Paper-XI CHN504 - B Computers for Chemists

I **Introduction to Computers and Computing**   **8 Hrs**

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

II **Computer Programming in FORTRAN/C/BASIC**   **12 Hrs**

(The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols. Expressions. Arithmatic assignment statement. Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements. (Students learn the programming logic and these language features by 'hands on' experience on a personal computer from the very beginning of this topic).

III **Programming in Chemistry**   **15 Hrs**

Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Hückel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge data base.

IV **Use of Computer Programmes**   **25 Hrs**

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Further, the students will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO and Word Processing software such as WORDSTAR/MS-WORD.