

INDIRA GANDHI UNIVERSITY, MEERPUR, REWARI

A State University established under Haryana Act No 29 of 2013
Recognized u/s 12-B & 2(f) of UGC Act, 1956

DEPARTMENT OF CHEMISTRY

Course Curriculum

for

Ph.D. Chemistry



Approved by the Academic council in its XX meeting held on Dec XX, 2021

INDIRA GANDHI UNIVERSITY, MEERPUR, REWARI

HARYANA

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SYLLABUS

Ph.D. CHEMISTRY

**DEPARTMENT OF CHEMISTRY
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Scheme of Examination Ph.D. Course Work (Chemistry) Under Credit System w.e.f. 2020-21

SEMESTER I Core Courses

S. No	Paper	Course Code	Course Title	Theory Marks	Internal Marks	Practical/ Workshop Marks	Max. Marks	Credits
1	Paper-I	CHE-701	Research Methodology	80	20	0	100	4
2	Paper-II	CHE-702	Computer Applications	50	0	50	100	4
3	Paper-IV	CHE-703	Research and Publication Ethics	25		25	50	2
4	Paper-V	CHE-704	Review of Literature and Seminar	0		50	50	2

Paper-III (Subject Specific) (Select any one)

S. No.	Course Code	Course Title	Theory Marks	Internal Marks	Practical/ Workshop Marks	Max. Marks	Credits
1	CHE-705	Advanced Inorganic Chemistry	80	20	0	100	4
2	CHE-706	Advanced Physical Chemistry	80	20	0	100	4
3	CHE-707	Advanced Organic Chemistry	80	20	0	100	4

Total Credits: 16

Note:

1. The internal assessment of 20 marks in each paper shall be based on two assignments of 5 marks each and one seminar of 10 marks presented by each candidate and their participation in seminar.
2. The syllabus of each theory course will be divided into three sections of two or three questions each. The question paper will consist of eight questions in all and students shall be asked to attempt five questions selecting at least one from each section.
3. Subject specific courses will be offered subject to availability of requisite resources/faculty

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Paper-I
CHE-701 :: Research Methodology
(Semester I)

L+T+P	:	4+0+0	End-semester exam	:	80
Credits:	:	4	Internal Exam	:	20
Contact hours	:	60			

Unit*	Contents	Lectures
I	Introduction Scope and Meaning of Research, Types of Research: Historical research, Descriptive research, Fundamental research, Application oriented research, Pure research, Applied research, Action research, Evaluation research and Concepts of invention & innovation, Research funding agencies and National and International Research awards.	11
II	Technical Writing Types of technical documents: Full length research paper, Short/Brief communications, Letters to editor, Book chapter, Review, Conference report, Project proposal Components of a full length research paper: Title/Topic statement, Abstract/key words, Aims and objectives, Hypothesis building, Rationale of the paper, Work plan, Materials and methodology, Results and discussion, Key issues and arguments, Acknowledgement, Conflict of interest statement, bibliography, Technical Resumes & Cover Letters Components of a research proposal: Project summary, Key words, Origin of the proposal, Major Objectives, Methodology, Instrument facility available in the PI's department, Overview of status of Research and Development in the subject, Importance of the proposed project in the context of current status, Bibliography	12
III	Analysis and presentation data: Using graphs, Presenting data in tables, Hints for solving numerical problems, Descriptive statistics, choosing and using statistical tests, drawing chemical structures, computational chemistry. Plagiarism: concepts, importance and tools, Impact factor and its importance, H index, citation, Fundamentals of Intellectual property rights, patents, copy rights, trade marks.	13
IV	Information technology and library resources: The Internet and World Wide Web, internet resources for chemistry, , finding and citing information Importance of publications, Reputed Research journals of international and national level, Literature review: concepts, importance, sources of literature survey.	12
V	Chemical safety and Disaster Management: Emergency response: chemical spills, radiation spills, biohazard spills, leaking compressed gas cylinders, fires, medical emergency, accident reporting General safety: General safety and operational rules, safety equipments, personal protective equipments, compressed gas safety, safety practices for disposal of broken glass wares, centrifuge safety, treated biomedical wastes and scientific ethics.	12

S. No.	Name of Books
1	Research Methodology-Methods and Techniques Kothari CR New Age International 2 nd ed. / 2004

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2	Research Methodology: A Step by Step Guide for Beginners Kumar R Pearson Education 2 nd ed. / 2005
3	Research Methodology in the Medical and Biological Sciences Laake P, Benestad H & Olsen B Elsevier 1 st ed. / 2007
4	Research Methodology Murthy C Vrinda Publications 1 st ed. / 2009
5	Research Methodology For Biological Sciences Gurumani N MJP Publishers 1 st ed. / 2013
6	Business Research Methods by William G. Zikmund, 2003 Edition (ISSN-13:978-81-315-0029-3), published by Cengage Learning India Pvt. Ltd, New Delhi.
7	RESEARCH METHODOLOGY- Methods and Techniques (2007 reprint edition) by C.R. KOTHARI, New Age International Publishers, and New Delhi
8	Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd. [Prentice Hall] (2002)

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Paper-II CHE-702 :: Computer Applications (Semester I)
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L+T+P	:	2+0+2	End-semester exam	:	50
Credits:	:	4	Practical/ Workshop	:	50
Contact hours	:	60			

Unit	Contents	Lectures
I	Basic of Computer Operating System: Using Windows – Directory structures – command structure (Document preparation, EXCEL, Power Point Presentation).	11
II	Word Processing: Basics of Editing and Word processing. Figure Plotting: Figure insertions in documents. Web Browsing for Research: Usage of Webs as a tool for scientific literature survey.	12
III	Error Analysis: Basics of a measurement and its interpretation, mean, standard deviation, variance, correlation coefficient; Usage of packages (e.g. ORIGIN; EXCEL) for data analysis. Features for Statistical data analysis using computers and software, Microsoft Excel Data, SPSS	13
IV	Curve Fitting: Linear and Non-linear fitting of data. Literature search technique: using SCOPUS, Google Scholar, PUBMED, Web of Science, Indian Citation Index, and RG. Styles of referencing: APA, MLA, Oxford, Harvard, Chicago Annotated bibliography. Tools for citing and referencing: Endnote	14
V	Presentation and Communication skills Tables, Figures and Pictures using Excel, PowerPoint slide preparation; Preparation of Posters, Electronic submission of manuscripts, Communication skills, oral and poster	10

Note: The practical of computer applications shall be conducted by one internal examiner appointed by the chair person and one external examiner appointed by the Vice-Chancellor on the recommendations of the Departmental Committee out of panel of 10 experts.

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Paper-IV CHE-703 :: Research and Publication Ethics (Semester I)
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L+T+P	:	2+0+0	End-semester exam	:	50
Credits:	:	2	Theory	:	25
Contact hours	:	30	Practical and viva voce	:	25

Note: The question paper shall have total eight questions of five marks each covering Unit 1, 2 and 3. The students shall be asked to attempt total five questions in all.

Practical and viva voce examination will be of 25 marks from Unit number 4, 5 and 6 and shall be conducted by two internal examiners appointed by the Vice-Chancellor.

Course Objective:

1. To understand the philosophy of science and ethics, research integrity and publication ethics.
2. To identify research misconduct and predatory publications.
3. To understand indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.)
4. To understand the usage of various plagiarism tools.

Course Outcomes:

At the end of the course, the student will have awareness about the publication ethics and publication misconducts.

Note: Unit 1, 2, 3 are to be covered via Theory mode and Unit 4, 5, 6 are to be covered via practice mode.

OVERVIEW

This course has total 6 units focusing on basics of Philosophy of science and ethics, research integrity, publication ethics. Hands on sessions are designed to identify research misconduct and predatory publications. Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy:

Class room teaching, Guest Lectures, group discussions and practical sessions. Total teaching hours shall be 30 hours.

Evaluation

Continuous assessment will be done through tutorials, assignments, quizzes and group discussions. Weightage will be given for active participation. Final written examination will be conducted at the end of the course.

Syllabus in Details:

Unit	Contents	Lectures
Theory		
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	3
II	SCIENTIFIC CONDUCT 1. Ethics with respect to science and research 2. Intellectual honesty and research integrity 3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)	5

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	4. Redundant publications: duplicate and overlapping publications, salami slicing 5. Selective reporting and misrepresentation of data	
III	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	7
Practice		
IV	OPEN ACCESS PUBLISHING 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 Suggester, etc.	4
V	PUBLICATION MISCONDUCT (A) Group Discussions (2 hrs.) 1. Subject specific ethical issues, FFP, authorship 2. Conflicts of interest 3. Complaints and appeals: examples and fraud from India and abroad (B) Software tools (2 hrs.): Use of plagiarism software like Turnitin, Urkund and other open source software tools	4
VI	DATABASES AND RESEARCH METRICS (A) Databases (4 hrs.) 1. Indexing databases 2. Citation databases: Web of Science, Scopus, etc. (B) Research Metrics (3 hrs.) 1. Impact Factor of journal as per Journal Citation Report, SNIP, SIR, IPP, Cite Score 2. Metrics: h-index, g index, i10 index, altmetrics	7

Suggested Reading

- Nicolas H. Steneck. Introduction to the Responsible Conduct of Research. Office of Research Integrity, 2007. Available at: <http://ori.hhs.gov/sites/default/files/rcrintro.pdf>
- The student's Guide to Research Ethics By Paul Oliver Open University Press, 2003.
- Responsible Conduct of Research By Adil E. Shamoo; David B. Resnik Oxford University Press, 2003.
- Ethics in Science Education, Research and Governance Edited by Kambadur Muralidhar, Amit Ghosh Ashok Kumar Singhvi. Indian National Science Academy, 2019. ISBN: 978-81-939482-1-7. http://www.insaindia.res.in/pdf/Ethics_Book.pdf
- Anderson B.H., Dursaton, and Poole M.: Thesis and assignment writing, Wiley Eastern 1997.
- Bijorn Gustavii: How to write and illustrate scientific papers? Cambridge University Press.
- Bordens K.S. and Abbott, B.b.: Research Design and Methods, Mc Graw Hill, 2008.
- Graziano, A., M., and Raulin, M.,L.: Research Methods – A process of Inquiry, Sixth Edition, Pearson, 2007.
- Bird, A. (2006). Philosophy of Science. Routledge.
- MacIntyre, Alasdair (1967) A Short History of Ethics. London.
- P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN: 978-9387480865.
- 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.
- Resnik, D.B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from <https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm>
- Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179-179.
- <https://doi.org/10.1038/489179a>

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Paper-V
CHE-704 :: Review of Literature and Seminar
(Semester I)

L:T:P:	:	0+2+0	Viva-voce	:	25
Credits:	:	2	Presentation	:	25
Contact hours	:	30			

Description

Students are required to prepare a power point presentation on the allotted topic and have to make a presentation in front of advisory committee. Students are expected to provide latest facts and updated information by consulting latest editions of textbooks, reference books, monographs and peer-reviewed national & international research journals.

Some Suggested Journals

S. No.	Name of the research journal/database	Publisher	Website
1.	Accounts of Chemical Research	ACS Publications	http://pubs.acs.org/
2.	ACS Medicinal Chemistry Letters	ACS Publications	http://pubs.acs.org/
3.	Advances in Chemistry	ACS Publications	http://pubs.acs.org/
4.	Journal of the American Chemical Society	ACS Publications	http://pubs.acs.org/
5.	Journal of Medicinal Chemistry	ACS Publications	http://pubs.acs.org/
6.	Journal of Medicinal and Pharmaceutical Chemistry	ACS Publications	http://pubs.acs.org/
7.	The Journal of Organic Chemistry	ACS Publications	http://pubs.acs.org/
8.	The Journal of Physical Chemistry A	ACS Publications	http://pubs.acs.org/
9.	The Journal of Physical Chemistry B	ACS Publications	http://pubs.acs.org/
10.	The Journal of Physical Chemistry C	ACS Publications	http://pubs.acs.org/
11.	Organic Letters	ACS Publications	http://pubs.acs.org/
12.	Bioorganic Chemistry	Science Direct	http://www.sciencedirect.com/
13.	Bioorganic & Medicinal Chemistry	Science Direct	http://www.sciencedirect.com/
14.	Bioorganic & Medicinal Chemistry Letters	Science Direct	http://www.sciencedirect.com/
15.	Biophysical Chemistry	Science Direct	http://www.sciencedirect.com/
16.	Tetrahedron	Science Direct	http://www.sciencedirect.com/
17.	Tetrahedron: Asymmetry	Science Direct	http://www.sciencedirect.com/
18.	Tetrahedron Letters	Science Direct	http://www.sciencedirect.com/
19.	Advanced Drug Delivery Reviews	Elsevier	www.journals.elsevier.com
20.	Analytical Chemistry Research	Elsevier	www.journals.elsevier.com

Databases

Pubmed/Medline, ScienceDirect, J-stage, SpringerLink, IngentaConnect, Google Scholar, Current Contents

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Paper-III (Select any one)

CHE-705 :: Advanced Inorganic Chemistry (Semester I)

L+T+P	:	4+0+0	End-semester exam	:	100
Credits:	:	4	Theory Marks	:	80
Contact hours	:	60	Internal Marks	:	20

Unit	Contents	Lectures
I	Electro analytical Techniques: Polarography:- 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;	13
II	Types of Currents:- Diffusion Current, Migration Current, Kinetic Currents, Catalytic Currents, Limiting Currents; Amperometry:- Principles and Applications; Square Wave Polarography, Voltammetry, Coulometry, Superimposed; AC Polarography:- Principles, theory and applications of these techniques.	17
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 for LED, Applications of Inorganic Phosphors	15
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 alkenes, methylenations and by Aryl diazonium salts.	15

S. No.	Name of Books
1	A textbook of Quantitative Inorganic Analysis, A.I. Vogel, ELBS, London.
2	Fundamentals of photochemistry by K.K.Rohatgi-Mukherjee New Age International Publishers Revised Edition (Reprint 2003)
3	Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son (2001).
4	Comprehensive Inorganic chemistry, J. C. Bailar, H. J. Emeleus, Sir R. Nyholm, R. F. Tortman- Dickenson (Pergamon Press, 1973) Volume 1 to 5.
5	Inorganic Material Chemistry, M. T. weller (oxford,1994)
6	Bioorganometallic chemistry, Volume Editor G. Simonneaux (Springer, 2009)

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CHE-706 :: Advanced Physical Chemistry (Semester I)

L+T+P	:	4+0+0	End-semester exam	:	100
Credits:	:	4	Theory Marks	:	80
Contact hours	:	60	Internal Marks	:	20

Unit	Contents	Lectures
I	Preparation of Materials and applications: a) Thin films and Langmuir-Blodgett Films: Preparation techniques; sol - gel, spin coating, Langmuir-Blodgett (LB) photolithography, properties and applications of films. b) Materials of Solid State Devices: Organic and inorganic materials for rectifiers, transistors, capacitors and their applications in optoelectronic and photovoltaic devices.	11
II	Kinetics of redox reactions: Outer and inner sphere reactions, kinetics and mechanism of oxidation reactions involving chromium, ruthenium and silver (III). Kinetics of catalyzed reactions: Homogeneous and heterogeneous. Positive, negative and auto catalysed reactions. Induced reactions, promoters and poisons. Theories of catalysis: intermediate compound formation and adsorption theory, characteristic of catalytic reaction and activation energy of catalyzed reactions. Micellar Catalysis: Models for micellar catalysis (Menger & Portony, Sepulveda, Berezin, Piszkiwicz and Raghavan&Srinivasan Models), Phase transfer catalysis, General mechanism, difference between phase transfer and micellar catalysis.	19
III	Thermodynamic of Liquid: Structure of liquids, relationship between structure and the thermodynamics properties, molecular theory of monoatomic and polyatomic liquids, thermodynamics of phase equilibria, statistical molecular description of phase transitions, chemical potential and partial molar quantities, mixing and excess thermodynamic properties of mixtures, statistical mechanical theories of non-electrolyte and electrolyte solutions, influence of solute on structure of water, structure of water near a surface	17
IV	Static dielectric constant: Dipolar interactions, dipolar molecules in gases and in dilute solutions. Debye equation and its generalizations, Structure and dielectric properties, methods for determination of dipole moments, Clausius-Mossotti equation, dielectric loss, cole-cole plots, dielectric relaxation.	13

S. No.	Name of Books
1	Solid State Physics, N. W. Ashcrott and N. D. Mermin, Saunders College
2	Materials Science, J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS
3	Kinetics and Mechanism by A. A. Frost and R. G. Pearson
4	R. S. Berry, S. A. Rice and J. Ross, <i>Physical Chemistry</i> , 2nd Ed., Oxford University Press, New York, 2000.

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CHE-707 :: Advanced Organic Chemistry (Semester I)

L+T+P	:	4+0+0	End-semester exam	:	100
Credits:	:	4	Theory Marks	:	80
Contact hours	:	60	Internal Marks	:	20

Unit	Contents	Lectures
I	Neighboring Group Mechanism, Neighboring Group (NG) participation by π and σ bonds: Classical and Non-classical Carbocations, C=C as NG, Cyclopropyl as NG, Aromatic ring as NG, C-C as NG, Hydrogen as NG. Anchimeric assistance.	11
II	Modern Organic Synthetic Reactions: Aza-Cope and Aza-Wittig reactions, Baylis-Hillman reaction, BINAL and BINAP assisted reactions, Buchwald-Hartwig coupling, Grubb's catalyst and olefin metathesis, Mukayama aldol reaction, Mitsunobu reaction, Suzuki coupling, Heck reaction, Negishi Coupling.	21
III	Protection and Deprotection of amine, aldehyde, ketone, hydroxyl, carboxyl groups.	13
IV	Rearrangements: Sommelet-Hauser, Favorskii, Fries and Benzilic acid rearrangements, Hofmann-Löffler-Freytag reaction, Barton reaction and Shapiro reaction, Beckmann rearrangement and Schmidt reaction, Vilsmeier-Haack Reaction.	15

S. No.	Name of Books
1	Asymmetric Synthesis Ed. J, D. Morrison, vol. 1-5. Academic Press.
2	Stereochemistry of Organic Compounds by D. Nasipuri.
3	March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure 2015 by Michael B. Smith