CHN-704(D) Computational Chemistry

Computational Chemistry **60 Hrs (2 Hrs/week)**

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.

d. Interpolation

Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

e. Numerical Differentiation

Solution of simple differential equations by Taylor series and Runge-Kutta methods.

f. Numerical Integration

Newton-Cotes formulae, Romberg integration, errors in integration formulae.
The students should develop computer programs for some of the above numerical methods.

II 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/Dynamics/Simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc.

III Introduction to Networking and Search using Internet **10 Hrs**

IV 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.

Books Suggested

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.
3. Numerical Analysis, C. E. Frogberg, Macmillan.
4. Numerical Analysis - A Practical Approach, M.J. Maron, John Wiley.
5. Numerical Methods for Scientists and Engineers, H. M. Antia, Tata McGraw Hill.