M. Phil/Pre PhD Course in Chemistry

Paper I. Research Methodology and Computer Applications in Chemistry.

Part A Research Methodology---------------------------------------------(20 hr)

Introduction to research methodology, definition of research, characteristics of research, types of research, the research process, formulating research problem, reviewing the literature.

Literature of Chemistry

Primary sources – journals and patents, secondary resources, listing of titles, abstracts, CA, collective indexes, bielstein, compendia and tables of information, reviews, annul reviews, awareness service, general treatise, monographs on specific areas, text books, other books,

Literature searching

(i) Using printed materials
(ii) Searching on – line

Database, Scifinder, Scopus, CA on CD
Locating research article
Citation Index, Impact Factor

Writing scientific report, planning, preparation, draft, revision and refining; Writing project proposal to funding agency; Paper writting for international journals, submitting to editors. Conference presentation, preparation of effective slides, how to give good talk.

BOOKS

2. Practical Research Methods, Catherine Dawson, UBS Publisher’s Distribution, New Delhi 2002.
5. Introduction to Research & Research Methodology M. S. Sridhar.
Paper B Computer Applications in Chemistry. ----------------------(20 hr)

1. Programming in Chemistry
   Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titrations, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles, etc. of molecules extracted from data base such as Cambridge data base.

2. Use of Computer Programs
   The students will learn how to operate a PC and how to run standard programs and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programming, Monte Carlo and Molecular dynamics. Programs with data preferably from physical chemistry laboratory.

3. Spectroscopic library searching and structure elucidation, graphical display of data. Graphical display of molecules. Artificial intelligence and expert system, pattern recognition, molecular mechanics and molecular dynamics.


5. Chemical information, structure elucidation, synthesis design, simulation of reaction, physicochemical data, molecular modeling, molecular graphics, data banks.

BOOKS
3. Computer algorithms for selecting molecule libraries for synthesis, Konstantin V. Balakin, Nikoloy P. Savchuk and Alex Kiselyou.
5. Chemometrics – Statistics and Computer Applications in Analytical Chemistry
   Matthias Otto, Wiley – VCH.