

# Course Work for Ph.D. (Chemistry)



(Effective from May 2019)

Department of Chemistry  
School of Physical Sciences  
Guru Ghasidas Vishwavidyalaya  
Bilaspur-495 009

**Course Work for Ph.D. (Chemistry)**  
(To be implemented from the Session 2018-19)

**A. School-Specific Common Courses:**

S. No	Title of the paper	Paper Type	Credits
SPC-R1	Research Methodology & Computer Applications	Common course Compulsory	4

**B. Discipline-Specific courses: Total 10 credits:** All these courses are compulsory to each student.

S. No	Title of the paper	Paper Type	Credits
CH-R1	Modern Techniques in Chemical Sciences	Compulsory for Chemistry	4
CH-R2	Emerging Area in Chemical Sciences	Compulsory for Chemistry	4

**C. Research theme-specific courses:**

6 credits

S. No	Title of the paper	Paper Type	Credits
CH-R3	Seminar on research topic with written report by student Mode of study includes: Assigning the topic to students based on their basic background and presentation in the form of seminar which will be followed by discussion and submission of the write-up. This will be evaluated by group of teachers.	Successful	No Credit

**SCHOOL OF PHYSICAL SCIENCES**  
**GURU GHASIDAS VISHWAVIDYALAYA, BILASPUR (C.G.)**  
**(A CENTRAL UNIVERSITY)**  
**(IMPLEMENTED W.E.F. SESSION 2019-20)**  
**Ph.D (CHEMISTRY)**

**PROGRAMME OUTCOMES:** Graduate will be able to

**PO-1:** To impart quality education at doctoral levels through the well-designed curriculum to meet the demands of academia, research laboratories and industry.

**PO-2:** To provide the state-of-art research facilities to carry out original research in the leading-edge areas of Chemistry.

**PO-3:** To become a hub for human resource development and sponsored research projects with funding from national and global agencies.

**PO-4:** To associate with national and international reputed institutions for academic excellence and collaborative research.

**PROGRAMME SPECIFIC OUTCOMES:** Graduate will be able to

**PSO-1.** Demonstrate knowledge and skills in advanced and interdisciplinary areas of chemistry.

**PSO-2.** Employ sophisticated techniques and sound research methodologies to achieve the comprehensive solutions for specific problems.

**PSO-3.** Apply disciplinary knowledge and transferable skills to the interdisciplinary areas of chemistry to solve the problems.

**PSO-4.** Develop international standards in writing, communications, team-work, and ethics to disseminate results of research work.

**PSO-5.** Prepares future researchers, scientists, team-leaders, and scientific intellectuals in the chosen area of chemistry.

**PSO-6.** Demonstrate abilities to analyse the conditions in a given area of chemistry to create employment opportunities for chemists and society.

**Paper I**

**Credit 4**

**Research Methodology & Computer Applications**

**OBJECTIVES:** Describe research, identification of research problems, and preparation of proposals. Practice ethics in all the domains of research. Analyze the results using mathematical and statistical tools. Develop skills to use ChemDraw, Origin Lab, Schrödinger, and Quantum Espresso, etc. in the research work. Outline writing of research publication, presentation, and Ph.D. thesis.

**Unit 1: Research methodology**

Definition of Research, Components of Research Problem, Various Steps in Scientific Research : Hypotheses, Research Purposes, Research Design, Literature searching, Literature Survey, defining the question and formulating hypothesis/ hypothesizes, Collection of research data, tabulating and cataloging. Sampling and methods of data analysis.

**Unit 2: Errors in measurements and statistical methods:**

Types of errors; mean deviation, standard deviation and probable errors; propagation of errors with summation, difference, product and quotient, Probability Theories – Conditional Probability, Poisson Distribution, Binomial Distribution and Properties of Normal Distributions, Estimates of Means and Proportions; Chi-Square Test, Association of Attributes – t-Test – Standard deviation – Co-efficient of variations. Correlation and Regression Analysis, plotting of graphs.

**Unit 3: Laboratory practices and safety guidelines:**

Safe working procedure and protective environment, Laboratory safety measures, Handling radiation, Chemical hazards and their types, Safe chemical use, Proper storage and disposal of hazardous materials, Bio-hazardous and other toxic experimental materials, Maintenance of equipments.

**Unit 4: Computer applications in scientific writing skills**

Applications of Microsoft Excel, power point and origin for data processing and data analysis, research paper –presentation using power point (which include texts, graphs, pictures, tables, references etc.)(oral in power point/poster);

Curve fitting, Method of least square fit, least square fit (straight line) to linear equations and equation reducible to linear equations. Non-linear curve fitting, back ground correction and mathematical manipulation in data using **origin**.

Structure and Components of Research Report, Types of Report: research papers, thesis, Research Project Reports, Pictures and Graphs, citation styles, writing manuscript in Latex, Steps to better writing.

**Unit 5: Ethics in Science:**

The source of ethical issues in science: examples from different disciplines. 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.

IPR and Patent regime: Recording and storage/retention of recorded materials. Management and use responsibilities in proper utilization of the facilities. Socio-legal issues, originality

**References:**

1. "How to write and Publish" by Robert A. Day and Barbara Gastel, (Cambridge University Press).
2. "Survival skills for Scientists" by Federico Rosei and Tudor Johnson, (Imperial College Press).
3. "How to Research" by Loraine Blaxter, Christina Hughes and Malcolm Tight, (Viva Books).

4. "Probability and Statistics for Engineers and Scientists" by Sheldon Ross, (Elsevier Academic Press).
5. "The Craft of Scientific Writing" by Michael Alley, (Springer).
6. "A Students's Guide to Methodology" by Peter Clough and Cathy Nutbrown, (Sage Publications).

**COURSE OUTCOMES:** *After completion of this course successfully, the students will be able to.....*

**CO-1:** Describe research, identification of research problems, and preparation of proposals.

**CO-2:** Practice ethics in all the domains of research.

**CO-3:** Analyze the results using mathematical and statistical tools.

**CO-4:** Develop skills to use ChemDraw, Origin Lab, Schrödinger, and Quantum Espresso, etc. in the research work.

**CO-5:** Outline writing of research publication, presentation, and Ph.D. thesis.

*Course Outcomes and their mapping with Programme Outcomes:*

CO	PO				PSO					
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	2	2	3	3	3	3	3	3
CO2	3	2	1	1	2	2	2	3	2	2
CO3	3	2	1	1	1	1	1	1	1	1
CO4	3	2	1	1	2	2	2	2	2	2
CO5	3	2	1	1	2	2	2	2	2	2

Weightage: **1-Sightly; 2-Moderately; 3-Strongly**

**Paper II**

**Credit 6**

**Modern Techniques in Chemical Sciences**

**OBJECTIVES:** *Students will learn about basic theories of instruments and computational chemistry. And also learn experimental data analysis of compounds by the various instruments.*

Basic theory, instrumentation and analytical applications: Spectroscopic techniques [NMR, ESR, MS (EI, FAB, MALDI-TOF), IR, UV-Vis, Fluorescence and Phosphorescence, Atomic Absorption, Biosensors.

**Techniques for Materials Characterization**

Basic theory and analytical applications of the following physical methods: X-ray diffraction methods (single crystal and powder method), Thermoanalytical methods (TGA, DSC, DTA), Microscopic methods (SEM, TEM, AFM), Surface Properties (XPS, BET), Cyclic Voltammetry, SQUID.

**Separation Techniques:**

Introduction, classification of chromatographic methods, terms and relationships in chromatography, sample characterization High performance liquid chromatography (HPLC), Gas chromatography (GC) and ion exchange chromatography, GPC.

Principle, Instrumentation and Application of :

Reverse Osmosis (RO), Nanofiltration (NF), Ultra Filtration (UF) and Micro Filtration (MF), gel electrophoresis, chiral separations.

**Computational Chemistry:** Theoretical Chemistry a quantum approach, MO theory, Ab initio calculation, Geometry optimization, basis set, electronic structure calculations.,

### **Books Recommended**

1. F.W Fifield & D.Keal, Principles and Practice of Analytical chemistry Blackwell Publishing Company, (2004)
2. Pradyot Patnaik, (2004), Dean's Analytical chemistry, Hand Book Second edition Graw- Hill Hand Books
3. J. D Seader /Ernest J. Henley, Separation Processes Principles; John Wiley & Sons Inc. (1998)
4. Skoog, Holler, Nieman, H.B Principles of Instrumental Analysis Fifth edition College publishers.
5. G.H. and H. Freiser, Solvent Extraction in Analytical Chemistry, 1<sup>st</sup> edition (1958), John Wiley, New York.
6. B. L. Karger, L.R. Snyder and C. Howarth, An Introduction to Separation Science, 2<sup>nd</sup> edition (1973) John Wiley, New York.
7. E.W. Berg, Chemical Methods of Separation, 1<sup>st</sup> edition (1963), McGraw Hill New York.
8. D.G. Peters, J.M. Hayes and C.M. Hieftj, Chemical Separation and Measurements, 2<sup>nd</sup> edition 1974, Saunders Holt, London.
9. R.M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, Edition (2003) John Wiley, New York. F J.R. Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi (1978).
10. J.M. Hollas, Modern Spectroscopy, 4th edition (2004), John Wiley and Sons, Chester.
11. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
12. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
13. D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, 5th edition (1998), Harcourt Brace & Company, Florida.
14. H.A. Strobel, Chemical Instrumentation – A Systematic Approach, 2nd Edition (1973), Addison Wesley, Mass.
15. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Analytical Analysis, 2nd Edition (1976), John Wiley, New York.

**COURSE OUTCOMES:** After completion of this course successfully, the students will be able to.....

**CO-1:** learn basic theories of different instruments and techniques.

**CO-2:** know analysis of chemical compounds by different techniques.

**CO-3:** learn use of different instruments and laboratory techniques.

**PO-5:** Evaluate the experimental and computational skills

### **Course Outcomes and their mapping with Programme Outcomes:**

CO	PO				PSO					
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	2	2	2	3	3	3	3	3	3
CO2	2	2	1	1	2	2	2	2	2	2
CO3	2	2	1	1	1	2	2	2	2	2
CO4	2	2	1	1	2	2	2	2	2	2

Weightage: **1-Slightly; 2-Moderately; 3-Strongly**

**CH-R2: Thrust Area in Chemical Sciences**

**OBJECTIVES:** *Students will learn about basic theories of various fields of chemistry such as green chemistry, Nanochemistry, organometallic reagents, multicomponents reactions, chemistry of molecular recognition and polymer chemistry.*

- 1. Emerging Green Chemistry:** Green chemistry, introduction, 12 principles, Solvent-free synthesis; Environmentally benign solvents: Water and Ionic liquids as green solvents and catalysts in organic synthesis. Microwave in chemical synthesis: Basic principles, advantages and examples. Sonochemistry and green aspects;
- 2. Nano-Chemistry:** Introduction, **Nucleation and growth, heterogeneous nucleation,** Size effect, Synthesis and assembly, techniques, General methods of preparation and synthesis. Types of nano materials, their Properties and applications. Carbon nanotube, micro- and mesoporous materials.
- 3. Formation of Carbon-Carbon bonds via organometallic reagents:** (i) Palladium-Catalyzed Coupling Reactions, (ii) Organoboron Reagents, (iii) Organozinc Reagents, (iv) Organocopper Reagents.
- 4. Multicomponent reactions (MCRs):** Definition, Advantages and examples particularly, Ugi reaction, Biginelli reactions, Strecker amino acid synthesis, Passerini synthesis, Mannich reaction,
- 5. The chemistry of molecular recognition:** Host and Guest Chemistry. Supramolecular interactions and their characterization, Supramolecular catalysis and transport processes, Cyclodextrin- a naturally occurring cyclic host, calixarene- a versatile host; Chemosensor, Electrochemical sensors, Origin and source of chirality, chiral ligands, chiral drugs, asymmetric epoxidation
- 6. Polymers:** Mechanism and kinetics of radical, condensation and living radical polymerizations. Spectroscopic characterization and testing of polymers. Measurement of molecular weights: viscosity, light scattering, osmotic and size exclusion chromatographic method. Properties and applications of commercial polymers: polyamides, polyesters, phenolic resins, epoxy resins and silicones. Fire retarding polymers, conducting polymers, and biocompatible polymers.



**Books Recommended**

1. Mike Lancaster, Green Chemistry: An Introductory Text, Royal Society of Chemistry, 2002.
2. Nina Hall( Editor-in-chief), The new Chemistry, Cambridge university Press, 2000.
3. CNR Rao, Muller and Cheetham, The Chemistry of Nano Materials, Vol.I & II, Wiley-VCH (2005)
4. Geoffrey A. Ozin, and Andre Arsenette, Nano Chemistry, RSC Publishing, 2005
5. S.C. Tjong, Nano Crystalline Materials Elsevier, 2006
6. George S. Zweifel, Michael H. Nantz, Modern Organic Synthesis - An Introduction, 1st Edition, 2007; ISBN: 978-0-716-77266-8; Ed. W. H. Freeman
7. Dale L. Boger, Modern Organic Synthesis, TSRI press.
8. P. S. Kalsi, Organic Reactions and Their Mechanisms, 1st Edition (1996), New Age International Pub., New Delhi.
9. M. B. Smith, Organic Synthesis, (1998) Mc Graw Hill Inc, New York
10. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001
11. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
12. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2<sup>nd</sup> Ed. (1981), John-Wiley & Sons, New York.
13. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An introduction and Guide, Wiley, New York (1995).
14. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
15. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998).
16. Ariga Katsuhiko, Kunitake Toyoki, Supramolecular chemistry- fundamentals and applications: advanced text book, Publisher: Iwanami Shoten Publishers, Tokyo, 2006.
24. Jean Marie Lehn, Supramolecular chemistry: concepts and perspective, Wiley-VCH (June 1995).
25. Crego-Calama, Mercedes Reinhoudt, Davis N. Ed. Supramolecular chirality, Topics in current Chemistry, vol 265, 2006, Springer Verlag.
26. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn., (1999), John-Wiley & Sons, New York.
27. Catalysis: Principles and Application, editor(s) : B. Viswanathan, S. Sivasanker, A.V. Ramaswamy ISBN: 978-81-7319-375-0: (2007).
28. Jacobsen, E.N., Pfaltz, A.; Yamamoto, H. (ed), Comprehensive Asymmetric Catalysis I-III; Springer Verlag: Berlin, 1999.
29. Textbook of Polymer Sciences, F. W. Billmeyer Jr, Wiley.Polymer Sciences, V. R. Gwariker, N. V. Vishwanathan and J. Sreedhar, Willey-Eastern.
30. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R. M. Otanbrite.
31. Contemporary Polymer Chemistry, H. R. Alcock and F. W. Lambe, Prentice Hall.
32. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and Professional.

**COURSE OUTCOMES:** After completion of this course successfully, the students will be able to.....

**PO-1:** understand the research work.

**PO-2:** identify the cutting-edge areas in related topics.

**PO-3:** develop knowledge to solve problems in various research fields.

**PO-4:** learn the advantages of the research work in interdisciplinary fields.

*Course Outcomes and their mapping with Programme Outcomes:*

CO	PO				PSO					
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	2	2	2	3	3	3	3	3	3
CO2	2	2	1	1	2	2	2	2	2	2
CO3	2	2	1	1	1	2	2	2	2	2
CO4	2	2	1	1	2	2	2	2	2	2

Weightage: 1-Sightly; 2-Moderately; 3-Strongly

**CH-R3 : Seminar on research topic with written report by student**  
**No Credit**

**OBJECTIVES:** Students will learn presentation and report writing along with research articles writing.

Mode of study includes: Assigning the topic to students based on their basic background and presentation in the form of seminar which will be followed by discussion and submission of the write-up. This will be evaluated by group of teachers.

**COURSE OUTCOMES:** After completion of this course successfully, the students will be able to.....

**PO-1:** present research work as well as competent to teaching and interview for various jobs.

**PO-2:** identify the cutting-edge areas in related topics.

*Course Outcomes and their mapping with Programme Outcomes:*

CO	PO				PSO					
	PO1	PO2	PO3	PO4	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	2	2	2	2	2	3	2	2	2
CO2	2	2	1	1	1	1	1	1	2	2

Weightage: 1-Slightly; 2-Moderately; 3-Strongly

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