Course No.	Course Name	L-T-P-Credits
CY 536	**Computational Chemistry**	**2-0-2: 03**

Prerequisite: NIL

Course Objectives: The main objective of the course is to introduce Linux operating system and basic commands used in terminal, to provide basic knowledge of Fortran/C coding, to explain the numerical methods commonly used in computation chemistry. The course objectives also lies in the knowledge of electronic structure calculations of molecular systems in terms of methods, basis set and different calculations. Finally, the course targets to provide knowledge on computational chemistry research areas

Course Outcomes: After successful completion of the course, students will be able to:

1. Learn to operate Linux operating system
2. Write basic codes in Fortran/C language
3. Learn the numerical methods to apply in order to deal with the solution of different equations in Chemistry
4. Do electronic structure calculations in terms of geometry and transition state optimization, single point energy calculation, and the calculation of potential energy surface of molecular systems
5. Apply specific numerical techniques to solve critical Chemistry problems in quantum mechanics, chemical kinetics, molecular dynamics, etc.
6. Grab an idea of current research interests in theoretical chemistry field

SYLLABUS		
Module	**Contents**	**Hours**
I	**Introduction to Programming Language in Scientific Computing** Elements of computational programming, basic program structure, data types, logical and arithmetic expressions, loops and control statements, arrays, input/output statements, format specifications, file processing, functions, subroutines and applications.	10
II	**Numerical Methods** Errors, accuracy and stability. Curve fitting: least square fit algorithm. Roots of equations: Newton-Raphson method, Bisection method. Numerical integration: Trapezoidal and Simpson's rules. Numerical differentiation: forward, backward and centred differencing. Interpolation: Lagrange's method. Linear simultaneous equations: Gaussian elimination and Gauss-Jordan elimination. Numerical solutions of ordinary differential equations using Euler, modified Euler and fourth order Runge-Kutta method. Application to some quantum chemistry problems.	14
III	**Review of electronic structure theory** Hatree-Fock, MP2, DFT, configuration interaction, basis sets, convergence	04

IV	**Applications** Geometry optimization, frequency calculation, location of transition state, intrinsic reaction co-ordinates, molecular orbitals and population analysis, natural bond orbital analysis, calculation of equilibrium constants and rate constants.	06
V	**Suggested Practical** 1. Development of computer program to solve differential equations arise in Lotka-Volterra Autocatalytic Reaction 2. Geometry optimization of biologically relevant molecules by using any quantum chemistry package, namely, GAUSSIAN, GAMMES, NWChem, etc. 3. Molecular dynamics on a dissociation reaction to validate Arrhenius theory of reaction rate 4. Quantum Dynamics on a simple system to show the procedure to obtain photoabsorption spectra.	12

Essential Readings:
1. V. Rajaraman, "Computer Programming in Fortran 77", PHI Learning publishers.
2. V. Rajaraman, "Computer Programming in C", PHI Learning publishers.
3. W. H. Press, S. A. Teukolsky, W. T. Vellerling and B. P. Flannery, "Numerical Recipes in FORTRAN: The Art of Scientific Computing", Cambridge University Press.

Supplementary Readings:
1. M. Schatzman, "Numerical Analysis: A Mathematical Introduction", Oxford University Press.
2. C. J. Cramer, "Essentials of Computational Chemistry - Theories and Models", John Wiley and Sons Ltd.
3. D. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley and Sons Ltd.