Pre-Ph.D. Course work

Chemistry

Guidelines and Syllabus

offered by

Department of Chemistry

Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research

Veer Bahadur Singh Purvanchal University, Jaunpur

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Pre-Ph.D. Course work (Guidelines and Syllabus)

Aim of the Course work: The Pre-Ph.D. course work is designed to develop investigative, evaluative, comprehensive, reasoning, statistical analyses and writing skills in students to create an in depth understanding of their research area.

Programme prerequisite: Master degree in Chemistry or equivalent areas

Programme Outcomes: At the end of this programme, the student should be able

PO 1: To develop a basic in-depth understanding of a branch of science and attain specialization in one sub-branch.

PO 2: To understand the importance of research and development.

PO 3: To develop a strong foundation in the fundamental and applications of several advance topics of chemistry.

PO 4: To explore the concept of research, research tools and different types of research.

PO 5: To learn all spectroscopic techniques and interpret the spectral data of chemical compounds.

Programme Specific Outcomes: At the end of this programme, the student should be able

PSO 1: To gain knowledge of types of research, research tools and methodology

PSO 2: To understand the basics and applications separation and purification techniques,

PSO 3: To understand the basics and applications of different spectroscopic techniques

PSO 4: To develop skills in advanced techniques relevant to cutting-edge research in chemistry through advanced topical courses.

PSO 5: To use computational software and methods for chemical science research.

General Instructions:

1. All matters relating to admission to this course shall be dealt by the Ph.D. Admission Committee constituted by the university.
2. The duration of Pre-Ph. D. course work will be of one semester (six months).
3. As per the university ordinance, the research scholars who are provisionally registered for the Ph.D. programme will undergo a Pre-Ph.D. Course work which is mandatory for all.
4. In Pre-Ph.D. Course work, the Ph.D. candidate has to pass three compulsory theory papers of total 16 credits that comprises two main papers from the subject (6 + 6 credits) in which the candidate has taken admission and one paper on Research Methodology (that includes topics on research ethics, plagiarism and computer applications) (4 credits).
5. For successful completion of the course work, the Ph.D. candidate is also required to complete one non-credited research project of 100 marks in addition to the three compulsory papers. The letter grade for the research project will be Q or NQ. The grade of the research project will not be included in the computations of the CGPA.
6. All papers will have a total maximum mark of 100, including both Continuous Internal Evaluation(CIE) and University Examination (UE). Maximum marks of 25 will be allotted to CIE and 75 to UE.
7. The Ph.D. candidate has to obtain a minimum of 55% marks or equivalent Grades/CGPA in aggregate during the course work in order to be eligible to continue in the Ph.D. programme and submit the thesis.
8. The minimum attendance required during the course work period is 75% of the total courses. As Per UP government direction teachers in service are allowed to attend their Pre-Ph.D.- Course Work class either in online or in offline mode.

Scheme of the Programme

Paper	Course Code	Course Title	Credit	Marks
I	B091101T	Analytical and Instrumentation Techniques	6	100
II	B091102T	Advance Chemistry	6	100
III	B091103T	Research Methodology	4	100
IV	B091104R	Research Project	-	100

Credit system:

- A four (4) credit theory course/paper will have four Lectures/periods (of one hour) in a week. In one full semester the course will be covered in 60 Lectures.

- Similarly, a six (6) credit theory course/paper will have six Lectures/periods (of one hour) in a week. In one full semester the course will be covered in 90 Lectures.

Continuous Internal Evaluation (CIE) of 25 marks:

- Continuous internal evaluation will be performed by the teacher/ course coordinator concerned.
- CIE shall be 25% of total assessment in a Theory paper and research project.
- 25 marks shall be distributed as 5 marks for attendance, 5 marks for presentation and assignment and remaining 15 marks for class test.

Marking system:

- All papers will have a total maximum mark of 100, including both CIE and University Examination (UE). Maximum marks of 25 will be allotted to CIE and 75 to UE in a theory paper/ research project.
- The CIE of the research project shall be evaluated by the research supervisor and co-supervisor (if any).
- 75 marks of **research project** shall be distributed as 50 marks (project work and presentation) and a viva voce of 25 marks.
- The evaluation (Max Marks 75 UE) of the research project shall be done by internal examiner/s (Supervisor and Co-supervisor (if any)) and one external examiner appointed by the University.

Research Project Submission:

- The evaluated research project report in two sets of hard copy (spiral binding) must be prepared. One copy of it shall be submitted to the university if it demands. A second copy of the evaluated research project report must be in the records of the college/research center.
- The format of university Ph.D. thesis writing guidelines can be used as format of Research project writing guidelines.

Paper Setting and Evaluation Pattern (For Paper I, II and III)

Types of Question	Total Number of Questions	Questions to be attempted	Marks
Very short type	10	10	10x2=20
Short type	8	5	5x7=35
Long type	4	2	2x10=20
		Total Marks	75

The grading system for the Pre-Ph.D. course work shall be followed as given in table -1

Table-1

Letter Grade	Details	Limit of Marks	Grade Point
O	Outstanding	91-100	10
A+	Excellent	81-90	9
A	Very Good	71-80	8
B+	Good	61-70	7
B	Above Average	55-60	6
F	Fail	<55	0
AB	Absent	Absent	0
Q	Qualified		
NQ	Not Qualified		

Computation of CGPA:

Calculations for SGPA and CGPA shall be followed as given table 2:

Table 2

For j^{th} Sem. SGPA (S_j) = $\frac{\sum Ci.Gi}{\sum Ci}$	Here: C_i = number of credits of the i^{th} course in the j^{th} semester G_i = grade point scored by the student in the i^{th} course in j^{th} semester
CGPA = $\frac{\sum Cj.Sj}{\sum Cj}$	Here: S_j = SGPA of the j^{th} semester C_j = total number of credits in the j^{th} semester

Allocation of CGPA into Division:

The allocation of CGPA into division in pre-Ph.D. course work follows as given in Table 3:

Table 3

Division	CGPA
First	Greater than or equal to 6.5 and less than or equal to 10
Second	Greater than or equal to 5.5 and less than 6.5

Programme: Post Graduate Diploma in Research (PGDR)	**Year: six (**6)	**Semester:** XI
Subject: Chemistry		
Course Code: B091101T	**Course Title: Analytical and Instrumentation Techniques**	

Course Outcomes (COs): After completing this course, the students should be able to learn:

CO 1: Different thermal technique for materials characterization

CO 2: Different spectroscopic techniques such as UV-Vis, IR, Raman, EPR for characterization of compounds

CO 3: 1H, 13C, 19F, 31P NMR spectroscopy for characterization of compounds

CO 4: X-rays techniques such as XRD, XRF, SAXS for materials characterization

CO 5: Electron microscopy including SEM and TEM

CO 6: Different purification techniques and their applications

Credits: 6	**Core Compulsory**
Max. Marks: 25 (CIE) + 75(UE)	**Min. Passing marks: 55**

Total number of lectures: Lectures-Tutorial-Practical (6 hours in a week) L-T-P: 6-0-0 **(90 hrs)**

Unit	Topics	No. of Lecture Hrs.
I	Thermal methods: Principle, instrumentation and applications of DTG, DTA, TMA, DSC, Principle and applications of photometric and colorimetric techniques in inorganic analysis.	**15**
II	Spectroscopic Methods I: Principle, instrumentation and applications of UV, IR, Raman, EPR, Fluorescence spectroscopy example will be taken from real research related problem.	**15**
III	Spectroscopic Methods II : Principle, instrumentation and applications of NMR (1H, 13C, 19F, 31P) spectroscopy example will be taken from real research related problem.	**15**
IV	Spectroscopic Methods III: X-ray methods: Principle, instrumentation and applications of (XRD, XRF, SAXS) example will be taken from real research related problem	**15**
V	Electron Microscopy (SEM, TEM): Principle, instrumentation and applications, Imaging and Introduction to Interpretation, Image Interpretation and Artifacts, Electron Tomography; Electron Probe Micro Analysis (EDS, WDS): Principle, instrumentation and applications; Quantitative Analysis (AAS, ICP, CHN): Principle, instrumentation and applications	**15**

VI	Purification Techniques: A brief knowledge about various techniques such as distillation, fractional distillation, crystallization, fractional crystallization. Chromatography: i. Column, ii. TLC, iii. Paper, iv. Gas Chromatography, v. Ion Exchange, vi. HPLC, vii. Gel Permeation	**15**

Suggested Readings:

1. Fundamentals of Analytical Chemistry: D.A. Skoog, D.M. West and F.J. Holler, 1992, 6e
2. Analytical Chemistry, Gary D. Christian, 2007, 6eInstrumental Methods of Analysis: H.H. Willard, L.L. Merrit, Jr. J.A. Dean, 1974, 5e
3. Instrumental methods of analysis, Hobert H. Willard, D. L. Merrit & J. R. J. A. Dean, C.B.S Publishers and Distributors, 1992.
4. Modern spectroscopy, J. Michael Hollas, J. Wiley, 2004.
5. Instrumental Methods of Analysis, Ewing, 1992.
6. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM Ray F. Egerton, 2005, Springer, New York,
7. Transmission Electron Microscopy: A Textbook for Material Scientists, D. B. Williams and C. B. Carter 2nd edition" (2009) Springer,

Programme: Post Graduate Diploma in Research (PGDR)	**Year: six (**6)	**Semester:** XI
Subject: Chemistry		
Course Code: B091102T	**Course Title: Advance Chemistry**	

Course Outcomes: After completing this course, the students should be able to:

CO-1. Learn the basics and different applications of phosphorescent materials.

CO-2. Learn designing and synthesis of nanomaterials and metal organic frameworks (MOFs).

CO-3. Learn the mechanism of concepts and mechanism of organic synthesis.

CO-4. Learn the basics and different applications computational methods.

CO-5. Learn principle, mechanism and application of different energy sources.

CO-6. Learn the methods of analysis of polymers and its composites.

Credits: 6	**Core Compulsory**
Max. Marks: 25 (CIE) + 75(UE)	**Min. Passing marks: 55**

Total number of lectures: Lectures-Tutorial-Practical (6 hours in a week) L-T-P: 6-0-0 **(90 hrs)**

Unit	**Topics**	**No. of Lecture Hrs.**
I	**Phosphorescent Materials:** Luminescence, Types of Luminescence, Fluorescence, Phosphorescence, FrankCondon Principle, Jablouski diagram, Organic Electroluminescence, Organic Light Emitting diode, Structure and working of OLED,Applications of OLEDInorganic phosphorescent materials, Long Persistant phosphors phosphors for LED, Applications of Inorganic Phosphors	**15**
II	**Nanomaterials :** Preparation, Characterization and Application of nanomaterials, Metal Organic Framework (MOF), Organometallic compounds	**15**
III	**Advanced Organic Synthesis:** Application of photochemistry and radical chemistry in Organic Synthesis; Total synthesis of natural product, Asymmetric Synthesis.	**15**
IV	**Computational Chemistry:** Electronic structure theory (Post-Hartree-Fock methods and Moller-Plesset perturbation theory), Density functional theory based methods: Basis set and basis function, Hybrid and Minnesota functional – Application of DFT methods (excitation energy calculations). Density functional methods with Dispersion correction (Grimme's approaches, different software and related molecule to solid materials)	**15**

V	**Alternate energy materials and sources:** Non-renewable and renewable energy sources; description of renewable sources and their importance. Sustainable sources of hydrogen; Fuel cell technologies; Hydrogen production by water splitting by organic and inorganic catalysis, storage and distribution; Applications and feasibility assessment; Science, technology and policy of energy conservation; Strategies for enhancing role of renewable energy.	**15**
VI	**Advanced polymer science & technology:** Structure and Properties of different Polymers, Processing of polymer and its composite.	**15**

Suggested Readings:

1. Highly Efficient OLEDs with Phosphorescent Materials, Hartmut Yersin, Wiley, 2007.
2. Nanomaterials and Nanochemistry, C. Bréchignac, P. Houdy, M. Lahmani, Springer, 2007.
3. Nanomaterials Chemistry: Recent Developments and New Directions, C. N. R. Rao, Achim Müller, Anthony K. Cheetham, Wiley-VCH, 2007.
4. L. Metal-Organic Frameworks: Design and Application, L. MacGillivray, Wiley, 2010.
5. An Introduction to Practical Organic Chemistry – Robert, Vingrove etc.
6. Modern Analytical Chemistry by David Harvey, 3 rd Ed.
7. A Handbook of Computational Chemistry, Tim Clark, – Wiley-Interscience, New York
8. Introduction to Computational Chemistry, F. Jensen (Wiley)
9. Essentials of Computational Chemistry – Theories and Models, C. J. Cramer (Wiley)
10. Text Book of Polymer Science, F.W. Billmeyer, Wiley–Interscience, New York.1971.
11. Polymer Science, V.R. Gowariker, N.V. Viswanathan & J. Sreedhar, John Wiley & Sons, New York, 1986.
12. Physics & Chemistry of Polymers, J.M.G. Cowie, Blacke Academic Press, 1993.

Programme: Post Graduate Diploma in Research (PGDR)	**Year: six (**6)	**Semester:** XI
Subject: Chemistry		
Course Code: B091103T	**Course Title: Research Methodology***	

Course Outcomes (COs) After completing this course, the students should be able:

CO1: To decide the research field, topic, design, and sampling, and data collection techniques.

CO2: To understand the research process and acquire the skill of writingresearch articles.

CO3: To execute the best practices, morals, and ethical values in scientific conduct

CO4: To learn about the standards of journals for good-quality publications of their research work

CO5: To learn how to use computers and different application software for manuscript writing.

CO 6: To learn about reference management and the maintenance of integrity using scientific tools

Credits: 6	**Core Compulsory**
Max. Marks: 25 (CIE) + 75(UE)	**Min. Passing marks: 55**

Total number of lectures: Lectures-Tutorial-Practical (6 hours in a week) L-T-P: 6-0-0 **(90 hrs)**

Unit	Topics	No. of Lecture Hrs.
I	**Introduction of Research Methodology:** Meaning of research, objectives of research, types of research, significance of research, problems encountered by researchers in India.	**15**
II	**Research Problem:** Definition, necessity and techniques of defining research problem, Formulation of research problem, Objectives of research problem. **Research Design:** Meaning, need and features of good research design, Types of Research Designs, Basic Principles of Experimental Designs, Design of experiments, Synopsis design for research topic.	**15**
III	Ethical issues in science research and reporting: objectivity and integrity, the problem of plagiarism and related issues, international norms and standards, Scientific temper and virtues; expectations from scientific community, Desired temper of scientists: truthfulness, simplicity, humility, open mindedness; attitude of service towards social and human well-being.	**15**
IV	Nature and importance of Communication in Science, Preparation of manuscripts: review articles, research papers, books, monograms, research projects; review of manuscripts, Survey of literature, and presentation of data, Popularization of Science, Socio – Legal issues: Originality, Integrity, IPR, Patents, Plagiarism.	**18**

V	Computer application in chemistry, study of different software's (MS-Excel, MS office, Power Point, Chemdraw, GaussView). Introduction to Networking and Search using Internet, online submission, e-submission etc.	**15**
VI	Paper/Thesis Writing and Report Generation: Basic concepts of paper their writing and report generation, review of literature, Concepts of Bibliography and References, significance of report writing, steps of report writing, Types of Research reports, Methods of presentation of report.	**12**

*Applicable from session 2023-24. For session 2022-23, the Research Methodology course offer by university is applicable.

Suggested Readings:

1. C.R. Kothari, Research methodology Methods and Techniques, 4th Edition, New Age International (P) Ltd. Publisher, 2014.
2. W. Creswell, Research Design, Qualitative, Quantitative and mixed method approaches,
   3rd Edition, Sage Publications, Inc.
3. David B. Resnik, 1998, The Ethics of Science: An Introduction. Routledge publisher, USA.
4. Callahan D. & Bok S., 1996, Ethics Teaching in Higher Education. Plenum Press, New York, USA.Kapur J.N., 1996, Ethical Values for Excellence in Education and Science, Vishwa Prakashan, New Delhi.
5. Human Values. Tripathi A.N., 2008, New Age International Publishers, New Delhi.
6. Handbook of Science Communication, Antony Wilson, 1998
7. Communicating Science: A practical Guide, Laszis P: 2006, Springer
8. Latex tutorials https://www.tug.org/twg/mactex/tutorials/ltxprimer-1.0.pdf
9. Libre Office tutorial: www.documentation.libreoffice.org/en/english-documentation