

Semester II 2015-2016

Semester II

M.M.40+10

Paper-X

Hour 36

CH-410: COMPUTERS FOR CHEMISTS

Credit-3

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

### UNIT-I

#### Introduction to computers and Computing

1. Basic structure and functioning of computer with a PC as illustrative example.
2. Memory I/O devices. Secondary storage Computer languages.
3. Operating systems with DOS as an example Introduction to UNIX and WINDOWS.
4. Principles of programming Algorithms and flow-charts.

### UNIT-II

1. Computer Programming in C/BASIC or C++ (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).
2. Elements of the computer language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Braching statements as If or GO TO statement. LOGICAL variables. Double procession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE COMMON and DATA statement (Student learn 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

1. FORTRAN/C/BASIC,C/C++ involving simple formulae in Chemistry, such as Van der 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 detrmination of molecular weight

### Unit-IV

#### Use of Computer Programmes

1. Operation of PC. Data Processing. Running of standard Programs and Packages such as MS-WORD, MS EXCEL-speical emphasis on calculations and chart formations X-Y plot.
2. Chem sketch – Drawing structure of molecules using free software available on Net.

प्राचार्य  
विद्यालयाई शास. महावि.  
रजौर

Semester II 2015-2016

Unit-V


Internet

1. Application of Internet for Chemistry with search engines,
2. various types of files like PDF, JPB.

Book Suggested:

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

 Gh-<sup>u</sup> a/z

  
माता जीजाबाई शास. महाविद्यालय  
भोती तळेला, इन्डोर