Ph.D. Coursework (Chemistry) Syllabus

Department of Chemistry
Rajiv Gandhi University
Arunachal Pradesh

Ph.D. Coursework Syllabus
Paper I: Research Methodology

Total Marks: 100
Sessional / Assignment: 25 marks
End Semester: 75 marks

UNIT I: Research Basics
Basics of scientific research, research process and steps involved, Hypothesis, Research proposals and aspects, literature survey, sources of information, review. Ethical issues and intellectual property rights.

UNIT II: Scientific Report Writing and Publication Process
Writing of research report and synopsis (steps involved), paper writing (steps involved), review writing, report preparation, publication process, selection of journals, citation index, impact factor, *h*-index.

UNIT III: Data Collection and Processing
Data types and collection: qualitative and quantitative, data processing, data analysis. Sampling: types, steps involved in sampling, sample size, advantages and limitations.

UNIT IV: Computer Basics and Application
Introduction to basic hardwares and softwares (MS Word, Power Point, Excel, Origin), bits, bytes, words, CPU, memory, operating systems (DOS, WINDOWS, UNIX). Scientific computer uses, algorithms and flow-charts, programming (with FORTRAN). Introduction to chemistry related softwares (Gaussian, Gaussview, ChemDraw etc.) and databases (SciFinder, Scopus, Cambridge Structural Database (CSD)).

UNIT V: Numerical Methods and Statistical Analysis
Curve fitting (least square), solution of polynomial equation, numerical integration (Trapezoidal rule, Simpson's rule, Gaussian qudrature), solution of ordinary differential equations (Euler's method, Runge-Kutta method, predictor-corrector method), matrix multiplication, inversion and diagonalisation.

Assignment: Literature survey / review writing on selected topics

Suggested Books

1. Kumar, R., *Research Methodology - A Step-By-Step Guide for Beginners*, Pearson Education, Delhi (2006).
2. Montgomery, D. C., Design & Analysis of Experiments, 5th Ed., Wiley India (2007).
3. Kothari, C. K., *Research Methodology-Methods and Techniques*, 2nd Ed., New Age International, New Delhi.

Ph.D. Coursework Syllabus
Paper II: Physical Methods in Chemistry

Total Marks: 100
Sessional / Assignment: 25 marks
End semester: 75 marks

UNIT I: Principle and Applications of NMR Spectroscopy

Basic principles, chemical shift, spin-spin coupling, relaxation processes, first order spectra, simplification of NMR spectra, application of ^{1}H and ^{13}C NMR spectra of some organic compounds, use of ^{1}H, ^{13}C and ^{31}P NMR spectroscopy in coordination chemistry. Simple applications to diamagnetic and paramagnetic inorganic compounds.

UNIT II: Applications of IR spectroscopy in Organic and Inorganic Chemistry

IR spectroscopy: Characteristic vibrational frequency / bands of hydrocarbons and important functional groups. IR spectra of aliphatic and aromatic alcohols, aldehydes, ketones, carboxylic acids, esters and amides. Application of IR spectroscopy in metal complexes.

UNIT III: Applications of UV-vis in Organic and Inorganic Chemistry

λ_{max} and molar absorptivity, factors affecting them. Calculation of λ_{max}-Woodward Fieser rule, electronic spectra of transition metal complexes: term symbols, Orgel diagram, Tanabe-Sugano diagrams, Calculation of Dq, B and β values, selection rules, band intensities and band width, charge transfer spectra.

UNIT IV: Mass Spectrometry

Basic principle and instrumentation, methods in mass spectroscopy, mass spectral fragmentation of organic compounds, examples of mass fragmentation of different groups of organic and inorganic molecules with respect to their structure determination, effect of isotopes on the appearance of mass spectrum. Application to organometallic compounds.

UNIT V: Characterization of Materials

Material characterization: Basic principles and applications of XPS, UPS, AES, SEM, TEM, XRD, DTA-TGA, DSC.

Recommended Books

1. Banwell C. N.; McCash, E. M., *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill (2006).
2. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Spectroscopy*, 4th Ed., Cengage Learning (2010).
3. Drago, R. S., *Physical Methods for Chemists*, Saunders Company (1999).
4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, Prentice Hall (2004).
5. Kemp, W., *Organic Spectroscopy*, Macmillan (2011).
6. Aruldas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., Prentice Hall India (2001).

7. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds*, Wiley-Interscience, New York (2008).
8. Gunther, H., *and NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., John Wiley & Sons (1995).
9. Viswanathan B.; Kannan S.; Deka, R. C., *Catalysts and Surfaces Characterization Techniques*, Narosa Publishers (2010).