

MAHARSHI DAYANAND UNIVERSITY ROHTAK
DEPARTMENT OF CHEMISTRY

Ph.D. Chemistry Course Work

Scheme of Examination w.e.f.2020-21

- (i) The duration of the Ph.D. course work will be of one semester.
- ii) The Department concerned has designed the Ph.D. course as per latest guidelines of UGC.
- iii) The scheme for Ph.D. course work is as under:

Paper No/Code.	Nomenclature	Load	Credit	Maximum Marks
Paper –I 20CHEPC1	Research Methodology	4 hrs/week	4	100 (80+20)*
Paper –II 20MPCC1	Research and Publication Ethics	2hrs/week	2	50 (40+10)*
Paper-III 20CHEPC3	Techniques in Chemistry	4 hrs/week	4	100 (80+20)*
Paper-IV 20CHEPC41 20CHEPC42 20CHEPC43 (one optional out of three)	(i) Inorganic Chemistry (Optional) (ii) Physical Chemistry (Optional) (iii) Organic Chemistry (Optional)	4 hrs/week	4	100 (80+20)*
Total			14	350

Each candidate will study three compulsory (Paper I, II and III) and one optional (Paper-IV one of the three optionals i.e. Inorganic Chemistry, Physical Chemistry or Organic Chemistry).

* Marks for Internal Assessment = Twenty percent of Theory papers. The internal assessment in each paper shall be based on assignment(s) and seminar(s) presented by each candidate and their participation.

➤ **Course outcomes**

CO1 To know the literature survey through books, journals, patents, References etc.

CO2 Understand the C++ Programming.

CO3 To learn the research paper writing.

CO4 Understand the Internet and Web programming.

PhD (Chemistry)
Paper- I (20CHEPC1)
Research Methodology

Max. Marks: 80

Time: 3 hrs.

Note: Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Question number 01 will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks

Section A

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.

Section B

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

Section C

Internet and Web programming: Hardware and software requirement for internet, ISP and internet account, Web home page, URL, Browser, Security on web, searching tools and search engines, FTP, Gopher, Telnet, e-mail and application of internet. Creating a web page, Text formation and alignment, Font control, Arranging text in lists, Images on web pages, Back ground and color control, Interactive layouts and frames.

Section D

C++ Programming: Constants, variables, data types, declaration of variables, user defined declaration, operators, hierarchy of arithmetic operators, expression and statements. Control statements: If, switch, conditional operator, go to, if-else. Decision making and looping statement: While, do -while, for, built in functions and program structure input and output statement. Pointers and arrays.

PhD (Chemistry)
Paper-II (20MPCC1)
Research and Publication Ethics

Max. Marks: 40

Time: 3 hrs.

Note: Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Question number 01 will be compulsory containing 04 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks

Course Outcomes:

By completion of course the student is able to

1. Ethics in conduct of scientific research
2. Know the scientific misconducts
3. How to avoid plagiarism and what are the penalties of plagiarism
4. Know the quality of research publications
5. Write research and review articles.

Unit - I

PHILOSOPHY AND ETHICS

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

SCIENTIFIC CONDUCT

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

Unit - II

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 ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

Unit - III
<p>DATABASES AND RESEARCH METRICS</p> <p>(A) Databases</p> <ol style="list-style-type: none"> 1. Indexing databases 2. Citation databases: Web of Science, Scopus, etc. <p>(B) Research Metrics</p> <ol style="list-style-type: none"> 1. Impact Factor of journal as per Journal Citation Report, SNIP, SIR, IPP, Cite Score 2. Metrics: h-index, g index, i10 index, altmetrics
Unit - IV
Practice
<p>OPEN ACCESS PUBLISHING</p> <ol style="list-style-type: none"> 1. Open access publications and initiatives 2. SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies 3. Software tool to identify predatory publications developed by SPPU 4. Journal finder/journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggested, etc. <p>PUBLICATION MISCONDUCT</p> <p>(A) Group Discussions</p> <ol style="list-style-type: none"> 1. Subject specific ethical issues, FFP, authorship 2. Conflicts of interest 3. Complaints and appeals: examples and fraud from India and abroad <p>(B) Software tools (2 hrs.) :Use of plagiarism software like Tumin, Urkund and other open source software tools</p>
<p>References:</p> <ol style="list-style-type: none"> 1. Bird, A. (2006). Philosophy of Science, Routledge 2. P. Chaddah (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarised. 3. Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019). 4. Beall, J (2012), Predatory publishers are corrupting open access. Nature, 489(7415), 179. 5. 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 Academic press.

➤ **Course outcomes**

CO1 Deliver the importance of general spectroscopic techniques.

CO2 Explain the principles of the most important liquid chromatography.

CO3 Acquire some technical knowledge of TLC, column chromatography and HPLC.

CO4 Interpretation of Thermal Spectra (Thermogram) of the given sample by DTA/TGA

CO5 Acquire technical knowledge of Morphological characterization.

Ph.D. (Chemistry)
Paper – III(20CHEPC3)
Techniques in Chemistry

Max. Marks: 80

Time: 3 hrs.

Note: Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Question number 01 will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks

Section A

Purification/ Crystallization

Isolation and purification of organic compounds (solids and liquids) with special emphasis on chromatographic techniques: TLC, column chromatography and HPLC. Drying and dehydrating agents.

Section B

Spectroscopic Techniques

Theory and applications of NMR spectroscopy of H-1, C-13, N-15, P-31 nuclei, two-dimensional NMR spectroscopy, theory and applications of infrared and mass spectrometry of organic compounds.

Section C

Thermal Techniques

Differential Thermal Analysis (DTA): Theories of DTA, factors affecting DTA curves, instrumentation and application of DTA.

Thermogravimetry (TG): Instrumentation and balances, X'- Y' recorder, thermogram, factors affecting thermogram, correlation of DTA and TGA data.

Section-D

Morphological characterization and diffraction techniques for solids:

Electron microscopy (SEM, TEM, HRTEM, AFM, EDAX), X-ray diffraction [(a) Powder X-ray diffraction, (b) single crystal X-ray diffraction, (c) X-ray diffraction at synchrotron sources] and Neutron Diffraction Analysis.

Books suggested:

1. A textbook of Quantitative Inorganic Analysis, A.I. Vogel, ELBS, London.
2. Dynamics of Chromatography- Part I; J.C. Gidding; Dekker, New York.
3. Vogel's textbook of practical Organic Chemistry, B.S. Furhen ey. al. Longman Group.
4. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill.
5. Spectrometric Methods in Organic Chemistry, D.H. Williams and I. Fleming.
6. Organic Spectroscopy, William Kemp, John Wiley.

➤ **Course outcomes**

- CO1** Know the processing of some nanoparticles, their properties and applications.
CO2 Understand the various Crystal Structures.
CO3 Describe the process of performing an amperometric titration.
CO4 Be able to understand the applications of inorganic and organic Luminescent Materials.
CO5 To identify various organometallics and explained their synthesis and stability

Ph.D. (Chemistry)
Paper-IV (i)
20CHEPC41
Inorganic Chemistry (Optional)

Max. Marks: 80
Time: 3 hrs.

Note: *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Question number 01 will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section A

Electro analytical Techniques

Amperometry: - Principles and Applications

Square Wave Polarography, Voltametry, Coulometry, Superimposed

AC Polarography:- Principles, theory and applications of these techniques.

Chemical Crystallography

Bonding in solids, introduction of crystallography, space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, Silicates and Zeolites, glasses, Quasicrystals.

Section-B

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

Section-C

Luminescent Materials

Luminescence, Types of Luminescence, Fluorescence, Phosphorescence, Frank Condon Principle, Jablouski 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

Section -D

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 alkenes, methylenations and by Aryl diazonium salts.

Structure elucidation by spectral techniques like IR, NMR, Mossbauer for compound of Si, Ge, Sn, , Bi and Te.

BooksSuggested:

1. P. Atkins, T. Overton, J.Rourke, M. Welle, F. Armstrong and M.Hagerman Inorganic Chemistry, Oxford University Press 2010.
2. R. West, Solid state chemistry and its applications, John Wiley & Sons, 1989.
3. D.J. Stokes, Principles and practice of variable pressure/environmental scanning electron microscopy (VP-ESEM), John Wiley & Sons, 2008.
4. R.F. Egerton, Physical principles of electron microscopy: An introduction to TEM, SEM, and AEM, Springer. 2005.
5. B. Voigtlander, Atomic force microscopy, Springer, 2019.
6. N.R. Rao and J.Gopalkrishnan, New directions in solid state chemistry Cambridge University Press 1997.
7. Principles & Applications of Organotransition metal Chemistry by J.P. Collman, L.S. Hegedus, J.R. Norton & R.G. Finke.
8. Organometallic Chemistry – R.C. Mehrotra & A.Singh.
9. Principles of Organometallic Chemistry – G.E. Coates, M.L.H. Green, P. Powel & K. Wade.

Course outcome:

- i. Learning about aspects related to Thermo-physical properties.
- ii. The student will learn about the basics and interpretation of surface characteristics of the materials.
- iii. Learning of theoretical aspects needs to excel in solid state science.
- iv Student will learn about the applied aspects of the electrochemistry in relation to Interface

PhD (Chemistry)
Paper-IV (ii)
20CHEPC42
Physical Chemistry (optional)

Max. Marks: 80
Time: 3 hrs.

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Section-A

Thermodynamics of liquid mixtures

Molecular interactions in liquid mixtures: Ion-ion interactions, Ion-dipole interactions, Dipole-dipole interactions, Ion-induced dipole interactions, Dipole-induced dipole interactions, Quadruple-octuple interactions; specific interactions, hydrogen bonding, charge-transfer interactions and contact charge-transfer interaction. Thermodynamic of mixing functions; excess molar volumes, excess molar enthalpies, excess isentropic compressibilities, excess Gibbs free energy, excess heat capacity and their significance.

Section-B

Reaction on surfaces:

Introduction, Competitive adsorption, Adsorption isotherms(monolayer and multilayer), Non ideal adsorption, Thermodynamics of adsorption(standard states and activated states), Mechanism of surface reactions, Kinetic effects of surface heterogeneity, Frumkin, Temkin, Flory-Huggins, BET, D-R isotherms and their applications, catalytic activities at surfaces, adsorption and catalysis.

Section-C

Solid State Chemistry:

Defects in crystals; Various types of defects in crystal; Thermodynamics of Schottky and Frenkel defects formation; Colour centers; Non-stoichiometric defects; Classification of solids; lattice energy; evaluation of Madelung constant (NaCl); calculation of repulsive potential exponent; Lattice heat capacity; Einstein and Debye model of lattice heat capacity; Debye T^3 law.

Section D

Electrodiodes:

Electron transfer under an interfacial electrical field; Butler-Volmer equation; electrode kinetic involving semiconductor solution interface; photo-electrochemistry; p-type photo-cathodes; n-type photo-anodes; 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.

Electrochemical Impedance Spectroscopy: Introduction, Real and Imaginary impedance, Impedance of a capacitor, AC impedance for electrode processes, Warburg Impedance, Nyquist plot, Bode plot, Cole-Cole plot of electrochemical interfaces, applications of EIS in electrochemistry.

Books Suggested:

1. Chakrabarty, D.K., Adsorption and Catalysis by Solids, Wiley Eastern Limited, New Delhi.
2. Adamson, Physical Chemistry of Surfaces, John Wiley & Sons
3. Rao, Y.V.C., "Chemical Engineering, Thermodynamics," University Press, 1997.
4. Rao, Y.V.C., "An Introduction to Thermodynamics," John Wiley, 1993.
5. R.T. Yang, Adsorbent: Fundamentals and Applications, Wiley Inter-science
6. J.O.M.Bockris and A.K.N.Reddy, Modern Electrochemistry Vol I, IIA & IIB, Plenum Press.
7. Bard, A. J. Faulkner, L. R. , Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley: New York, 2002
8. V. S. Bagotsky, Fundamentals of Electrochemistry, The Electrochemical Society Series, 2nd Ed., Wiley, 2006.
9. A. R. West, Solid State Chemistry and its applications, 2nd edition, Wiley, 2014

➤ **Course outcomes**

- CO1** Apply different reagents in the organic transformations.
CO2 Understand the nomenclature, synthesis and reactivity of different heterocyclic compounds.
CO3 To know the drug design and development of cimetidine and oxamniquine drug.
CO4 To know the principles and techniques of green chemistry.

Ph.D. (Chemistry)
Paper – IV (iii) 20CHEPC43
Organic Chemistry (Optional)

Max. Marks: 80
Time: 3 hrs.

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Section – A

Stereo selective Synthesis

Principle of stereo selectivity, 1, 2- and 1, 3-asymmetric induction, acyclic stereoselection, distereoselection in cyclic systems.

Enantioselective synthesis: Enantioselective hydroboration, hydrogeantion, epoxidation, enantioselective synthesis via hydrazones. Role of enzymes in chiral synthesis.

Section - B

Disconnection approach of synthesis

Introduction, main synthetic strategies, Synthetic strategies of 1, 2- and 1,4-difunctionalised compounds, Group disconnection, Umpolung Strategies, α -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, IpC₂BH, PINB), Organosilicon compounds, Trifluoromethyl sulphonates (triflates).

Section – C

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: 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.

Section – D

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 suggested:

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.

