## GROUP - (D) ELECTIVE PAPER
## PAPER II. COMPUTATIONAL CHEMISTRY

M.M. - 75 | 60 Hrs. (2 Hrs./Week)

| Units | Topics |
|---|---|
| I | **Fortran/C Programming and Numerical Methods** **15 Hrs.** |
| | Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc. |
| | a. **Solution of Equations:** Bisection, regular falsi, Newton - Raphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill - conditioning. |
| | b. **Linear Simultaneous Equations:** Gaussian elimination, Gauss - Seidel method, Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning. |
| | c. **Eigenvalues and Matrix Diagonalization:** Jacobi and Householder methods, analysis or errors. |
| II | a. **Interpolation:** Newton forward and backward difference, central differenced formulae. |
| | Lagrange and Hermite interpolation. Polynomial wiggle problem. |
| | b. **Numerical Differentiation:** Solution of simple differential equations by Taylor series and Runge-Kutta methods. |
| | c. **Numerical Integration:** Newton-Cotes formulae, Romberg integration, errors in integration formulae. |
| | The students should develop computer programs for some of the above numerical methods. |
| III | **Running of Advanced Scientific Packages** **15 Hrs.** |
| | The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN/GAMES with carefully designed exercises for illustrating various features of the packages. Semi empirical/Dyanmics/Simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc. |
| IV | **Introduction to Networking and Search using Internet** **10 Hrs.** |
| V | **Project** **20 Hrs.** |
| | The students will develop utilities such as analysis of spectra, simulation programmes which will supplement laboratory or theory exercises in physical, organic, inorganic chemistry or biochemistry. This list is only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out. |