DISCIPLINE SPECIFIC ELECTIVE COURSE- 9 (DSE-9): Applications of Computers 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		
Applications of Computers in Chemistry (DSE 9)	**04**	**03**	**-**	**01**	Class 12th with Physics, Chemistry	

Learning Objectives

The Objectives of this course are as follows:

- To familiarize the students with the fundamental building blocks and syntax of coding in Python with
- To apply python programming to solve simple Chemistry problems by thinking algorithmically and coding structurally

Learning outcomes

By studying this course, the students will be able to:

- Understand the importance of python programming in chemistry and its applications in the field of AI and ML
- Perform simple computations in python after learning the basic syntax, loop structure, string data manipulation etc.
- Solve chemistry problems such as finding pKa of a weak acid, solving Schrodinger's equation etc.
- Plot experimental data and perform regression analysis

SYLLABUS OF DSE-9

UNIT–1: Basic Computer system **(Hours: 3)**

Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and

Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High-Level languages (Machine language, Assembly language; QBASIC, C, C++, FORTRAN 90&95); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application

UNIT-2: Introduction to Python **(Hours: 3)**

Why Python? Python coding environment setup, Python as an interpreted language, Brief history of Python, Uses of Python (including artificial intelligence and machine learning), Applications of Python in Chemistry

UNIT-3: Coding in Python **(Hours: 18)**

(i) Basic syntax including constants and variables, Operators, Data Types, Declaring and using Numeric data types: int, float, string etc. (ii) Program Flow Control Conditional blocks: if, else and else if, simple FOR loops, FOR loop using ranges, string, list and dictionaries. Use of while loops, Loop manipulation using pass, continue, break and else. (iii) Complex data types: String, List, Arrays, Tuples and Dictionary, String operations and manipulation methods, List operations including slicing, in-built Python Functions. (iv) Python packages - usage of numpy and scipy for mathematical computations.

UNIT-4: Plotting graphs **(Hours: 9)**

Matplotlib for Plotting - Simple plots, formatting of plots, multiple plots, histograms, bar graphs, distributions, curve fitting – linear regression.

UNIT-5: Numerical Methods in Chemistry **(Hours: 12)**

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numerical differentiation – finite difference method (backward, central and forward), Numerical integration - Trapezoidal and Simpson's rule to calculate area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis-mean, variance, standard deviation, error, Curve fitting – linear regression, Solving Schrödinger's equation using Python packages.

Practical component

Practicals: Python Programming for Chemists **Credits: 01**

4. **Writing simple programs using scipy and numpy**
    a. syntax, data types
    b. loop structure, conditional loops

c. To learn string data manipulation
d. Array and lists
e. Sorting, matrix manipulations

5. **Plotting graphs using matplotlib**
    a. Planck's distribution law
    b. Maxwell-Boltzmann distribution curves as a function of temperature and mass
    c. Radial distribution curves for hydrogenic orbitals
    d. Gas law Isotherms – Ideal and Real
    e. Data from phase equilibria studies
    f. Wavefunctions and Probabilities as multiplots
    g. Kinetics data with linear fitting

6. **Numerical Methods in Chemistry**
    a. Solving equations involved in chemical equilibria such as pH of a weak acid at a given concentration, cubic equation obtained from solving van der Waals equation of real gases using Iteration, Newton-Raphson, and Binary Bisection Method
    b. Numerical Differentiation – finding equivalence point given pH metric and potentiometric titrations data by finding the first and the second derivative using the finite difference method
    c. Numerical Integration – Trapezoidal and Simpson's 1/3 rule to calculate enthalpy and entropy of an ideal gas
    d. Statistical Analysis – Calculating Mean, Variance, Standard Deviation
    e. Solving Schrodinger's Equation

Essential/recommended readings

Theory:

7. Dr. M. Kanagasabapathy(2023), **Python for Chemistry: An introduction to Python algorithms, Simulations, and Programing for Chemistry** (English Edition), BPB Publications
8. Robert Johansson (2021), **Numerical Python: Scientific Computing and Data Science Applications with Numpy, SciPy and Matplotlib**, 2nd Edition, Apress

Practical

1. Urban M., Murach J., **Murach's Python programming,** 2nd Indian reprint 2018, Shroff publishers and distributors
2. Gaddis T., **Starting out with python plus My programming Lab** with Pearson e-text-Access card package, 3rd ed.

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