Credit Distribution, Eligibility and Pre-requisites of the Course

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Chemistry : IT Skills and Molecular Modelling	04	02	--	02	Class 12th with Physics, Chemistry, Mathematics	NA

Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the students to basic computer skills that are a must for a new age chemist.
- To acquaints the students with data tabulation, calculation, graph plotting, data analysis and document. Preparation using various software (preferably open-source).
- To learn about molecular modelling, its applications to various molecular systems, energy minimization techniques, analysis of Mulliken Charge and ESP Plots.

Learning Outcomes:

By the end of the course, the students will be able to:

- Become familiar with the use of computers
- Use software for tabulating data, plotting graphs and charts, carry out statistical analysis of the data.
- Solve chemistry problems and simulate graphs.
- Prepare documents that will incorporate chemical structure, chemical equations, mathematical expressions from chemistry.
- Understand theoretical background of computational techniques and selective application to various molecular systems.
- Learn ESP Plots by suitable software, electron rich and electron deficient sites.
- Compare computational and experimental results and explain deviations.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.

Unit 1: Introduction to important software in chemistry Hours:10

Introduction to different software available for drawing chemical structures (Proprietary and Open-source) like ACD Chemsketch and 3-D viewer, ChemDraw.
Carrying out simple calculations on anyone of the following software: ArgusLab, Pymol, Avogadro, Molview, MarvinSketch.
Draw structures of various compounds (aliphatic, aromatic, heterocyclic with different functional groups) using software. Save the structures in various file formats. Incorporate the structures in word document and powerpoint presentation. SMILES notation for the chemical structures. PDB Files.

Unit 2: Handling of Numerical Data Hours:10

Using a spreadsheet software: applying basic functions and formulae to the data, drawing charts, tables and graphs, displaying the equation of graph along with the R^2 value, incorporating tables and graphs in Word files, graphical solution of equations, plotting pressure-volume curves of van der Waals gases, Maxwell-Boltzmann distribution, concentration versus time graphs, spectral data, titration curves, etc.

Unit 3: Molecular Modelling Hours: 10

Introduction to molecular modelling, overview of classical and quantum mechanical methods (semi empirical, ab initio and DFT) and molecular mechanics method

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, concept of transition state with examples.

Practical
(Credits: 02, Laboratory periods: 60)

Plotting graphs using a spreadsheet

1. van der Waals isotherms
2. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
3. Plot the conductometric titration curve for

   a) strong acid vs strong base and b) weak acid vs strong base

4. Plot the pH metric titration curve for

   a) strong acid vs strong base and b) weak acid vs strong base

5. Plot the graphs for the kinetics of first order reaction.

Molecular Modelling

6. Optimise and compare the geometry parameters of H_2O and H_2S using Argus Lab.

7. Compare the basicities of ammonia, methylamine, dimethylamine and trimethylamine using Argus Lab by comparing Mulliken charges and ESP maps.
8. Compare C-C bond lengths and bond order in ethane, ethene and ethyne using Argus Lab.
9. Determine enthalpy of isomerization of cis and trans-2-butene in Argus Lab.
10. Compare the HAH bond angles for the second row hydrides (BeH_2, CH_4, NH_3, H_2O) and compare with the results from qualitative MO theory.

References (Theory):

1. Levie, R. de. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press.
2. Lewars, E. (2003), **Computational Chemistry,** Kluwer academic Publisher.
3. Cramer, C.J.(2004), **Essentials of Computational Chemistry,** John Wiley & Sons.
4. Hinchcliffe, A. (1996), **Modelling Molecular Structures,** John Wiley & Sons.
5. Leach, A.R.(2001), **Molecular Modelling,** Prentice-Hall.

References (Practical):

1. Lewars, E. **(2003), Computational Chemistry,** Kluwer academic Publisher.
2. Cramer, C.J. **(2004), Essentials of Computational Chemistry,** John Wiley & Sons.
3. Hinchcliffe, A. **(1996), Modelling Molecular Structures,** John Wiley & Sons.

Note: Some of the papers are same as in B Sc (H) Chemistry and B Sc Physical Sciences.