

## DISCIPLINE SPECIFIC ELECTIVE COURSE CHEM-DSE 9: Computer Applications in Chemistry

### 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		
<b>Chem-DSE 9: Computer Applications in Chemistry</b>	<b>04</b>	<b>02</b>	<b>-</b>	<b>02</b>	<b>Class XII with Science</b>	

### Learning Objectives

The Learning Objectives of this course are as follows:

- To introduce the students to basic computer skills that will help them in solving chemistry problems using spreadsheets and BASIC language.
- To acquaint the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.
- To expose the students to the concept of molecular modelling, its applications to various molecular systems, energy minimization techniques, analysis of Mulliken Charge and ESP Plots.

### Learning outcomes

By studying this course, students will be able to:

- Become familiar with the simple use of BASIC Language.
- 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 Energy minimization methods through use of different force fields.
- Learn ESP Plots by suitable soft wares, 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.

## Syllabus

### Unit 1: Programming using BASIC

(Hours: 20)

Programming Language – Elements of BASIC language, Numeric and string Constants and Variables, arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the various QBASIC commands: REM, CLS, INPUT, PRINT, GOTO, IF, IF...THEN, IF...THEN..ELSE, IF and END IF, FOR and NEXT etc., DIM, READ, DATA, GOSUB, RETURN, RESTORE, DEF FNR and Library Functions, Simple programs based on usage of the commands mentioned above.

Statistical analysis using BASIC: Mean, Least square fit - Linear regression, variance, standard deviation.

### Unit 2 : Handling of Numerical Data

(Hours: 4)

Spreadsheet software: MS Excel. Creating a spreadsheet, entering and formatting information, 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: 6)

Introduction to molecular modelling, overview of classical and quantum mechanical methods (molecular mechanics, semi empirical, ab initio and DFT), general considerations and comparison of these methods.

### Practical component

Credit:02

(Laboratory periods: 15 classes of 4 hours each)

#### Exercises of Programing

7. Calculate pressure of a real gas using Van der Waal's Equation.
8. Calculate the most probable speed, average speed and root men square velocity of an ideal gas.
9. Roots of quadratic equations
10. Binomial coefficient using GOSUB statement.
11. Mean, standard deviation
12. Least square curve fitting method for linear equation.

#### Plotting graphs using a spreadsheet

4. Van der Waals isotherms
5. Maxwell-Boltzmann distribution curves as function of temperature and molecular weight

6. Plot the conductometric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base
5. Plot the pH metric titration curve for
  - a) strong acid vs strong base and b) weak acid vs strong base and determine the  $pK_a$  of the weak acid
7. Plot the graphs for the kinetics of first order reaction and determine the rate constant
8. Plot the UV-vis absorbance spectra and determine the molar absorption coefficient.

### **Molecular Modelling**

6. Optimize and compare the geometry parameters of  $H_2O$  and  $H_2S$  using ArgusLab.
7. Compare the basicities of N atom in ammonia, methylamine, dimethylamine and trimethylamine using ArgusLab by comparing Mulliken charges and ESP map in ArgusLab.
8. Compare C-C bond lengths and bond order in ethane, ethene and ethyne using ArgusLab.
9. Determine enthalpy of isomerization of cis and trans-2-butene using ArgusLab.
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:**

7. Levie, R. de. (2001), **How to use Excel in analytical chemistry and in general scientific data analysis**, Cambridge Univ. Press.
8. Venit, S.M. (1996), **Programming in BASIC: Problem solving with structure and style**. Jaico Publishing House.
9. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
10. Cramer, C.J.(2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
11. Hinchcliffe, A. (1996), **Modelling Molecular Structures**, John Wiley & Sons.
12. Leach, A.R.(2001), **Molecular Modelling**, Prentice-Hall.

#### **Practicals**

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

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.