

Ph.D. Elective

CH 637 : Computational Methods in Chemistry (2-0-2-6)

Prerequisites : Nil

Introduction to linux operating system. Introduction to Fortran; Development of small computer codes involving simple formulae in chemistry: such as van der Waals equation, pH titration, kinetics, radioactive decay; Basic numerical analysis: Roots of equations, Interpolation and polynomial approximation, Numerical solution of differential equations: ODE and PDE, numerical integration, solution of linear systems using Gaussian elimination; Use of standard available software to perform simple quantum chemical calculations.

Text Books

1. S. J. Chapman, *Fortran 90/95 for Scientists and Engineers*, 2nd Edition, McGraw-Hill, 2003.
2. W. E. Mayo and M. Cwiakala, *Programming with FORTRAN 77*, Schaum's Outline Series, McGraw Hill, 1995.
3. W. H. Press , S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in FORTRAN/C*, Cambridge University Press, 2nd Edition, 1996.
4. S. C. Chapra and P. Canale, *Numerical Methods for Engineers*, 4th edition, Tata McGraw -Hill, 2002.
5. F. Jensen, *Introduction to Computational Chemistry*, 3rd Edition, Wiley, 2017.

References

1. V. Rajaraman, *Computer Programming in Fortran 90 and 95*, PHI, 1997.
2. M. Metcalf and J. Reid, *Fortran 90/95 Explained*, Oxford : O.U.P, 1999.
3. C. Xavier, *Fortran 77 and Numerical Methods*, Wiley Eastern, 1994.
4. J. Leszczynski, A. Kaczmarek-Kedziera, T. Puzyn, M. G. Papadopoulos, H. Reis, M. K. Shukla (Eds.), *Handbook of Computational Chemistry*, 2nd Edition, Springer, 2017.