGC syllabus for Research and Publication Ethics, D.O. no. F.1-1/2018(Journal/CARE)

**Unit-I: Different Chromatographic Techniques****(06 Lectures)**

Chromatography terms, Techniques by chromatographic bed shape, Column chromatography, Planar chromatography, Paper chromatography, Thin layer chromatography, Displacement chromatography, Techniques by physical state of mobile phase, Gas chromatography, Liquid chromatography, Affinity chromatography, Supercritical fluid chromatography, Techniques by separation mechanism, Ion exchange chromatography, Size-exclusion chromatography, Expanded Bed Adsorption (EBA) Chromatographic Separation, Special techniques, Reversed-phase chromatography, Two-dimensional chromatography, Simulated moving-bed chromatography, Pyrolysis gas chromatography, Fast protein liquid chromatography, Counter-current chromatography, Chiral chromatography

**Unit-II: Basics of NMR and Mass Spectroscopy:****(07 Lectures)**

Basic NMR techniques, Chemical shift, J-coupling, Second-order (or strong) coupling, Magnetic inequivalence, Deuterated solvents, Correlation spectroscopy, Biomolecular NMR spectroscopy, Proteins, Nucleic acids, Carbohydrates

Basics of Mass spectroscopy; X-axis:  $m/z$  (mass-to-charge ratio), Alternative x-axis notations, History of x-axis notation; Y-axis: signal intensity, Y-axis and relative abundance

**Unit-III: Green Chemistry****(04 Lectures)**

**Basic Principles of Green Chemistry; Designing a Green Synthesis:** Choice of starting materials, choice of reagents, choice of catalysts, choice of solvents;

**Green catalysts:** Acid catalysts, oxidation catalysts, basic catalysts, polymer supported catalysts, polystyrene-aluminium chloride, polymeric super acid catalysts, polystyrene-metallo porphyrins, polymer supported photosensitizer, PTC, Organic synthesis in solid phase; Versatile ionic liquids as green solvents, Applications of Microwaves for Environmentally benign Organic Chemistry, Sonochemistry.

**Unit IV: Chemistry of Macromolecules****(03 Lectures)**

Functionality of Monomers, Degree of Polymerization, Types of Polymerization, addition, Condensation and co-Polymerization, Glass transition temperature ( $T_g$ ), Number average, weight average and Viscosity average molecular weight of polymers.

**Unit V: Basic Concepts of Drug Development****(06 Lectures)**

**General Aspects of Medicinal Chemistry:** A brief history and classification of drugs, main phases of drug activity, measurement and expression of drug effects.

Drug targets: General mechanisms of drug action on lipids, proteins, carbohydrates and nucleic acids.

**Lead Compound Discovery Strategies:** Search for new lead compounds, natural product pharmaceuticals, basics of Combinatorial Chemistry and high-throughput screening.

**Drug Design:** Primary exploration of structure-activity relationships (SARs), identification of pharmacophore, drug optimization strategies, prodrugs, drug alliances and endogenous compounds as drugs.

### **Unit-VI Inorganic Chemistry**

**(07 Lectures)**

Metal ions in biological system and their classification as Trace, Toxic, essential and non-essential. Metal ions and their excess and deficiency. Toxic metal ions, fundamentals of Toxicity and Detoxification or chelation therapy. Designing of chelating agents and metal chelates as medicines. Coordination compounds in medicine. Metal complexes and their interaction with nucleic acids, Role of alkali/alkaline earth metals in bio-systems, Role of metal ions in replication and transcription process of nucleic acids, Synthetic and natural oxygen carriers and their mechanism, Non-heme Iron-sulfur proteins, Nitrogen Fixation.

### **Unit-VII: Synthetic Organic Chemistry and Some Important Named Reactions (07 Lectures)**

Heterocyclic compounds of therapeutic value, Phenothiazine and sulpha drugs, Some aspects of the Chemistry of cycloalkanes with particular reference to their synthesis and properties, Carcinogens.

**Named Reactions:** Arbuzov Reaction, Bamford-Stephens Reaction, Barton Olefin Synthesis, Baylis-Hillman Reaction, Barton reaction, Mitsunobu Reaction, Fischer Oxazole Synthesis, Fischer Indole Synthesis, Sharpless Epoxidation, Swern Oxidation.

### **References:**

1. F.W. Billmeyer, Jr., Text Book of Polymer Science, Wiley-Inter Science, New York.
2. P. K. Sinha, Computer Fundamentals.
3. J.E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, 4th ed., Pearson, 2001.
4. Miessler and D. A. Tarr, Bioinorganic chemistry, 3<sup>rd</sup> ed., Pearson, 2004
5. D. F. Shriver, P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller and F. A. Armstrong. Inorganic Chemistry. 4<sup>th</sup> ed., Oxford University Press, 2006.
6. J.D. Lee. Concise inorganic Chemistry, 5<sup>th</sup> ed., Wiley, 2010.
7. S. Cotton. Lanthanide and Actinide Chemistry. Wiley & Sons Ltd, 2006.
8. W. U. Malik. G. D. Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand. 2019
9. P. Sykes. Mechanism in Organic Chemistry
10. J. March. Advanced Organic Chemistry. Wiley.
11. House. Synthetic Reactions.
12. R.T. Morrison & R.N. Boyd. Organic Chemistry, P.H. Ltd .
13. Fieser & Fieser. Topics in Organic Chemistry, Reinhold.
14. I. L. Finar. Organic Chemistry (Vol. I & 2). Elbs & Longmann.

15. S. J. Lippard. J.M. Berg. Principles of Bioinorganic Chemistry, University of Science Books.
16. W. Kemp. Organic Spectroscopy. 3<sup>rd</sup> ed. Palgrave, 2012.
17. D. L. Pavia. G.M. Lampman. G. S. Kriz and J.R. Vyvyan, Introduction to Spectroscopy, 5<sup>th</sup> ed. Cengage Learning. 2015.
18. R. M. Silverstein and F. X. Webster, Spectrometric identification of Organic Compounds, 6<sup>th</sup> ed., Wiley, 2010.
19. D. H. Williams and I. Fleming. Spectroscopic Methods in Organic Chemistry, 6 ed. McGraw-Hill. 2011.
20. D. N. Sathyanarayana. Handbook of Molecular Spectroscopy: from radio waves to gamma rays, 2<sup>nd</sup> ed. Wiley, 2019.
21. C. N. Banwell & E. M. McCash, Fundamental of Molecular Spectroscopy, 4<sup>th</sup> ed. McGraw-Hill, 2017.
22. D. A. Williams & T. L. Lemke, Foye's Principles of Medicinal Chemistry.
23. Wilson & Gisvold's Text Book of Organic, Medicinal & Pharmaceutical Chemistry

**Online Courses (Optional):** Online courses/topics may be included as per the requirement. The students may opt any of the available online course/topics of not less than 04 credits from the various online portals such as SWAYAM, MOOCS, COURSERA, NPTEL etc. in place of paper-II. Few of the links are given below:

1. <https://swayam.gov.in/explorer.Category=Chemistry>
2. <https://archive.nptel.ic.in/noc/courses.104>