

Ph.D. COURSE WORK

SEMESTER-1

Paper CH-1.1.1

RESEARCH METHODOLOGY

Learning Objective: This course is to provide the basic research methodology including Computer applications to Chemistry.

Learning outcome: This paper will ensure that the students learn to know about formulating research problem, publications of scientific work, E-journals, E-books, E consortium and various important things like tracking manuscript status. General Safety Measures in Research and handling of chemicals is the most essential thing for the students to learn in this time. Correlation and regression, Curve fitting, fitting of linear equations under data analysis will help the students to learn more about data-related research. The knowledge about UV-Visible spectroscopy, chromatography and mass spectroscopy will be very much useful for the students.

UNIT-1

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, problem faced by researcher in India, ethics in research. Reporting practical and project work, organizing a poster display and 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, writing of thesis, patent law, filing of patent.

UNIT-II: Literature survey

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).

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. Report writing using templates, Online submission system. Tracking manuscript status. End-note and Scifroof, Digital object Identifier (DOI), Hot articles.

UNIT- III: General Safety Measures in Research and handling of chemicals

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. Handling of high voltage and electronic equipments, 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-IV Data Analysis

Fundamentals of statistical analysis - types, mean, median, mode, range, variance, standard deviation. Choosing and using statistical tests, test for rejection of outliers (Q test), levels of confidence and significance, test of significance (F-test, student T-test. paired T-test), Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals. General polynomial fitting, linearizing transformations, exponential function fit. r and its abuse. Basic aspects of multiple linear regression analysis.

Unit-V: Computer applications in chemistry

Computer Softwares and chemistry, Computer technique used in chemistry with special reference to UV-Visible spectroscopy, chromatography, mass spectroscopy. Basic idea on computer use in drug discovery, chemical information, structure elucidation, synthesis design, simulation of reaction, physicochemical data, molecular modeling, molecular graphics, data banks. Applications of some common computer packages (MS-Excel, Origin Chem draw. Chem-sketch) to chemistry.

Paper CH-1.1.2

PHYSICAL METHODS IN CHEMISTRY

Learning Objective: This course is framed to give an overview of some of the common techniques used for characterization of different materials and compounds.

Learning Outcome: This paper will ensure that the students learn to know about Principle and instrumentation of X-ray diffraction, X-ray fluorescence, Optical microscope, SEM, TEM, SPM, STM, AFM, UV-Vis DRS, Fluorescence spectroscopy, FT-IR spectroscopy, Optical Rotary Dispersion and Circular Dichroism. Students will get an idea about Cyclic Voltammetry, Differential pulse voltammetry, Potentiometric stripping analysis, Chronocoulometry, Chrono potentiometry. Electrochemical sensor ion-sensitive electrodes, glass-membrane electrodes and solid liquid membrane electrodes.

UNIT-I: X-ray techniques for materials characterization

X-ray diffraction: Principle, measuring system and applications for characterization of powdered materials), Introduction to Extended X-ray absorption fine structure (EXAFS), Surface extended

X-ray absorption (SEXAFS). 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) for characterization of different samples. Energy dispersive X-ray microanalysis (EDS) - Basic aspects of Atomic force microscopy (AFM), scanning probe microscopy (SPM). Scanning Tunneling Microscopy (STM)

UNIT III Spectroscopic methods-I

Principle, instrumentation and applications of UV-Visible (Diffuse Reflectance) (UV-Vis DRS) spectroscopy, Fluorescence spectroscopy and FT-IR spectroscopy. Optical Rotary Dispersion and Circular Dichroism: Introduction, principles, Cotton effect, Octant rule, alpha-halo ketone rule, applications in determining the absolute configuration of simple monocyclic ketones and metal complexes.

UNIT IV Spectroscopic methods-II

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

NMR: Theory of FT NMR quantum mechanical description of NMR, spin lattice relaxation, Bloch equations-nuclear Induction, NOE advance concepts-pulse sequences INEPT and DEPT cross polarization. Introduction to ^{31}P and ^{19}F NMR. Principle and applications of COSY and NOESY for structural elucidation of organic molecules

Unit-V Electroanalytical Techniques

Linear sweep voltammetry, Cyclic Voltammetry, Reversibility, elucidation of reaction mechanisms, Differential pulse voltammetry, Potentiometric stripping analysis, Chronocoulometry, Chrono potentiometry. Electrochemical sensor ion-sensitive electrodes, glass-membrane electrodes, solid liquid membrane electrodes, ion-selective field effect transistors (ISFET), Sensors for the analysis of gases in solution, Amperometric gas sensors

PAPER CODE- 1.1.3

RESEARCH AND PUBLICATION ETHICS (RPE)

Learning Objective: This course is framed to give an overview of some of the philosophy and ethics, publication ethics and open access publishing.

Learning Outcome: This paper will ensure that the students learn to know about Intellectual honesty and research integrity, best practices/ standards setting initiatives and guidelines, identification of publication misconduct, complaints and appeals, Predatory publishers and journals and scientific misconducts: Falsification, Fabrication and Plagiarism (FFP). Journal finder and use of plagiarism software are the most important things to learn by the students. Combination of theory and practical will help the young researchers to know more about research and publication.

THEORY

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

PRACTICE

- RPE 03: OPEN ACCESS PUBLISHING (10 HRS)
 1. Open access publications and initiatives
 2. Journal finder/journal suggestion tools viz. JANE. Elsevier Journal Finder, Springer Journal Suggester, etc.
 3. Complaints and appeals: examples and fraud from India and abroad
 4. Use of plagiarism software like Turnitin, Urkund and other open source software tools
 5. Conflicts of interest

PAPER CODE- 1.1.4

REVIEW OF LITERATURE

Learning Objective: This course is framed to give an overview of searching different papers and concisely doing a literature survey.

Learning Outcome: This paper will ensure that the students learn to find different research papers by journal finder, collecting the useful papers among a wide variety of papers and combining them to do a proper literature survey. This literature search will help them to proceed further to do their research experimental work. Hence, this course will be beneficial for the students to learn about literature survey and carry out experiment basing on that.