**School of Chemical Sciences**

**Devi Ahilya Vishwavidyalaya, Indore**

**M.Sc. Chemistry**

**SEMESTER II**

**MCH/MPC-205: COMPUTER APPLICATIONS IN CHEMISTRY**

**Credits 3**

(This is a theory cum-laboratory course with more emphasis on laboratory work leading to impart professional and entrepreneurship skills).

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| **Unit – I**  |  **Use of standard Programs and Packages**Power Point preparation and Presentation of research workMS EXCEL |
| **Unit – II** | **Use of Computer Softwares** ACD LabOrigin Programs related to pi-chart, Bar diagram  |
| **Unit – III** | **Fundamental concepts of Programming**Fundamental s of BASIC programming, Flow Charts for problems related to chemistry and mathematics, Basic concepts of FORTON, BASIC and C- Language.  |
| **Unit – IV** | **Programming in Chemistry**Developing of small computer programs 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 of Electronegativity of atom and Lattice Energy. |
|  | **Books Suggested :** 1. Fundamentals of Computer: V. Rajaraman (Prentice Hall Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
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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