Name of the Programme: Ph.D. (Chemistry)
Course Code: CHC-700
Title of the course: Research Methodology
Number of Credits: 04
Effective from AY: 2022-23

Pre-requisites for the Course:	Provisional registration for PhD in Chemistry	
Course Objectives:	1. To introduce research students to various aspects of research methodology. 2. To provide understanding of various databases used in chemistry for literature survey 3. To provide fundamental roles of computers in chemical research 4. To provide understanding and importance of lab safety. 5. To make students aware of the statistical methods used in chemical research. 6. To understand the usefulness of various instrumental techniques in characterization of chemical compounds.	
Content:	**1. Introduction to Research Methodology** a) Research- meaning, objectives, motivation, types and methodology. b) Process- formulating the research problem; literature survey; developing the hypothesis and the research design; sample design and collection of the data; execution of the project; analysis of data; testing of hypothesis; generalizations and interpretation, and preparation of the report or presentation of the results & conclusions. c) Nature of scientific information- types of books, types of presentations published in journals, standard format for reporting original research, introduction to various scientific (chemistry) databases & sources from the internet. **2. Role of Computers in Research and chemistry** a) Applications of computers in research. Applications of computer in Chemistry - Need of computers in chemistry-introduction & history; Introduction to programming & programming languages; Solving a problem with computers-algorithm, flowchart and program; Use of software for data handling, plotting graphs and drawing molecular structures, visualisation of 3-D data; Software for literature survey, software for reference citing b) Optimisation techniques and applications in molecular geometry optimisation **3. Safety aspects in Chemistry** a) Introduction to lab safety. b) Handling of various chemicals, solvents & glassware. c) Fires and fighting with fires. d) Hazardous substances, classification and handling e) Safety data sheet **4. Introduction to Statistical methods** a) Errors & their types, precision & accuracy in chemical analysis. b) Application of statistical methods to data treatment & evaluation. c) Confidence limits; hypothesis testing. d) F-tests, Chi square test, correlation and linear regression. e) Use of software for statistical analysis. **5. Instrumental methods of analysis** Data analysis in following techniques:	10 10 8 10 22

	a) Elemental analysis: CHNS analysis and AES b) Infrared (IR), Raman, Ultraviolet-Visible (UV-Vis) c) Nuclear magnetic resonance (^{1}H, ^{13}C) d) LC-MS, GC-MS e) X-ray diffraction f) Thermal analysis: TG/DTA g) Microscopy: SEM, TEM h) Methods for determination of magnetic & dielectric properties. i) Cyclic voltammetry j) AFM k) BET	
Pedagogy:	Mainly lectures/recorded video lectures/ tutorials, discussions, seminars, internal exams/ assignments, / self-study or a combination of some of these. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References/ Readings:	1. C. R. Kothari, *Research Methodology: Methods & Techniques*, New Age International Pvt. Ltd., 2004. 2. M. Coghill & L. R. Garson, *The ACS Style Guide: Effective Communication of Scientific Information*, American Chemical Society Washington, DC & OXFORD University Press New York, 2006. 3. Y. K. Singh, *Fundamentals of Research Methodology & Statistics*, New Age International Pvt. Ltd., 2006. 4. National Research Council, *Prudent practices in the laboratory: handling and management of chemical hazards*, The National Academies Press, USA, 2011. 5. B. S. Furniss, A. J. Hannaford, P. W. G. Smith & A. R. Tatchell, *Vogel's Text book of Practical Organic Chemistry*, 5th Ed.; Longman, 1989 6. E. A. V. Ebsworth, D. W. H. Rankin & S. Craddock, *Structural Methods in Inorganic Chemistry*, Blackwell Scientific Publishers, 1986 7. R. S. Drago, *Physical Methods in Chemistry*, 2nd Ed. W. B. Saunders Co. Ltd. 2016 8. R. M. Silverstein, F. X. Webster; *Spectrometric Identification of Organic Compounds*; 6th Ed, Wiley, 2011. 9. J. Mendham, R. C. Denny, J. D. Barnes & M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, 6th Ed.; Pearson Education Asia, 2002. 10. H. V. Keer, *Principles of the Solid State,* 1st Ed. (Reprint 2005); New Age International (P) Ltd., 1993. 11. G. D. Christian, *Analytical Chemistry*, 6th Ed.; Wiley, 2004. 12. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, *Fundamentals of Analytical Chemistry*, 9th Ed.; Cengage learning. 13. A. Skoog, F. J. Holler, S. R. Crouch, *Principles of Instrumental Analysis*, 7th Ed.; Cengage learning. 14. Pavia, G. Lampman, G. Kriz and J. Vyvyan, *Introduction to Organic Spectroscopy*, 5th Ed.; Cengage Learning, 2015. 15. N. Elgrishi, K. J. Rountree, B. D. McCarthy, E. S. Rountree, T. T. Eisenhart, and J. L. Dempsey, *A Practical Beginner's Guide to Cyclic Voltammetry*, J. Chem. Educ. 2018, 95, 197−206. 16. V. Rajaraman, *Computer Programming in Fortran 90 And 95*, PHI Learning Pvt. Ltd., 2013. 17. A. Szabo, N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications, Inc. Mineola, 1989.	
Course Outcomes:	1. Students will be able to apply the concepts of research methodology 2. Students will be able to apply computer technology to solve their research problems in chemistry. 3. Students will take safety precautions in chemical lab.	

	4. Students will apply statistical methods of data handling in their research. 5. Students will be able to apply characterization techniques for sample analysis.