CERTIFICATE COURSE ON SOFTWARE TOOLS FOR SCIENTIFIC GRAPHING AND MOLECULAR MODELLING

Department of Chemistry P.S.M.O College Tirurangadi offers a Certificate Course On "Software Tools For Scientific Graphing And Molecular Modelling" for Degree and PG students. This Non-Degree Course involves both theory And practical session.

COURSE DESCRIPTION:

Calicut university syllabus instruct project works for UG &PG students. There is a great demand of familiarizing various research tools such as Chemdraw,Chemsketch,Origin and many computational chemistry softwares which are the widely used in their studies. Chemdraw and chemsketch are used for the purpose of molecular modeling and structure designing. The scientific graphing and data analysis are done by using origin software. Computational softwares which are used for optimizing geometry and calculating various molecular parameters.

COURSE OUTCOME:

- Applying chemdraw and chemsketch softwares for molecular modeling,writing structures and chemical equations.
- To understand scientific graphing and data analysis.
- Applying computational chemistry softwares for calculating molecular parameters.

COURSE SYLLABUS

MODULE-I (5 Hrs)

Introduction to basic features of Chemdraw, Chemical structure to name conversion, Chemical name to structure conversion ,NMR spectrum simulation(both H NMR &C13 NMR),Mass spectrum simulation, structure clean up,export to SVG,PDF. Introduction to Chemsketch-Molecular modelling , create and modifying images of chemical structures, write and perform chemical equations and diagrams.

MODULE-II (5 Hrs)

Introduction to Origin, basic features like Scientific graphing, drawing various 2D &3D plots, Data analysis,statistics,signal processing,curve fitting,peak analysis,conversion of graph to various file format like JPEG,GIF,EPS.

MODULE-III (5 Hrs)

Introduction to computational methods-Molecular mechanics and electronic structure methods-*ab initio* and semi empirical methods-basis set approximation.

MODULE-IV (9 Hrs)

PRACTICAL SESSION

Introduction to Guassian Programme- the structure of a Guassian input file, types of key words.

Specification of molecular geometry using Cartesian co-ordinates and internal co-ordinates(Z-Matrix).

Geometry optimization of simple molecules, computation of normal modes of vibration of simple molecules, computation of MO coefficients of simple molecules, computation of NMR coupling constants ,introduction and application of Guassian as a software which interfaces with Guassian.