School of Chemistry
University of Hyderabad

Ph.D. Coursework: Manual

General Guidelines for Students:

Every student admitted to the Ph.D. program in the School of Chemistry has to undertake course work adding up to a total credit of 12 (minimum). As per the UGC stipulations, the student can formally register for the Ph.D. programme, only on satisfactory completion of the coursework requirements.

1. The course work is to be started in the Semester following the one during which the student was admitted, and should be completed in **two semesters**. For example, a student admitted to the Ph. D. program in January 2021 admission has to start the coursework in the Winter semester (January-June) of 2021 and complete the coursework in the Monsoon semester (July-December) of 2021. Similarly, a student admitted in July 2021 admission has to start the coursework in the Monsoon semester (July-December) of 2021 and complete the coursework in Winter semester (January-June) of 2022. Failure to complete the coursework within one year (two semesters) will lead to the cancellation of admission of the Ph. D. programme.

2. The student has to complete a minimum of 12 credits for satisfactory completion of the coursework. Out of 12 credits, 10 would be from mandatory courses (CY801, 802 and any one (minimum) from CY803-805. The course for the remaining 2 credits will be prescribed by the Doctoral Committee of the student from any course (CY803-805, in addition to the choice of CY80X) or M. Sc. level courses (CY400/500) taking into account the background, interest and needs of the student.

3. The student should obtain a minimum of **55%** marks to pass any course.

4. The official course completion certificate will indicate only Pass/Fail and not marks or grades for each course.

5. Attendance (minimum of 75%; University requirement) is mandatory for all courses. Failure to adhere, a student will not be allowed to write the end semester exams.

6. There is a supplementary exam (with minimum of 75% attendance of same course previously attended) for each course. No provision available further to write the exams. There is no possibility to write the improvement examination for any course.

7. Mandatory credits (10)

(i) **CY801: Research Methodology** [4 credits]

The objective is to help research students understand the purpose and process of technical and research writing and documentation.

Part A will have lectures on academic writing and Part B: Preparation of a Research Proposal. The student will prepare and defend a research proposal based on self-study. The proposal will be evaluated by the doctoral review committee (DRC). The defense will involve presentation in a seminar.

(ii) **CY802: Research and Publication Ethics** (**RPE**) [2 credits]

This course is a mandatory requirement as per the UGC directives. The objective of the course is to help research scholars understand the fundamental relevance of ethical practice in academics, and to provide researchers with an overview of the current and emerging ethical issues in scientific research and publishing. The course will have lectures on ethics in scientific research and will have practice sessions.

(iii) There will be three theory courses in Chemistry. Student must choose any one (minimum). The offered courses are:

(a) **CY803: Essentials of Inorganic Chemistry** [4 credits]

(b) **CY804: Essentials of Organic Chemistry** [4 credits]

(c) **CY805: Essentials of Physical Chemistry** [4 credits]

8. Elective credits (2)

One of any of the courses (courses will have a credits from 2 to 3).

400/500 Level courses (other than Laboratory courses, Seminar or foundation course) offered in the M.Sc. Program. Students who did their M.Sc. program in the School of Chemistry can take a 400/500 level course only if they have obtained a grade less than **C** in the same course during their M.Sc. Students should check with School's Office for the list of courses offered in every semester.

More details of list of courses can be found at http://chemistry.uohyd.ac.in/MSc2Yr.htm

The detailed syllabus for Ph. D. courses are provided in pages 3-10 and grading system in page 11.

Course: **CY801: Research Methodology** [4 credits]

This course is a mandatory requirement for the Ph.D. course work. The objective is to help research students understand the purpose and process of technical and research writing and documentation.

Course outcome

The course will enable students to:

- Explain and understand the basic concepts of research
- Identify various sources of information for literature review and data collection
- Appreciate the components of scholarly writing and evaluate its quality
- Read and understand scientific literature, analyze the content and imbibe the critical message in the reports
- Formulate ideas and present them in a logical manner as scientific reports
- Prepare scientific writing in the form of research proposals, scientific articles or reviews, in a clear and precise language

Course implementation

The course has two parts.

- Part A: Lectures on **Academic Writing** (scientific and technical writing).
- Part B: Preparation of a **Research Proposal**. The student will prepare and defend a research proposal based on self-study. The proposal will be evaluated by the doctoral review committee (DRC). The defense will involve presentation in a seminar.
- Evaluation of the course will be as follows:
  - Part A: 10 marks from the evaluation based on the theory classes
  - Part B: 50 marks from the DRC based on proposal evaluation + 40 marks from the assessment of the presentation of the proposal.

Part A: Lecture plan

Academic Writing (Scientific and Technical Writing) (4 Lectures)

1. Types of research communication: Full length research paper, brief communications, letters to editor, review article, popular non-technical article, research proposal
2. Structure of Writing: Title of the manuscript, Abstract, Key words, Introduction, Materials and methodology, Results, Data presentation: figures, tables and legends, Discussion/Conclusion, Acknowledgement, Conflict of interest statement, References
3. Literature survey and Plagiarism
4. Writing skill: Elements of writing (argument and discussion, cause and effect, definitions); Writing Vocabulary and language (grammar, voice, clarity, academic vocabulary, word choice, Commas, parentheses, dash skewers Argument)

Reference books

1. A. H. Hofmann, *Scientific Writing and Communication: Papers, Proposals, and Presentations*, Oxford University Press, 2019.
2. M. S. Robinson, F. L. Stoller, M. S. Costanza-Robinson, J. K. Jones, *Write Like A Chemist: A Textbook and Resource*, Oxford University Press, 2008.
3. American Chemical Society and Royal Society of Chemistry publications and webinars.

Course: **CY-802: Research and Publication Ethics (RPE)** [2 credits]

This course is a mandatory requirement for the Ph.D. course work as per the UGC directives. The objective of the course is to help research scholars understand the fundamental relevance of ethical practice in academics, and to provide researchers with an overview of the current and emerging ethical issues in scientific research and publishing.

Course Outcome

After the completion of the course, research scholar would be able to understand and explain:

- The ethical dimensions of conducting research
- The critical relevance of accurate reporting of scientific methods and data

Course implementation

- It will be a 2-credit course with 30 contact hours
- The course will have lectures on ethics in scientific research and practice sessions

References

1. D. B. Resnik, *The Ethics of Science: An Introduction*, Routledge, 2005.
2. B. E. Rollin, *Science and Ethics*, Cambridge University Press, 2006 and 2009.
3. *Ethics in Research & Publication*, Elsevier. https://www.elsevier.com/__data/assets/pdf_file/0008/653885/Ethics-in-research-and-publication-brochure.pdf

Research and Publication Ethics (RPE)-Course for awareness about the publication ethics and publication misconducts.

Course Level:

- 2 Credit course (30 hrs)

Eligibility:

- Ph.D student and interested faculty members (it will be made available to Post-graduate students at later date)

Fees:

- As per University Rules

Faculty:

- Interdisciplinary Studies

Qualifications of faculty members of the course:

- **Ph.D in relevant subject areas having more than 10 years of teaching experience**

About the course:

Course Code: CPE-RPE

Overview

- This course has total 6 units focusing on the basics of Philosophy of Science and Ethics, Research Integrity, Publication Ethics. Hands-On-Sessions are designed to identify research misconduct and predatory publications. Index and citation database, Open Access Publications, Research metrics (citations, h-index, impact factor, etc.) and plagiarism tools will be introduced in this course.

Pedagogy:

- Classroom teaching, guest lectures, group discussions, and practical sessions.

Evaluation:

- Continuous assignment will be done through tutorials, assignments, quizzes, and group discussions. Weightages will be given for active participation. Final written examinations will be conducted at the end of the course.

Course structure:

- The course comprises of six modules listed in table below. Each module has 4-5 units

Modules	Unit title	Teaching hours
Theory		
RPE 01	Philosophy and Ethics	4
RPE 02	Scientific Conduct	4
RPE 03	Publications Ethics	7
Practice		
RPE 04	Open Access Publishing	4
RPE 05	Publication Misconduct	4
RPE 06	Database and Research Metrics	7
	Total	30

Syllabus in detail

THEORY

- **RPE 01: PHILOSOPHY AND ETHICS (3 hrs)**
  1. Introduction to philosophy definition, nature and scope, concept, branches
  2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

- **RPE 02: SCIENTIFIC CONDUCT (5 hrs)**

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

RPE 03: PUBLICATION ETHICS (7 hrs)

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiative and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publications misconduct: definition, concept, problems that lead to unethical behaviour 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

PRACTICE

- **RPE 04: open access publishing (4 hrs)**

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.

- **RPE 05: PUBLICATION MISCONDUCT (4 hrs)**

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

- **RPE 06: DATABASE AND RESEARCH METRICS (7 hrs)**

A. Databases (4 hrs)

1. Indexing databases
2. Citation databases: Web of Science, Scope, etc.

B. Research Metrics (3 hrs)

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g-index, i10 index, altmetrics

References

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: 9789387480865

National Academy of Science, National Academy of Engineering and Institute of Medicine. (2009). On Beinga 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

Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance (2019), ISBN 978-81-939482-1-7

http://www.insaindia.res.in/pdf/Ethics_Book.pdf

Course: **CY-803: Essentials of Inorganic Chemistry** [4 credits]

Main Group Chemistry	: Recent advances.
Transition metal Chemistry	: Correlation of structure, reactivity, electronic and magnetic properties of 3d,4d, 5d elements.
Inner Transition Metal	: Chemistry of f-block elements, differences from d-block elements and Chemistry magnetic properties.
Reaction Mechanisms	: Substitution reaction, anation and hydrolysis. Square planar substitution – trans effect. Electron transfer reactions – outer-sphere and inner-sphere mechanisms. Correlation of rates with structure and electronic configuration. Molecular rearrangements – fluxional molecules.
Organo-Transition Metal	: Complexes with -acceptor, and -donor ligands -18e and 16e rule – Chemistry several examples. Transition metal to carbon bonds in synthesis.
Catalysis	: Homogeneous and heterogeneous catalysis, hydrogenation, carbonylation and polymerization catalysed by transition metal compounds.
Metal Clusters	: Metal-metal bond, carbonyl clusters - low dimensional solids. Inorganic solid state chemistry.
Inorganic Photochemistry	: Ligand field photochemistry of d_6 complexes. Photochemistry of carbonyl complexes. Solar energy conversion and photodecomposition of water.
Bioinorganic Chemistry	: Biochemistry of iron - its storage, transport and function. Elementary ideas of photosynthesis and nitrogen fixation. Toxicity of heavy metals.

Suggested Readings:

1. Inorganic Chemistry: Shriver, Atkins and Langford.
2. Chemistry of the Elements: Greenwood and Earnshaw.
3. Inorganic Chemistry: Huheey.
4. An introduction to inorganic chemistry: Purcell and Kotz.
5. Advanced Inorganic Chemistry: Cotton and Wilkinson.
6. Inorganic Chemistry: Catherine E. Housecroft and Alan G. Sharpe
7. Original articles in the Primary Journals and Review Journals.

Course: **CY804: Essentials of Organic Chemistry** [4 Credits]

This course will deal with the survey of advanced concepts and theories of organic chemistry. It will be based on leading text books listed below as well as references to current literature. The emphasis will be on problem-solving. The topics to be covered are:

Bonding	: Strong and weak forms and bonds; their effects on molecular structure and conformations. Supramolecular chemistry
Stereochemistry	: Determination of absolute configuration, conformational analysis, and symmetric synthesis
Synthetic Transformations	: Modern reagents and methods in organic synthesis. Name reactions, target-oriented synthesis
Mechanism	: Their types and methods of determining them
Spectroscopy	: Use of modern spectroscopic methods including techniques like 2D NMR, GC-MS and X-ray crystallography in structure elucidation

Suggested Textbooks:

1. J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, Wiley, 2015.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part A and B*, Springer, 2008.
3. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, Wiley, 2008.
4. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, New Age, 2018.
5. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 2015.
6. H. O. House, *Modern Synthetic Reactions*, Benjamin-Cummings Publishing Co., 1972.
7. J. J. Li, *Name Reactions*, Springer, 2014.
8. E. J. Corey and X.-M. Cheng, *The Logic of Chemical Synthesis*, Wiley, 1995.
9. P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, Pearson, 2003.
10. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, Pearson, 1997.
11. S. Sankararaman, *Pericyclic Reactions - A Textbook: Reactions, Applications and Theory*, Wiley, 2005.
12. W. Kemp, *Organic Spectroscopy*, Springer, 2019.
13. R. M. Silverstein, F. X. Webster, D. J. Kiemle and D. L. Bryce, *Spectrometric Identification of Organic Compounds*, Wiley, 2014.

Course: **CY805: Essentials of Physical Chemistry** [4 Credits]

Thermodynamics	: First law, second law, phase transitions/mixtures, equilibria.
Electrochemistry	: Ions and electrodes, Debye-Huckel theory, electrochemical cells.
Quantum Theory	: Atomic structure and spectra, molecular structure.
Statistical	: Ensemble, partition functions, applications. Thermodynamics
Symmetry	: Point groups, representations, character tables, symmetry of crystals.
Spectroscopy	: Rotational, vibrational, electronic and magnetic resonance
Solid State	: Crystal lattices, diffraction methods.
Kinetic Theory/ Transport properties	: Kinetic theory of gases, laws of diffusion, transport properties
Chemical Kinetics	: Rate laws, complex reactions, fast reactions, microscopic kinetics.
Surface Chemistry	: Adsorption, surface catalysis.
Macromolecules	: Conformation and configuration, colloids.

The course will be based on the text 'Physical Chemistry' by P.W. Atkins and will be structured around problems on the above topics.

Suggested Readings:

1. Physical Chemistry, David Eisenberg & Donald Crothers.
2. Physical Chemistry, Robert A. Alberty.
3. Physical Chemistry, I.N. Levine.
4. Physical Chemistry, G.M. Barrow

Grading System for Ph. D. courses (as per UGC/UoH):

Letter Grade	Ph.D. Range of % of Marks (Theory)
A+	**80** to **100**
A	**75** to **79**
B+	**65** to **74**
B	**60** to **64**
C	**55** to **59**

Pass marks (minimum): 55%

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