Subject Code : N4B10

PAPER X : COMPUTER APPLICATIONS AND ANALYTICAL CHEMISTRY

UNIT – I

BASIC CONCEPTS OF COMPUTING AND NETWORKING

01. Introduction to computers and computing – hardware – basic organization of a computer - CPU – Main memory – secondary storage – I/O devices – Software – System and application Software – High and low level languages – Compliers – Algorithms and Flowcharts.

02. Introduction to networking – computer networks –network components-hubs, switches, repeaters, routers, bridges – brouters and gateways-network topologies-star, bus and ring – LAN, WAN, Intranet and internet – World Wide Web – internet for chemists – online search of chemistry database – search engines for chemistry – chemweb. (18 hours)

UNIT – II

C PROGRAMMING I

03. C Programming – Structure of a C program – Data types, Variables, Constants, Keywords, Operators, Expression.

04. Control structure – if, if-else, nested if-else, while, while-do, for, nested for, goto, continue, break, switch case statements(18 hours)

UNIT – III

C PROGRAMMING II

05. Arrays – User defined functions (recursion, callby value and callby reference)-String functions – Preprocessors – Storage class – Structure, union.

06. Pointers: pointer expressions, arithmetic passing pointers through arrays and functions – File Handling, Introduction to OOPS. (18 hours)

UNIT – IV

C PROGRAMMING - APPLICATIONS

07. C Programming – Simple applications to Chemistry: Determination/Calculation of (1) Bohr radius; (2) Average, R.M.S.and Most Probable Velocities of gas molecules; (Anyone) (3) $\triangle$E for atomic spectral transitions using Rydberg equation; (4) Energy of electromagnetic radiations (given : Wavelength or frequency); (5) Anharmonicity constant and dissociation energy of a molecule; (6) Enthalpy change using Clapeyron-Clausius Equation; (7) Rate constant for a first order reaction; (8) pH of a buffer solution (using Henderson's equation); (9) Solving systems of linear equations, using Gauss elimination method; (!0) Least squares fitting. (18 hours)

UNIT – V

SEPARATION TECHNIQUES

08. Solvent extraction – Principle and applications.

09. Chromatographic techniques – Theory of chromatography, Mechanism – adsorption and partition – Column, paper, thin layer and ion exchange chromatography – technique, illustrations and applications; - Gas chromatography – principles, instrumentation – types of column, detectors and applications; - High Performance Liquid Chromatography – Principle, types of columns, detectors and applications. (18 hours).

Text Books and References:

1. E.Balagurusamy, "Programming in C", Tata McGraw Hill, New Delhi 1991.
2. E.Balagurusamy, "Programming in ANSIC", Tata McGraw Hill,2nd edition, New Delhi 1999.
3. E.Balagurusamy, "Object oriented Programming with C++", Tata McGraw, New Delhi 1995.
4. Yashavant Kanethkar, "Let Us C", BPB Publications, 3rd edition, New Delhi, 1999.
5. Robert Lafore, "Object oriented Programming in Turbo C++", Galgotia, New Delhi 2000.
6. Byron S.Gottfried, "Schaum's Outline of Theory & Problems of Programming with C" New York; McGraw Hill, 1998.
7. K.V.Raman, 'Computers in Chemistry', Tata McGraw Hill, New Delhi, 1993.
8. E.Balagurusamy, "Fortran for Beginners", Tata McGraw Hill, New Delhi,1990.
9. S.K.Basandra, "Local Area Networks", Galgotia Publications,1999.
10. A.S.Tanenbaum, "Computer Networks", Prentice Hall of India, 1996.
11. S.M.Bachrach, "Internet for Chemists", ACS Publications, Washington DC 1996.
12. Uyless Black, "Computer Networks, Protocols, Standards and Interfaces", Prentice Hall of India, 1987.
13. K.B.Lipkowitz and D.B.Boyd, Ed. "Reviews in Computational Chemistry",VCH, New York, 1990.
14. Y.Kanetkar, "Working with C" , BPB Publications, 1st edition, New Delhi, 1994.
15. M.Chandrasekaran, S.Govindaraju, A.Abdul Huq, T.R.Narayanan, Elements of Computer Science, New Age International Pvt.Ltd., New Delhi, 1996.
16. T.Swan, Type and learn C, Pustak Mahal, New Delhi,1994. Chapters 3,4,5,6,7,8 and 9.
17. H.R.Zepa, "The Internet as a Computational Chemistry Tool", J.Mol.Struct.(Theo.Chem.), 398-399, 1997,27-33.
18. Vogel. A.I.Text book of Quantitative Inorganic Ananlysis, ELBS, Longman, London, 1982.
19. D.A.Skoog and D.M.West, Fundamentals of Analytical Chemistry, Holt Reinhart & Winston, New York, 1986.
20. G.Christian, Analytical Chemistry, John Wiley, 5th edition, 1994.
21. R.A.Day and A.L.Underwood, Quantitative Ananlysis, Prentice Hall of India Pvt.Ltd., New Delhi.
22. G.Chatwall and S.Anand, Instrumental Methods of Chemical Analysis, Himalaya Publishing House, Mumbai.
23. B.K.Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House, Meerut.