

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : V (Code- MCH - 410)
 Compulsory /Optional : Compulsory
 Max. Marks : 100

Paper – V : Computers For Chemists

This is a theory cum-laboratory course with more emphasis on laboratory work.

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| Unit – I | Introduction to computers and Computing Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Algorithms and flow-charts. |
| Unit – II | Computer Programming in FORTRAN/C/BASIC (The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the compute language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learns the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.) |
| Unit – III | Programming in Chemistry Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Vander Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity and Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles. |
| Unit – IV | Use of Computer Programmes Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL -special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory. |
| Unit –V | Internet Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera. |

Books suggested:

1. Fundamentals of Computer : V. Rajaraman (Prentice Hall)
2. Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)
3. Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)

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