

Chaudhary Bansi Lal University, Bhiwani

(A State University established under Haryana Act No. 25 of 2014)



Department of Chemistry
Examination Scheme
& Syllabi for
Ph.D. Course Work
W. e. f. 2024-25

Chaudhary Bansi Lal University, Bhiwani

Department of Chemistry

Scheme of Examination for Ph.D. Course Work in Chemistry

Credits = 14

Marks = 350

Paper Code	Name of the Paper	Credits	Contact Hours Per Week	Examination Scheme		Total
				External Theory/ Presentation	Internal Assessment	
24 CHEP-101	Paper-I: Research Methodology	4	4	70	30	100
24 CHEP-102	Paper-II: Inorganic Chemistry/Physical Chemistry/Organic Chemistry	4	4	70	30	100
24 CHEP-103	Research and Publication Ethics	2	2	35	15	50
24 CHEP-104	Paper-III: Review of Literature	4	4	100		100
Total		14	14	275	75	350

Duration: 6 Months (1 Semester)

Total Credits: 14

Total Marks: 350

Each candidate has to study three papers (Paper I, II, III & IV); Paper II has three options and one paper is to be chosen (Inorganic Chemistry/Organic Chemistry/Physical Chemistry) by the candidate.

24 CHEP-101
Paper-I: Research Methodology

Maximum Marks: 100
Theory: 70
Internal: 30
Max. Time: 3 hrs.
Credit: 4

Note: The question paper will contain eight questions in all. The candidates are required to attempt any five questions. All questions carry equal marks.

Unit I

Research Methodology: Meaning, Scope, Primary sources of literature survey, Journals, patents etc., secondary sources of literature survey, Books, Reference books, Text books, listing of letters.

Chemical Literature: (1) The structure of chemical information, Important paper based and electronic based sources, How to find chemical information on specific compounds and their synthesis; (2) Abstracts and Journals in chemistry, Electronic forms of Journals, major libraries, subscribing Journals related to chemistry in the region and country; and (3) Patents and Patents writing. Parts of patent applications characteristics of the disclosure for a chemistry invention.

Unit II

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

Writing of Thesis: Format of a thesis: Review of literature, formulation, writing methods, results, preparation of tables, figures, writing discussion, summary and conclusion, synopsis, reference citing and listing, bibliography, avoiding plagiarism.

Unit III

Data Collection: Methods of Data Collection. Case study method, Measurement and Scaling Techniques: Measurement Scales, Meaning of Scaling, Test of Second Measurements. Meaning of Scaling, Scale Classification Bases, Important Scaling and Scale Construction Techniques.

Computer applications in research: Basic operating systems — handling different operating Systems, MS Office.

Drawing graphs and diagrams- Exploring Univariate and Multivariate Data using Tables and

Plots- Stem and Leaf, Box Plot, Spider Plot, Q-Q Plot and Probability Plot, Graphical Methods of Clustering, Photoshop and Paints.

Unit IV

Scientific softwares in research: Data Analysis using Tools like MS Excel, Minitab, ChemDraw and MATLAB.

Digital Methods and Web Search: Internet basics, Internet protocols, pre-requisites, search engines- google scholar, chemspider, scifinder, scopus, reaxys, research gate; using advanced search techniques, web resources, e- journals, e-books, journal access, subscribing TOC alerts, hot articles, citation index — h-index and i-index; Impact factor.

Recommendation for the Candidate:

The candidate is expected to consult standard books, monographs, research papers and accounts for the above mentioned course.

alkenes, methylenations and by Aryl diazonium salts. Structure elucidation by spectral techniques like IR, NMR, Mossbauer for compound of Si, Ge, Sn, Pb, As, Sb, Bi and Te.

Books recommended:

1. Lindsay, S. M., *Introduction to Nanosciences*, Oxford University Press (2010)
 2. Muralidharan, V. S. & Subramania, A., *Nano Science and Technology*, Ane Books Pvt. Ltd. (2009)
 3. Cotton, F.A., Garg, V.C. & Wilkinson, *Advanced Inorganic Chemistry*, John Wiley 4th ed. (1930).
 4. Gupta, B.D. & Elias, A.J., *Basic Organometallic Chemistry; Concepts, Synthesis and Applications* University Press 1st ed. (2010)
 5. Rohtagi-Mukherjee, K. K., *Fundamentals of Photochemistry*, New Age International (2018)
 6. Turro, N. I., Ramamurthy, V., Scaiano, J. C., *Principles of Molecular Photochemistry An Introduction*, University Science Books 1st ed. (2009)
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24 CHEP-102
Paper-II: Inorganic Chemistry
(Optional)

Maximum Marks: 100
Theory: 70
Internal: 30
Max. Time: 3 hrs.
Credit: 4

Note: The question paper will contain eight questions in all. The candidates are required to attempt any five questions. All questions carry equal marks.

Unit-I

Electro analytical Techniques Polargraphy: - Introduction and Basic Principles, Polarograph, Polarographic cells, Half wave Potential and its significance. DME:- Advantages and Disadvantages of DME, SCE Carbon electrodes-Carbon paste Electrode, Types of Currents:- Diffusion Current, Migration Current, Kinetic Currents, Catalytic Currents, Limiting Currents Amperometry :- Principles and Applications, Square Wave Polarography, Voltametry, Coulometry, Superimposed, AC Polarography:- Principles, theory and applications of these techniques.

Unit-II

Nanomaterials: - Definition, Methods of Preparation, Properties of Nanomaterials: - Physio chemical and optical, Electrical and Electronics properties. Applications of Nanomaterials, Gold, Silver & Pt Nanomaterials: General Properties and Applications

Unit-III

Phosphorescent Materials: Luminescence, Types of Luminescence, Fluorescence, Phosphorescence, Frank Condon Principle, Jablonski diagram, Organic Electroluminescence, Organic, Light Emitting diode, Structure and working of OLED, Applications of OLED Inorganic phosphorescent materials, Long Persistent phosphors, phosphors for LED, Applications of Inorganic Phosphors.

Unit-IV

Organometallic Compounds of Main Group Elements: General characteristics of different types of main group organometallics, stability, routes of M-C bond formation: Oxidative addition, transmetallation, Carbanion halide exchange, metal-hydrogen exchange, metal hydride addition to

Unit-IV

Nano materials Technology: Nano materials, Properties of nano structured materials (optical, magnetic, chemical and photo catalytic properties), Techniques for their synthesis (Hydrothermal, Solvothermal, solgel, Precipitation, Reverse Micelle Synthesis, Physical Vapour deposition (PVD), Chemical Vapour Deposition (CVD), Electro deposition and Characterization of nanomaterials by X-ray diffraction(XRD), Scanning Electron Microscope (SEM), Energy dispersive X-ray Analysis, Transmission Electron Microscope (TEM), Atomic Force microscopy (AFM) techniques. Applications of nanoscience and nanotechnology in various fields.

Books recommended:

1. Kapoor, K.L., *A Textbook of Physical Chemistry Volume 4*, Tata Mc Graw Hill(2015).
2. Mcquarrie, D. A., *Quantum Chemistry*, University Science Books 2nd ed. (2008)
3. Chandra, A.K., *Introductory Quantum Chemistry*, Tata Mc Graw Hill, 4th ed. (1998)
4. Levine, I. N., *Quantum Chemistry*, Pearson 7th ed. (2016).
5. Bockris, J. O' M. & Reddy, A. K. N., *Modern Electrochemistry 1: Ionics* Springer 2nd ed. (1998)
6. Bockris, J. O' M., & Reddy, A. K. N., *Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science* Springer 2nd ed. (2001)
7. Chattopadhyay, K. K., Banerjee, A. N., *Introduction to Nanoscience and Technology*, PHI Learning Pvt. Ltd. (2009).
8. Lindsay, S. M., *Introduction to Nanosciences*, Oxford University Press (2010)
9. Muralidharan, V. S. & Subramania, A., *Nano Science and Technology*, Ane Books Pvt. Ltd. (2009)

24 CHEP-102
Paper-II: Physical Chemistry
(Optional)

Maximum Marks: 100
Theory: 70
Internal: 30
Max. Time: 3 hrs.
Credit: 4

Note: The question paper will contain eight questions in all. The candidates are required to attempt any five questions. All questions carry equal marks.

Unit-I

Electrodics: Electron transfer under an interfacial electrical field; Butler-Volmer equation, electrode kinetic involving semiconductor solution interface; Rate determining step in photo-electrochemical reaction; Ionic conductivity in solids; Solid electrolytes; Fast-ion conductors, oxygen ion conductors, sodium ion conductors; Solid state ionic devices, Batteries: Lithium batteries; Sodium batteries; fuel cells; sensors.

Unit-II

Quantum mechanics: The Born-Oppenheimer approximation, The Hellmann-Feynman theorem, Huckel molecular orbital (HMO) theory for linear and cyclic conjugated systems, . Applications of HMO theory (i) to set up and solve Huckle determinant equation (ii) to calculate resonance energy; (iii) to draw wave functions for molecular orbitals for the following molecules: (1) Ethylene molecule (2) Allyl system (Allyl radical and related ions) (c) Butadiene(d) Cyclobutadiene (e) Cyclopropenyl system (cyclopropenyl radical and the related ions) (f) Benzene ring.

Unit-III

Surface Chemistry: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), surface films on liquids (electro kinetic phenomenon), Surface active agents: General features, structure & classification, micellisation, mass action model and phase separation model, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, thermodynamics of micelle formation, counter ion binding to micelles, reverse micelles.

Unit-IV

Green Chemistry

Basic principles of green chemistry, Application of non-conventional techniques in organic synthesis (ultrasonic, microwave and grinding). Solid state synthesis and synthesis under solvent free conditions, Use of ionic liquids.

Drug discovery and development

A rational approach to drug design and drug development of following drugs: cimetidine oxamniquine.

Books recommended:

1. Asymmetric Synthesis Ed. J. D. Morrison, vol. 1-5. Academic Press.
2. Stereochemistry of Organic Compounds by D. Nasipuri.
3. Designing organic synthesis by S. Waren.
4. Heterocyclic Chemistry by T. L. Gilchrist.
5. Comprehensive Heterocyclic Chemistry by A. R. Katritzky and C. W. Rees.
6. Green Chemistry by M. Kidwai and V. K. Ahluwalia.
7. Wilson and Gisvold's Text Book of organic medicinal and pharmaceutical chemistry Ed. R. F. Dorge.

24 CHEP- 102
Paper-II: Organic Chemistry
(Optional)

Maximum Marks: 100
Theory: 70
Internal: 30
Max. Time: 3 hrs.
Credit: 4

Note: The question paper will contain eight questions in all. The candidates are required to attempt any five questions. All questions carry equal marks.

Unit-I

Stereo selective Synthesis: Principle of stereo selectivity, 1,2- and 1,3-asymmetric induction, acyclic, stereoselection, distereoselection in cyclic systems. Enantioselective synthesis: Enantioselective hydroboration, hydrogenation, epoxidation, enantioselective synthesis via hydrazones. Role of enzymes in chiral synthesis.

Unit-II

Disconnection approach of synthesis: Introduction, main synthetic strategies, Synthetic strategies of 1,2- and 1,4-difunctionalised compounds, Group disconnection, Umpolung Strategies, functionalisation of carbonyl compounds. Synthetic approach to cyclic systems. Retro synthetic and reconnection strategies.

Reagents: Preparation and application of following reagents: Hypervalent iodine, organoboron reagents (IBBN, CATB, IPc_2BH , PINB), Organosilicon compounds, Trifluoromethyl sulphonates (triflates).

Unit-III

Heterocyclic compounds: General synthesis of (a) compounds with three or more heteroatoms in the ring (1,2,3)- and (1,2,4)-triazoles (1,2,4)- and (1,3,4)-oxadiazoles, (1,2,5)- and (1,3,4) thiadiazoles (1,2,3)-, (1,2,4)- and (1,3,5)-triazines. Tetrazoles and tetrazines.

(b) Bridgehead nitrogen containing compounds: 9 Indolines, Imidazo (1,2-a) and [1,5 a]pyridines Triazolo [1,5-a] pyridines, S-triazolo [3,4-b] [1,3,4] thiadiazoles Imidazo [2,1-b] [1,3,4] thiadiazoles, S-triazolo [3,4-b] [1,3,4] thiadiazines Thiazolo [3,2-b] [1,2,4] triazoles.

Indexing databases

Citation databases: Web of Science, Scopus, etc.

Impact Factor of Journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score.

Metrics: h-index, g-index, i10 index, altimetry's.

Course Outcomes

At the end of this course, students will be able to understand ethical issues related to Research and Publication, Patents and rights, IPR – Intellectual Property Rights. Also students will be familiar with writing of research papers/thesis following publication ethics, related issues. Also students will be able to publish ethically without plagiarism.

References:

1. Bird, A. (2006). Philosophy of Science. Routledge.
 2. MacIntyre, Alasdair (1967) A Short History of Ethics. London.
 3. P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978-9387480865
 4. 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.
 5. Resnik, D.B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10.
- Beall, J.(2012). Predatory publishers are corrupting open access. Nature, 489(7415), 176-179

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24 CHEP-103
Research and Publication Ethics

Maximum Marks: 50
Theory: 35
Internal: 15
Max. Time: 3 hrs
Credit: 2

Course Objectives

This course is aimed to provide understanding of ethical issues related to Research and Publication, Patents and rights, IPR – Intellectual Property Rights. Also students will learn how to write research papers/thesis following publication ethics, related issues. Also students will know how to publish ethically and ways for avoiding plagiarism.

Note: There shall be nine questions in all covering the entire syllabus. Each question shall carry equal marks. Question number 1 shall be compulsory consisting of 7 questions of short answer types. The students shall have to attempt five questions in all by choosing one question from each unit. The questions of the units shall consist of medium and long answer questions. Simple Calculator, if required, may be allowed.

Unit-I

Introduction to Philosophy: Definition, nature, and scope, concept, branches.

Ethics: definition, moral philosophy, nature of moral judgements and reactions.

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

Unit-II

Publication Ethics: Definition, introduction, and importance.

Best practices/ standards setting initiatives and guidelines: COPE, WAME, etc.

Conflicts of interest

Publication misconduct: Definition, concept, problems that lead to unethical behavior and vice-versa, types. Violation of publication ethics, authorship and contributorship. Identification of publication misconduct, complaints and appeals. Predatory publishers and journals.

Open access publication and initiatives.

SHERPA/ ROMEIO online resource to check publisher copyright & self-archiving policies.

Unit-III

Software tool to identify predatory publications developed by SPPU.

Journal finder/ journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggested, etc.

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

Unit-IV

24 CHEP-104
Paper-III: Review of Literature

Maximum Marks: 100

1. The candidate will be required to study any of the following thrust areas of the research work being carried out in the department and submit a copy of review of literature with at least 50 relevant up to date references.

(50)

- i). Heterocyclic Chemistry
- ii). Medicinal Chemistry
- iii). Hypervalent Iodine Chemistry
- iv). Application of Reagents in
- v). Chemistry Green Chemistry
- vi). Synthetic Organic
- vii). Chemistry Theoretical
- viii). Chemistry Computational
- ix). Chemistry Physical
- x). Chemistry Inorganic
- xi). Chemistry Pharmaceutical
- xii). Chemistry Nanochemistry
- xiii). Natural Products
- xiv). Chemistry Radiation
- xv). Chemistry Nuclear
- xvi). Medicine
- xvii). Material Chemistry
- xviii). Supramolecular Chemistry
- xix). Nanomaterials
- xx). Energy Storage Devices
- Any other thrust(s) area duly approved by the DRC

2. Presentation/Seminar on relevant review of literature submitted before the evaluation committee.

(50)

Recommendation for the Candidate:

The candidate is expected to consult standard books, monographs, research papers and accounts for the above-mentioned course.