Curriculum and Credit Framework

For

Ph.D (Chemistry)

(To be effective from the Academic Session 2024-25)

Department of Chemistry

Gurugram University, Gurugram

(A State Govt. University Established Under Haryana Act 17 Of 2017)

Scheme of Programme

Ph.D CHEMISTRY

Course Work Structure for Ph.D. Degree in Chemistry

Course Code	Course Title	Course ID	Teaching Hours per week	Credits	Marks (T.I. + T.E.)
Core Course(s)					
	Research Methodology		4	04	30 + 70
	Research Publication and Ethics		2	02	15 + 35
Specific Elective Courses					
	Inorganic Chemistry		4	04	30 + 70
	Organic Chemistry		4	04	30 + 70
	Physical Chemistry		4	04	30 + 70
Term paper Courses					
	Seminar in Thrust Area of Research		Seminar Based	02	50
	Review of Literature		Assignment Based	02	50
Total Credits				14	350

Marks will be converted into letter grade and grade point as per following table:

Marks	Letter Grade	Grade Point
85-100	O	10
75-84	A^+	9
65-74	A	8
55-64	B^+	7
50-54	B	6
41-49	C	5
40	P	4
Less than 40	F	0

Example to calculate the Grade Point Average (GPA)

Course	Credit	Letter Grade	Grade Point	Credit Point
Research Methodology	4	A	8	4x8=32
Research Publication and Ethics	2	A^+	9	2x9=18
Specific Elective Courses	4	A	8	4x8=32

Seminar in Thrust Area of Research	2	B	6	2x6=12
Review of Literature	2	A	8	2x8=16
Total	14			110

A candidate is required to obtain a minimum grade point of 7 in each paper and minimum GPA of 7 to qualify the course work.

CORE COURSES

Name of Course	**Research Methodology**	
Credits: 04	**Total Max. Marks: 100** **Theory Internal: 30** **Theory External: 70**	**Theory Exam Duration**: 3 Hrs

COURSE SYLLABUS

Note: Eight questions will be set, two from each of the sections I, II, III & IV. The candidates are required to attempt five questions in all selecting at least one question from each section. All questions shall carry equal marks.

Section	**Contents**	**Contact Hrs**
I	**Introduction to Research:** Definition, need and purpose of research, types of research, research process, approaches to research, planning a research proposal, literature review.	**60**
II	**Measurement Scales:** Indexes vs. Scales, Types of Scale, construction of Scale, Bogardus social distance scale, Thurstone Scale, Likert Scale, Semantic Differential Scale, Guttmann Scale.	
III	**Data Collection Methods:** Experiments and Surveys, Experiments: Classical Experiments, Independent & Dependent Variables, Pre-Testing & Post Testing, Double Blind Experiment, Subject Selection, Variation on Experiment Design. Survey Research: Topics appropriate for survey research, Guidelines for asking questions, Questionnaire Construction, Strengths & Weakness of Survey Research, Types of Surveys.	
IV	**Sampling:** Types of sampling methods: Non-Probability Sampling, Probability Sampling, Theory & Logic of Probability Sampling, Sampling Distributions & Estimates of Sampling Error.	
V	**Data Analysis:** Qualitative v/s Quantitative data analysis, Qualitative Data Analysis: Discovering Patterns, Grounded Theory Method, Semiotics, Conversation Analysis, Qualitative Data Processing. Quantitative Data Analysis: Quantification of Data, Univariate Analysis, Bivariate Analysis, Multivariate Analysis, Regression Analysis, Description Analysis. Hypothesis. Multiple Attribute Decision Making.	

VI	**Report Writing, Ethical Issues and Outcomes:** Report Preparation, Structure of Report, Report Writing Skills, Citations, Research Papers, Intellectual Property Rights, Plagiarism, Patent, Commercialization, Ethical Issues.	

Suggested Books

1. Research Methodology by R. Panneerselvam, PHI.
2. Research Methodology by C.R. Kothari & Gaurav Garg, New Age Publishers.
3. Research Methodology by Deepak Chawla and Neena Sondhi, Vikas Publishing.
4. The practice of social research by Earl Babbie, Cengage.
5. Multiple Attribute Decision Making, Gwo-Hshiung Tzeng and Jih-Jeng Huang, CRC Press
6. Research Methodology by Ranjit Kumar, Sage Publications.

CORE COURSES

Name of Course	**Research Publication and Ethics**	
Credits: 02	**Total Max. Marks: 50** **Theory Internal: 15** **Theory External: 35**	**Theory Exam Duration**: 2 Hrs

COURSE SYLLABUS

Note: Eight questions will be set, two from each of the sections I, II, III & IV. The candidates are required to attempt five questions in all selecting at least one question from each section. All questions shall carry equal marks.

Section	Contents	Contact Hrs
	Theory	
I	**Philosophy and Ethics:** Introduction to philosophy: definition, nature and scope, concept, branches; Ethics: definition, moral philosophy, nature of moral judgement and reactions	3
II	**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	5
III	**Publication Ethics:** Publication ethics: definition, introduction and importance, Best practices / standards setting initiatives and guidance: COPE, WAME, etc., Conflicts of interest, Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types, Violation of publication ethics, authorship and contributorship, Identification of publication misconduct, complaints and appeals, Predatory publishers and journals	7
	Practice	

IV	**Open Access Publishing:** Open access publications and initiatives, SHERPA/RoMEO online resource to check publisher copyright & self-archiving polices, Software tool to identify predatory publications developed by SPPU, Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer, Journal Suggester, etc.	4
V	**Publication Misconduct**: Group Discussion (2 hrs), Subject specific ethical issues, FFP, authorship; Conflicts of interest, Complaints and appeals: examples and fraud from India and abroad; Software tools (2 hrs) Use of plagiarism software like Turnitin, Urkund and other open source software tools	4
VI	**Databases and Research Metrics**: Databases (4 hrs), Indexing databases Research Metrics, Citation databases: Web of Science, Scopus, etc., Research Metrics (3 hrs.), Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IIP, Cite Score Metrics: h index, g index, i10 index, altmetrics	7

Suggested Books

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
5. Medicine. (2009). On Being a Scientist: A Guide to Responsible Conduct in Research:Third Edition. National Academics Press.
6. Resnik, D. B. (2011). What is ethics in research and why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from https://www.neihs.nih.gov/research/resources/bioethics/whatis/index.cfm
7. Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489 (7415), 179-179. https://doi.org/10.1038/489179a
8. Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN:978-81-939482-1-7. 1956 http://www.insaindia.res.in/pdf/EthicsBook.pdf

Specific Elective Courses

Name of Course	Inorganic Chemistry	
Credits: 04	**Total Max. Marks: 100** **Theory Internal: 30** **Theory External: 70**	**Theory Exam Duration**: 3 Hrs

COURSE SYLLABUS

Note: Eight questions will be set, two from each of the sections I, II, III & IV. The candidates are required to attempt five questions in all selecting at least one question from each section. All questions shall carry equal marks.

Section	Contents	Contact Hrs
I	**Nanomaterial**	15

	Introduction to Nanoscience, general properties and application, basic instrumentation and imaging techniques, i.e. SEM and TEM. Various synthesis methods in Nano chemistry like Sol-Gel, Hydro/solvothermal, co-precipitation, Chemical vapour deposition and Micro emulsion method.	
II	**Bioinorganic Chemistry:** Metalloenzymes: Metalloenzymes of Zinc, Copper and Cobalt-structure, reactivity and biochemical functioning. Medicinal aspects of vitamin B12. Inorganic compounds as medicine: Lithium drugs in psychiatry, Drugs in hypo and hyper activity of thyroids. Chelation therapy in Alzheimer disease. Vanadium based diabetes drugs. Bio-sensors: Basic components, designing and application.	15
III	**Organometallics** Synthesis, reactivity and applications of σ-bonded and Π-bonded complexes (organometallics) in catalysis **Supramolecular Chemistry** Classification of host-guest compounds, thermodynamics and kinetic stability of supramolecular compounds, different types of macro-molecules hosts, host design, pre-organised hosts cyclodextrin, calixarenes, cryptands and determination of binding constant for supramolecular compounds.	15
IV	**Spectroscopic techniques in inorganic analysis** Application of IR spectroscopy in detection of inorganic complexes. Electron spin resonance (ESR): General introduction, principle and application to complexes, Mossbauer spectroscopy: Basic principle and applications to determine the structures of inorganic complexes.	15

Suggested Books

1. Nanotechnology: Principles and Practices by Sulabha K. Kulkarni
2. Nanomaterials: An Introduction to Synthesis, Properties, and Applications" by Dieter Vollath
3. Bioinorganic Chemistry: A Laboratory Manual by Leona R. Levy and David C. Harris
4. Bioanalytical Chemistry by Susan R. Mikkelsen and Donald L. S. M.
5. Metallobiochemistry: A Practical Approach by Ivan Bertini, Harry B. Gray, and Erwin P. K. Marchand
6. Chemical sensors and biosensors: Fundamental and application: Florinel- Gabriel Banica, John Wiley.
7. Organometallics: A Concise Introduction by Jonathan W. Steed and Jerry L. Atwood
8. The Organometallic Chemistry of the Transition Metals by Robert H. Crabtree
9. Organometallic Chemistry by Gary O. Spessard and Gary L. Miessler
10. Supramolecular Chemistry: Jerry L. Atwood, Jonathan, W. Steed, Wiley 2nd edition.
11. Fundamentals of molecular spectroscopy: C.N. Banwell: McGraw Hills.
12. Textbook of quantitative inorganic analysis: A.I. Vogel ELBS London.
13. Inorganic Spectroscopic Methods by J. Derek Woollins
14. Principles of Instrumental Analysis by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch

Name of Course	Organic Chemistry	
Credits: 04	**Total Max. Marks: 100** **Theory Internal: 30** **Theory External: 70**	**Theory Exam Duration:** 3 Hrs

COURSE SYLLABUS

Note: Eight questions will be set, two from each of the sections I, II, III & IV. The candidates are required to attempt five questions in all selecting at least one question from each section. All questions shall carry equal marks.

Section	Contents	Contact Hrs
I	**Spectroscopic techniques** 2 D NMR-Principle of COSY, HETCOR, HSQC, DQF-COSY, RL-COSY, DEPT, INEPT, NOESY, HMBC, HMQC, INADEQUATE Structural elucidation by spectroscopic methods: application of UV, IR and NMR spectroscopy, mass spectrometry in structural analysis of organic compounds. (Combined problems) Principle of GC-MS, HPLC-MS and GC-FTIR	15
II	**Organic Synthesis** Name reactions/Rearrangements in organic synthesis with special reference to C-C bond formation (Aldol condensation, Benzoin condensation, Perkin reaction, Cannizaro reaction, Grignard reaction, Wittig reaction, Friedel Craft Reaction); Coupling reactions (Heck, Sonogashira, Suzuki). Organic Oxidation-Reduction reactions (Wolf Kishner reduction, Birch Reduction, Oppenauer oxidation); C-N rearrangement (Beckman, Hoffmann, Schmidt & Lossen rearrangement). **Disconnection approach** An introduction of synthons and synthetic equivalents, general principles of the disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, Reversal of polarity, chemoselectivity, regioselectivity, regiospecificity, stereoselectivity and stereospecificity, synthesis of cyclic system (five and six membered rings).	15
III	**Biological and Medicinal Chemistry** Brief introduction to microbes: bacteria, fungi, viruses and parasites, Classification of bacteria, Introduction to the terms MIC, IC_{50}, K_i, therapeutic index, LD_{50} and ED_{50}. Classification of drugs based on therapeutic action. Elementary idea about drug action: the receptor role, neurotransmitters and receptors, ion channels and their control. Membrane bound enzymes-activation/deactivation. Chemical basis of messenger induced change of shape by the receptor.	15
IV	**Computer aided drug discovery and quantitative tools** The Lead compound, Pharmacophore, Bioinformatics in drug discovery and development. chemical databases, ADME and Toxicity, Virtual Screening, Molecular Docking, Ramachandran Plot, Structure and Ligand Based Drug Designing, Case studies Introduction to QSAR methodologies and its application in molecular design.	15

Suggested Books

1. Organic Chemistry, J. Clayden, N. Geeves, S. Warren, 2nd Edition. Oxford University Press, 2012.
2. Organic Synthesis, M. B. Smith, Academic Press, 2009.
3. Classics in Total Synthesis, K. C. Nicolaou and E. J. Sorensen, Wiley, 2008,
4. Carey and Sundberg, Advanced Organic Chemistry; Parts A and B, Springer 2007.
5. The logic of Chemical Synthesis, E. J. Corey and X.-M. Cheng, Wiley, 2005.
6. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, 3rd Edition, CRC Press, 2004.
7. Asymmetric Synthesis Ed. J, D. Morrison, vol. 1-5. Academic Press.
8. Stereochemistry of Organic Compounds by D. Nasipuri.
9. Designing organic synthesis by S. Waren.
10. Heterocyclic Chemistry by T. L. Gilchrist.
11. Comprehensive Heterocyclic Chemistry by A. R. Katritzky and C. W. Rees.
12. Green Chemistry by M. Kidwai and V. K. Ahluwalia.
13. Wilson and Gisvold's Textbook of organic medicinal and pharmaceutical chemistry Ed. R. F. Dorge.

Name of Course	**Physical Chemistry**	
Credits: 04	**Total Max. Marks: 100** **Theory Internal: 30** **Theory External: 70**	**Theory Exam Duration**: 3 Hrs

COURSE SYLLABUS

Note: Eight questions will be set, two from each of the sections I, II, III & IV. The candidates are required to attempt five questions in all selecting at least one question from each section. All questions shall carry equal marks..

Section	Contents	Contact Hrs
I	**Chemical & Electrochemical Energy Systems** Brief overview of Electrochemical Techniques, Electrochemical Cells: Batteries, Super capacitors, Fuel Cells, Solid Electrolytes and Photo electrochemical Cells, Perovskite Solar Cells, Photocatalysis, hydrogen production, decomposition of N_2O, dry reforming.	15
II	**Nanochemistry I** Introduction to Nanoscience, quantum dots and their properties, basic instrumentation and imaging techniques. Intermolecular Interactions, Various synthesis methods in nanochemistry like Sol-Gel, Hydro/solvothermal, co-precipitation, Chemical vapor deposition and Microemulsion method.	15
III	**Nanochemistry II** Principles of self-assembly, soft lithography, nano/micro-contact printing-stamps and tips, layer by layer assembly, meso-structures from soft building blocks, nanocrystals, templating methods, photonic crystals, nanorods-, nanotubes-, nanowires- self-assembly.	15
IV	**Application of nanomaterials** Energy storage applications: rechargeable solid state batteries, Supercapacitors. Fuel cells, catalytic, electrocatalytic and photocatalytic applications, CO2 conversion, Gas sensing and biomedical application.	15

Suggested Books
1. Chemical and Electrochemical Energy Systems by R. Narayan, B. Viswanathan 2. Nanomaterials and Nanochemistry by C. Bréchignac, P. Houdy, M. Lahmani 3. Fundamentals of Nanochemistry by Dr. Rupali Ajesh Gulalkari 4. Nanotechnology: An introduction to synthesis, properties, and applications of nanomaterials by Thomas Varghese, K.M. Balakrishna

Term Paper Courses

Name of Course	Seminar in Thrust Area of Research	
Credits: 02	**Total Max. Marks:** 50	**Seminar Duration:** 01 Hr

COURSE SYLLABUS		
Section	**Contents**	**Contact Hrs**
I	Each candidate will deliver a seminar on any of the following thrust area along with report before the departmental research committee. 1. Synthetic Organic Chemistry 2. Green Chemistry 3. Heterocyclic Chemistry 4. Theoretical and Computational Chemistry 5. Organic Photochemistry 6. Thermodynamics of liquid mixtures 7. Thermal techniques 8. Nano Chemistry 9. Synthetic Inorganic Chemistry 10. Analytical Chemistry 11. Organometallics 12. Bio-Inorganic Chemistry 13. Thermophysical and transport properties 14. Enzymes Chemistry Any other thrust areas(s) duly approved by Departmental Research Advisory Committee	30

Name of Course	Review of Literature	
Credits: 02	**Total Max. Marks:** 50	

COURSE SYLLABUS		
Section	**Contents**	**Contact Hrs**
I	Each Candidate shall submit three copies (hard bound) of a review article with at least 50 relevant up-to-date references on a topic assigned by the proposed supervisor based on published works in one of the following broad fields for evaluation	30

	1. Inorganic Chemistry 2. Organic Chemistry 3. Physical Chemistry 4. Pharmaceutical Chemistry Candidates will ensure plagiarism by using plagiarism checker and will submit the similarity index (not more than 10%) report along with hard bound review. For writing the review student will make use of drawing tools like ChemDraw and modern Reference management tools like endnote and mendeley.	