

**DEPARTMENT OF CHEMISTRY**  
**UNIVERSITY OF CALICUT**

**Syllabus: RESEARCH METHODOLOGY IN CHEMISTRY**

**UNIT I: RESEARCH METHODOLOGY AND DATA ANALYSIS**

Research processes - scientific research, formation of the topic, hypothesis, conceptual definitions, operational definition, gathering of data, analysis of data, revising of hypothesis, Conclusion. Literature survey - Journals, books and e-resources. Presentation and publication of research output. Errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation, comparison of results: “t” test, “f” test and “chi” square test, least squares analysis, weighted least squares analysis, regression coefficient, rejection of results, presentation of data.

**References**

- 1 Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
- 2 Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
- 3 Anthony M Graziano and Michael L Rau, Research Methods: A Process of Inquiry, Prentice Hall, 2006.
- 4 [Peter C Jurs](#), Computer Software Applications in Chemistry, 2nd Ed., John Wiley & Sons, New York, 1996.

**UNIT II APPLICATIONS OF COMPUTERS IN CHEMISTRY**

History of development of computers, mainframe, mini, micro's and super computer systems. Personal computers. General awareness of computer hardware, CPU, input and output devices, memory, other peripheral devices, auxiliary storage devices. Basic knowledge of computer systems, softwares - System softwares and application softwares Programming languages: machine language, assembly language and high level languages. Interpreter and compiler. Flow charts and Algorithms. General awareness of operating systems: Disk operating system, Windows, Macintosh, Linux. General awareness of Software packages and other scientific application packages. Applications and uses of common softwares in chemistry, Origin, Chems sketch, Chemdraw. Basic ideas on the use of Internet in Chemistry education.

**References**

- 1 Madric and Donevan, Understanding Computers, McGraw Hill.
- 2 KV Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
- 3 P Lykose, Personal Computers in Chemistry, John Wiley and Sons, New York, 1981.
- 4 Ramesh Kumari, Computers and their applications to Chemistry, 2nd Ed., Alpha Science
- 5 Biggs Pete, Computers in Chemistry, Oxford University Press, 2000

- 6 Cartwright Hugh, Using Artificial Intelligence in Chemistry and Biology: A Practical Guide, CRC Press, 2008
- 7 Cropper William H, Mathematical Computer Programs for Physical Chemistry, Springer
- 8 Stephen Wilson, Chemistry by Computer: An Overview of the Applications of Computers in Chemistry, **Plenum Pub Corp, 1986**
- 9 [Peter C Jurs](#), Computer Software Applications in Chemistry, 2nd Ed., John Wiley & Sons

### UNIT III CHROMATOGRAPHIC TECHNIQUES

Gas chromatography: Theory of chromatography, column efficiency and column equation, sample injection, sampling system for capillary columns and packed columns, detectors, gas flow control system, high resolution gas chromatography/mass spectroscopy.

HPLC: Principles of high performance liquid chromatography, the liquid chromatograph, the requirements of solvent pumping and different pumping systems, gradient elution, isocratic elution, sampling, detectors for liquid chromatography, the mobile phase in HPLC, solvent degassing, column technology, column selection, quantitative analysis by HPLC.

#### References

- 1 Hobart H Willard, Lynne L Merritt, Jr., Jonn A Dean, Frank A Settle, Jr (Ed.), Instrumental Methods of Analysis, 7th Ed., WADSWORTH publishing company, 1988.
- 2 DA Skoog & M West, Principles of Instrumental Analysis, Saunders Golden Sunburst Series.

### UNIT IV ANALYTICAL TECHNIQUES FOR CHEMICAL RESEARCH

Optical Methods of analysis, basic principles of uv-visible, AAS, AES, flourometric and phosphorometric methods. Electroanalytic methods-Principles and applications of polarography, amperometry, coulometry and cyclic voltametry.

Thermal methods of analysis- Principles and important applications of thermogravimetry (TG)- differential thermal analysis (DTA), differential scanning calorimetry (DSC), dilatometry (DIL) and dynamic mechanical analysis (DMA).

#### References

- 1 **AI Vogel**, A Text Book of Quantitative Inorganic Analysis, ELBS Longman's Green and Co **Ltd., London, 1962.**
- 2 DA Skoog and M West, Fundamentals of Analytical Chemistry, Saunders Golden Sunburst Series.
- 3 JD Dick, Analytical Chemistry, McGraw-Hill, 1972.
- 4 WW Wendlandt, Thermal Methods of Analysis, Interscience, New York, 1964.
- 5 PJ Haines, Thermal Methods of Analysis: Principles, Applications and Problems, Blackie Academic and professional, New York, 1995.
- 6 GWH Hohne, WH Hemminger and HJ Flammersheen, Differential Scanning Calorimetry, 2<sup>nd</sup> Edition, Springer.

- 7 C Duval, Inorganic Thermogravimetric Analysis, Elsevier, 1963.
- 8 Paul Gabbott, Principles and Applications of Thermal Analysis, Wiley.

## **UNIT V      PHYSICAL METHODS OF STRUCTURE ELUCIDATION**

An integrated problem solving approach to the elucidation of structures of organic compounds based on UV, IR, NMR ( $^1\text{H}$  and  $^{13}\text{C}$ ) and Mass spectral techniques. Modern NMR experiments: NOE, APT, DEPT, HOMCOR ( $^1\text{H}$ - $^1\text{H}$ ) and HETEROCOSY ( $^1\text{H}$ - $^{13}\text{C}$ ).

Use of electronic, IR, NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ), Mossbauer and ESR in the structure elucidation of inorganic and coordination compounds.

### **References**

- 1 William Kemp, Organic Spectroscopy, ELBS London, 1987.
- 2 RM Silverstein, CG Bassler and TC Morrill, Spectroscopic Identification of Organic Compounds, 4<sup>th</sup> Edition, John Wiley & Sons, New York, 1981.
- 3 Donald L Pavia, Gary M Lampman and George S Kriz, Introduction to Spectroscopy, 3<sup>rd</sup> Edition, Saunders Golden Sunburst Series.
- 4 CN Banwell and Elaine M McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Edition.
- 5 Raymond Chang, Basic Principles of Spectroscopy, RE Krieger Publishing Co., Huntington, New York, 1978.

**Model Question Paper**  
**Paper I: RESEARCH METHODOLOGY IN CHEMISTRY**  
**(Ph. D. Programme in Chemistry)**

Time: 3 hours  
marks

Maximum: 70

**Section A**

Answer all questions. Each question carries 2 marks

1. Define column efficiency and column equation?
2. Differentiate interpreter and compiler?
3. Define regression coefficient?
4. What is an Operating System? Give examples.
5. What is significant figure? Explain.

(5×2 = 10 marks)

**Section B**

Answer any five questions. Each question carries 4 marks

6. Explain basic ideas on the use of internet in chemistry education?
7. (i) Define flowchart and algorithm? (ii) What is meant by isocratic elution and gradient elution?
8. Describe the principles and applications of TG?
9. Discuss the principle involved in the functioning of flame ionization detector?
10. What is the need of literature survey in a research work? Explain the methods used in literature survey?
11. Discuss the various applications of Mossbauer spectroscopy in structural elucidation of inorganic and coordination compound?
12. Explain (i) "chi" square test. (ii) Least square analysis.
13. Define software? Explain briefly system software and application software

(5×4 = 20 marks)

**Section C**

Answer any five questions. Each question carries 8 marks

- 14 Explain the following (i) "t" test. (ii) "f" test (iii) Mean and standard deviation.
15. Write a brief note on programming languages?
16. Give a brief account on the instrumentation used in HPLC with the help of a block diagram?
17. Comment on the principle and applications of amperometry?
18. Explain briefly the common software's used in chemistry education?
19. Write the history and development of computers?
20. Briefly explain the errors in chemical analysis?
21. Discuss the steps involved in scientific research?

(5×8 = 40 marks)