**DEPARTMENT OF CHEMISTRY**

**SHRI G. S. INSTITUTE OF TECHNOLOGY AND SCIENCE, INDORE**

**COURSE COMPLETION UNIT PLAN**

**Course: M.Sc. (Applied Chemistry) Semester III**

**Paper: CH91307 Computer applications in Chemistry**

**Name of Faculty: Mr Krishnapal S Solanki and Mr. Bhupendra Morya**

|  |  |  |
| --- | --- | --- |
| **Lecture No.** | **Topic to be taught** | **Reference/ Remark** |
| **Unit 1: Computers and peripheral devices** | **Principles of Computer Science by V.B. Aggarwal** |
| 1 | Introduction to computers. |
| 2 | History of computer, Generations of computer. |
| 3 | Computer and its peripheral device (Input, output devices, storage devices) |
| 4 | Basic Information about hardware and software devices |
| 5 | The basic organization of digital computers |
| 6 | Introduction of Operating Systems |
| 7 | Introduction to Computer languages (High-level and low-level languages). |
| 8 | Introduction to internet |
| **Unit 2: Computer programming using C, Python/FORTRAN** |  |
| 9 | Principles of basic programming, Algorithm, flow charts | **- K.V Raman Computers in Chemistry** |
| 10 | Expressions, statements, Library functions, and Control statements in Programming. |
| 11 | Chemistry and FORTRAN programming, Introduction to Linux operating system, Logical statements. |
| 12 | 1D and 2D Arrays, Arithmetic statement functions, Use of subroutines, loops. |
| 13 | Programming in C, Input and output in c language, control statement. |
| 14 | Functions in C, Arrays and Pointers, Structures and Unions. |
| 15 | Programming in Python, Subroutines, loops, control statements, and transfer statements. |
| 16 | Handling of files and exceptions, file handling through libraries, and error and exception handling. |
| **Unit 3: Networking and Data Base System** |  |
| 17 | Introduction to Networking, Historical background. | **K.V Raman Computers in Chemistry** |
| 18 | Need &Advantages of computer network, Internet protocol, types of protocol. |
| 19 | Type of computer network, LAN, MAN, WAN, Basic HW & SW requirement for networking, Networking Sites. |
| 20 | Introduction to Database |
| 21 | Database application in chemistry |
| 22 | Introduction to DBMS and Characteristics of DBMS |
| 23 | Study of protein data bank. |
| 24 | Study PubChem database |
| **Unit 4: Programming in Chemistry** |  |
| 25 | Development of small computer codes in FORTRAN (Part 1): Kinetics of first order,radioactive decay. | **K.V Raman Computers in Chemistry** |
| 26 | Development of small computer codes in FORTRAN (Part 2): Kinetics of second order reaction. |
| 27 | Development of small computer codes in FORTRAN (Part 3): vanderWaals equation, pH titration |
| 28 | Development of small computer codes in C (Part 1): Kinetics of first order,radioactive decay. |
| 29 | Development of small computer codes in C (Part 2): Kinetics of second order reaction. |
| 30 | Development of small computer codes in C (Part 3): vander Waals equation, pH titration |
| 31 | Development of small computer codes in Python (Part 1): Kinetics of first order,radioactive decay, Kinetics of second order reaction. |
| 32 | Development of small computer codes in Python (Part 2): vander Walls equation, pH titration. |
| **Unit 5: Software Package in Chemistry** |  |
| 33 | Introduction to Different Software Packages in Chemistry, Need of Software packages. | **K.V Raman Computers in Chemistry** |
| 34 | Gaussian software package Handling |
| 35 | Chemistry software packages such as ChemSketch, ChemDraw, etc forStructure drawing, Geometry Optimization, and Estimation of various physic-chemical properties. |
| 36 | Introduction of Linear Regression Model |
| 37 | Linear Regression equation: Equation for Slope, Equation for intercept, Equation for R and R2 |
| 38 | Linear Regression equation:Solving two-dimensional arrays,Half-life period. |
| 39 | Introduction to non-linear regression. |
| 40 | Use of Online Chemical structure databases |