

## Ph.D. Course work

### Syllabus of

Department of Chemistry Dr. Shakuntala Misra National Rehabilitation University

Lucknow-226017

S.No.	Paper Name	Code	Marks			Credit
			External	Internal	Total	
1	Research Methodology	DCY-101	70	30	100	4
2	<b>ELECTIVE I</b> (a) Spectroscopy -I or (b) Spectroscopy -II	DCY -102A DCY -102B	70	30	100	3
3	<b>ELECTIVE II</b> (a) Organometallic Chemistry or (b) Chromatography	DCY -103A DCY -103B	70	30	100	3
4	Research and publication ethics	DCY-104	70	30	100	2
		<b>Total</b>		<b>400</b>		<b>12</b>

<b>DCY-101: Research Methodology</b>		
<b>Credits 4</b>	<b>Paper Code DCY-101</b>	<b>Marks (70 +30) = 100</b>

**Course Description:**

This course has been designed to introduce the student to the overall framework within which modern ‘scientific’ research is conducted. This involves an appreciation of the ‘jargon’ of scientific methodology as well as the various paradigms that operate upon the researcher’s mind as he goes about designing a research plan. This course also includes an introduction to Research methodology, empirical study and the statistical method as *the* modern tool for inductive research. We will touch upon concepts in probability as well as statistical inference but only briefly. It is hoped that the student will be able to conduct further study on his own to master the tools of his trade. The third and last part of the course will be targeted to candidates in social science and management and will continue with a study of methodological dimensions of research.

**Course Objectives:** This course has following objectives:

CO1: The students will be able to understand research terminology, be aware of the ethical principles of research, ethical challenges and approval processes

CO2: The students will be able to describe quantitative, qualitative and mixed methods approaches to research, identify the components of a literature review process

CO3: To introduce the students to the concept of valid research and to make them appreciate how validity is influenced by formulation of various design aspects;

CO4: To develop a basic understanding of the statistical method;

CO5: To help student understand the various ways in which research can be pursued so that he can place his own work in proper perspective.

**Expected Course Learning Outcome:**

After the completion of this course, the student will be able:

CLO1: Identify different research methods and their theoretical underpinnings.

CLO2: Demonstrate an ability to identify, analyse and synthesise literature related to a research question.

CLO3: Critically analyze and demonstrate an ability to formulate viable research questions and hypothesis.

CLO4: Describe, compare, and contrast descriptive and inferential statistics,

CLO5: Describe sampling methods, measurement scales and instruments, and appropriate uses of each.

CLO6: Explain the rationale for research ethics.

## **Course 1: Research Methodology**

**4 Credit**

(Including quantitative methods, Computer Applications, research ethics, review of public research in relevant field, training, field work etc.)

### **UNIT I**

**Literature Survey:** Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, reviews, monographs. Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples. Digital: 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, Chem Industry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus. Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

### **UNIT II**

#### **Chemical Safety and Ethical Handling of Chemicals:**

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, and laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

### **UNIT III**

#### **Writing Research Proposal for obtaining financial assistance form:**

Introduction about Funding Agencies. National Funding Agencies, Review writing, Seminars. Basic Knowledge about Computer, MS Office, Chem Draw, Diamond, Mercury, encipher, ORTEPS, Documentation and scientific writing: Results and Conclusions, Preparation of manuscript for Publication of Research paper, presenting a paper in scientific seminar, Thesis writing. Structure and Components of Research Report, Types of Report: research papers, thesis, Research Project Reports, Pictures and Graphs, citation styles, writing a review of paper, Bibliography.

## **SUGGESTED READING:**

1. Thesis & Assignment Writing–J Anderson, B.H.Dursten & M.Poole, Wiley Eastern
2. A Hand Book of Methodology of Research – P. Rajammal and P. Devadoss, R. M. M. Vidya Press,
3. The Craft of Scientific Writing by Michael Alley, (Springer).
4. Research Methodology by R. Panneerselvam, PHI, New Delhi
5. Research methodology techniques and methods by C L Kothari, New age International publishers.
6. C.R. Kothari , Gaurav Garg–“Research Methodology” New Age International Publishers, 2018
7. Naresh Malhotra, *Marketing Research: An Applied Orientation* (Pearson), 2019
8. Prasant Sarangi, *Research Methodology* (Taxmann), 2010

## ELECTIVE I

<b>DCY-102A: Spectroscopy-I</b>		
<b>Credits 3</b>	<b>Paper Code: DCY-102A</b>	<b>Marks (70 +30) = 100</b>

### Unit-I

**UV-Visible Spectroscopy:** Basics of Photometry, Lambert beer's law, Woodward-Fisher rule and applications.

**Microwave spectroscopy:** Selection Rules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, nuclear and electron spin interaction and effect of an external field, Application of Microwave Spectra.

### Unit-II

**Infrared spectroscopy:** Introduction, Theory, Coupled Interactions, Effect of Hydrogen Bonding, Instrumentation of IR, Fourier Transform Infrared Spectrometer, Sample Handling, Interpretation of Spectra, Characteristic Group Absorption of organic molecules, Selection rules, normal modes of vibration, group frequencies, Finger print region, overtones, hot bands, factor affecting the band positions and intensities, forensic application.

### Unit-III

**Raman Spectroscopy:** Classical and quantum theories of raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes raman spectroscopy (CARS).

### Books Recommended

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, *Analytical Chemistry*, 5th Edition (1994), John Wiley & Sons, New York.
3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Analytical Chemistry - An Introduction*, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
4. J. H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition (1990), Saunders Holt, London.

## ELECTIVE I

<b>DCY-102B: Spectroscopy-II</b>		
<b>Credits 3</b>	<b>Paper Code: DCY-102B</b>	<b>Marks (70 +30) = 100</b>

### Unit I

**Mass Spectrometry:** Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, McLafferty rearrangement, deduction of structure using mass spectral fragmentation, FAB-Mass, High resolution MS, soft ionization methods, EI-MS and MALDI-MS.

### Unit II

#### Proton Magnetic Resonance Spectrometry

<sup>1</sup>H NMR: Instrumentation, Magnetic and non-magnetic nuclei, Larmor frequency, absorption of radiofrequency, chemical shift and its measurement, factors influencing chemical shift, deshielding, anisotropic effect, spin-spin coupling, factors influencing coupling constant, AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, NOE effects, restricted rotation (DMF, DMA), cyclohexane ring inversion, chemical shift reagents for stereochemical assignments.

### Unit III

#### <sup>13</sup>C NMR Spectrometry

Introduction to <sup>13</sup>C NMR, Peak assignment, Peak Intensity, Deuterium Substitution, Chemical shift equivalence, Chemical classes and chemical shifts, Off-resonance coupled and decoupled and DEPT method,

#### Recommended Books:

1. Instrumental Methods of analysis- Willard, Merrit, Dean and Settle.
2. Spectroscopic identification of organic compounds- R. M. Silverstein and G. C. Bassler
3. Spectroscopic methods inorganic chemistry- D. H. Williams and I. Fleming
4. Absorption spectroscopy of organic molecules- V. M. Parikh
5. Applications of spectroscopic techniques in Organic chemistry- P. S. Kalsi

## ELECTIVE II

<b>DCY-103A: Organometallic Chemistry</b>		
<b>Credits 3</b>	<b>Paper Code: DCY-103A</b>	<b>Marks (70 +30) = 100</b>

### Unit-I

**Organometallic Chemistry:** Synthesis of Organometallic compounds eg. Grignard Reagents and Organolithium reagents. Ligand hapticity, synthesis, structure and bonding organometallic compounds, organometallic compounds in organic synthesis, homogeneous catalytic reactions.

### Unit-II

#### **Transition Metal Compounds with Bond to Carbon in Catalysis:**

General idea of important catalytic steps: ligand coordination and dissociation, insertion and elimination, nucleophilic attack on coordinated ligands, oxidative addition and reductive elimination reductions.

### Unit-III

Hydrogenation of alkenes using Wilkinson's catalyst, Hydroformylation of alkenes using Co and Rh catalysts, Carbonylation of methanol to acetic acid (Monsanto process), Oxidation of alkenes (Wacker process)

#### **Recommended books:**

1. J. H. Huheey, Inorganic Chemistry- Principles, structure and reactivity, Harper and Row Publisher, Inc. New York (1972)
2. J. D. Lee, Concise Inorganic Chemistry, Elbs with Chapman and Hall, London
3. M.C. Day and J. Selbin, Theoretical Inorganic Chemistry, Reinhold, EWAP
4. T. S. Swain and D. S. T. Black, organometallic Chemistry
5. John Wulff, structure and properties of materials, Volume-4, electronic properties, Wiley Eastern
6. F. A. Cotton, R. G. Wilkinson. Advanced Inorganic chemistry
7. William L. Jolly, Modern Inorganic Chemistry
8. P. L. Pauson, Organometallic Chemistry
9. H. S. Sisler, Chemistry in non-aqueous solvents, Reinhold Publishing Corporation, USA, 4<sup>th</sup> edition (1965)

## ELECTIVE II

<b>DCY-103A: Chromatography</b>		
<b>Credits 3</b>	<b>Paper Code: DCY-103B</b>	<b>Marks (70 +30) = 100</b>

**Unit-1:** Chromatography-Introduction and classification

Principle, Classification of chromatographic methods, Nature of adsorbents, eluents,  $R_f$  values, factors affecting  $R_f$  values.

**UNIT-2:** TLC and paper chromatography

Thin layer chromatography: Principle, Experimental procedure, preparation of plates, adsorbents and solvents, development of chromatogram, detection of spots, applications and advantages.

Paper Chromatography: Principle, Experimental procedure, choice of paper and solvents, various modes of development- ascending, descending, radial and two dimensional, applications.

**UNIT-3: Column chromatography**

Column chromatography: Principle, classification, Experimental procedure, stationary and mobile phases, development of the Chromatogram, applications.

HPLC: Basic principles, instrumentation—block diagram and applications.

### **Recommended books:**

1. Instrumental Methods of analysis (CBS)- H. H. Willard, L. L. Mirrit, J. A. Dean
2. Instrumental Methods of Analysis: Chatwal and Anand
3. Chemical Instrumentation: A Systematic approach- H. A. Strobel
4. Designing of Organic Synthesis, S.Warren,Wiley.
5. Modern Synthetic Reactions, H.O.House,W.A.Benzamin.
6. Some Modern Methods of Organic Synthesis,Wcarruthers ,Cambridge univ.Press
7. Advance Organic Chemistry,Reaction Mechenism & Struture.J.March,John Wiley.
8. Principle of Organic Synthesis,R.O.C.Norman and J.M.Coxan,backie Academic & Professional.
9. Advance Organic Chemistry,Part B,F.A.Carey & R.J.Sundberg, plenum Press.

<b>DCY-104: Research and Publication Ethics</b>		
<b>Credits 3</b>	<b>Paper Code: DCY-104</b>	<b>Marks (70 +30) = 100</b>

**Course Description:**

The main purpose of research is creating and disseminating knowledge in the world. By virtue of its importance in the development of humankind, the conduct and behavior of researchers is bounded by set of written and unwritten rules known as Research Ethics. As the primary mode of dissemination of research is through research publications, Publication Ethics decides the credibility of published research work and recognition of the contribution of other researchers in that field. This course touches the both aspects and provides basic understanding and modern tools for being respectful and credible researcher.

**Course Objectives (COs):**

- CO1: Understand the philosophy and ethics of research.
- CO2: Awareness about the research ethics and its practice.
- CO3: Understand the research databases and their application.
- CO4: Understand the research metrics their application to assess the research output.
- CO5: Awareness about the publication ethics and its practices by researchers.

**Expected Course Learning Outcomes (CLOs):**

- CLO1: Basic understanding of the research philosophy and its elements.
- CLO2: Application of research and publication ethics in research and its dissemination.
- CLO3: Application of research database.
- CLO4: Application of research metrics in assessing research output.
- CLO5: Ability to plan the research publication in suitable journal.

**Unit-1 (Research Philosophy and Ethics) :** Introduction to Philosophy of Research: definition, nature, scope, concepts and branches. Research Ethics: definition, moral philosophy, Nature of moral judgement and reactions. Ethics with respect to Science and research, Intellectual honesty and research integrity. Scientific misconducts: Falsification, Fabrication and Plagiarism (FFP).

**Unit-2 (Databases and Research Metrics) :** Indexing and Research Databases such as SCOPUS, WoS . Research Metrics associated with SCOPUS and WoS : JCR, JIF, Immediacy Index, Eigen Factor Metrics, IPP, Cite Score, SJR, SNIP. FWCI etc . Research Metrics: h-index, i10-index, G-index, almetrics.

**Unit-3 (Publication Ethics) :** Publication Ethics: Introduction, Definitions and importance. Best Practices/ Standard setting initiatives and guidelines: COPE WAME etc. Publication misconduct: Definitions, concept, problems that leads to unethical behaviour. Plagiarism and software tools such as Turnitin and URKUND for Plagiarism Check. Redundant Publications: Duplicate and Overlapping

publications, salami slicing. Selective Reporting and misrepresentation of data. Violation of publication ethics: authorship, contributor-ship, complaints and appeals

**SUGGESTED READING:**

1. Kerry E Howell, "An Introduction to the Philosophy of Methodology", SAGE Publications India Pvt. Ltd., 2013
2. Alexander M. Novikov, Dmitry A. Novikov, "Research Methodology
3. From Philosophy of Science to Research Design." CRC Press, 2013
4. Paul Oliver, "The Student's Guide to Research Ethics", 2<sup>nd</sup> Edition, McGraw Hill, 2010
5. C. Neal Stewart, Jr., "Research Ethics for Scientists: A Companion for Students," Wiley-Blackwell, 2011.
6. <https://www.scopus.com/>
7. <https://mjl.clarivate.com/>