11.2.6. Course Code: ANALYTICAL CHEMISTRY (DSE-AC6)
Course Title: COMPUTER APPLICATION IN CHEMISTRY
Total Credits: 04 (Credits: Theory-03, Practical-01)
(Total Lectures: Theory- 45, Practical-30)

Objectives: The aim of this paper is to make the students learn the working of computer and its applications in chemistry via programming language, QBASIC and use of software as a tool to understand chemistry and solve chemistry-based problems.

Learning Outcomes:

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

- Have knowledge of most commonly used commands and library functions used in QBASIC programming.
- Develop algorithm to solve problems and write corresponding programs in BASIC for performing calculations involved in laboratory experiments.
- Use various spreadsheet software to perform theoretical calculations and plot graphs

Unit 1: Basic Computer system

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, FORTRAN and C++); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application.

(Lectures: 05)

Unit 2: QBASIC commands and Library functions

QBASIC for solving some of the basic and complicated chemistry problems). QB4 version of QBASIC can be used. Arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the following QBASIC commands: INPUT and PRINT; GOTO, If, ELSEIF, THEN and END IF; FOR and NEXT; Library Functions (ABS, INT, CINT, MOD, ASC, CHR$, LEN, EXP, INT, LOG, RND, SQR, TAB and trigonometric Functions), DIM, READ, DATA, REM, RESTORE, DEF FNR, GOSUB, RETURN, MID$, LEFT$, RIGHT$, SCREEN, VIEW, WINDOW, LINE, CIRCLE, LOCATE, PSET Simple programs using QBASIC commands, Matrix addition and multiplication.

(Lectures: 20)

Unit 3: Use of QBASIC for solving problems in Chemistry

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numerical differential, Numerical integration (Trapezoidal and Simpson's rule), Calculation of area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis-mean, variance, standard deviation, error, least square method.

Plotting linear graphs using experimental data, plotting (i) trigonometric functions-particle in a one-dimensional box(ii) exponential function (iii) Ideal gas isotherms. Plotting van der Waals Isotherms, and observe whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation.

(Lectures: 20)

PRACTICALS (Credits:01; Laboratory Periods: 30)

Computer programs using QBASIC based on numerical methods

1. Simple programs to calculate numerical values of chemistry problems.
2. Roots of equations: (e.g. volume of gas using van der Waals equation and comparison with ideal gas, pH of a weak acid).
3. Solving polynomial equation using iterative method. (van der Waal's equation of state, pH of a weak acid using exact expression)
4. Solving polynomial equation using Newton-Raphson's method. (van der Waal's equation of state, pH of a weak acid using exact expression)
5. Matrix operations: addition, multiplication and transpose
6. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
7. Numerical integration using trapezoidal method. (e.g. entropy/ enthalpy change from heat capacity data).
8. Numerical integration using Simpson's rule
9. Mean, standard deviation
10. Least square curve fitting method for linear equation.
11. Calculate the relative intensities of peaks of a proton obtained after spin-spin coupling with 4 equivalent neighboring protons in a high-resolution NMR spectrum using GOSUB RETURN.

Computer programs using QBASIC for plotting graphs

1. van der Waals isotherm
2. Compressibility versus pressure curves
3. Maxwell distribution curves
4. Concentration-time graph using kinetics data
5. pH metric titration curve
6. Conductometric titration curves for strong acid-strong base titrations.
7. Calibration curve using Lambert Beer's law
8. Particle in a one-dimensional box.

Plotting graphs using spreadsheet

1. Particle in a one-dimensional box.
2. van der Waals isotherms below critical temperature, at critical temperature and above critical temperature.
3. Radial plots and radial distribution functions for orbitals of hydrogen atom.
4. Plotting characteristics graphs of zero, first and second order reactions using concentration time data and determine the order of the reaction.

References:

Theory:

- McQuarrie, D. A. (2008), Mathematics for Physical Chemistry, University Science Books.
- Mortimer, R. (2005), Mathematics for Physical Chemistry,3rd Edition, Elsevier.
- Steiner, E. (1996), The Chemical Maths Book, Oxford University Press.
- Yates, P. (2007), Chemical Calculations, CRC Press.
- Harris, D. C. (2007), Quantitative Chemical Analysis,6th Edition, Freeman, Chapters 3-5.

Practical:

- Levie, R.D. (2001), How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge University Press.
- Kapoor, K.L. (2019), A Textbook of Physical Chemistry, Vol.7, 1st Edition, McGraw Hill Education.

Teaching Learning Process:

- Blend of conventional blackboard teaching and modern teaching learning tools
- Problem solving and quizzes for enhanced understanding of the concepts
- Explaining the algorithm for solving a problem.

Assessment Methods:

- Class Tests at Periodic Intervals.
- Written assignment (s) / Presentation by individual students
- End semester University Theory and Practical Examination

Keywords: Hardware, Software, Programming Language, ASCII, BCD, QBASIC, library functions, Library commands, mathematical operators, QBASIC commands, Library commands, mathematical operators, QBASIC commands numerical methods, graphs.

11.2.7. Course Code: CHEMISTRY(DSE-C1)
Course Title: Functional Group Organic Chemistry- II
Total Credits: 04 (Credits: Theory-02, Practical-02)
(Total Lectures: Theory- 30, Practical-60)

Objectives: This is designed for better understanding of the organic functional groups, which include carboxylic acids and their derivatives (aliphatic and aromatic), amines (aliphatic & aromatic), diazonium salts and their reactivity patterns. The concept of amino acids, peptides has also been introduced with detailed reactions mechanistic pathways will be discussed to unravel the spectrum of organic chemistry and the extent of organic transformations.