FACULTY OF COMPUTER SCIENCE & IT

SYLLABUS

of

COMPUTER FOR CHEMISTS

for

M.Sc. Chemistry (Semester-I)

(Under Continuous Evaluation System)

Session: 2018-19

The Heritage Institution

KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)

Scheme of Studies and Examination

M.Sc. Chemistry
(Session 2018-19)

SemesterI								
Course Name	**Program Name**	**Course Code**	**Course Type**	**Marks**				**Examination time (in Hours)**
				Total	**Ext.**		**CA**	
					L	**P**		
Computer for Chemists	M.Sc. Chemistry (Semester-I)	MCHM-1135	C	75	40	20	15	3+3

M.Sc. Chemistry (Semester-I)

(Session 2018-19)

Course code: MCHM - 1135

COMPUTER FOR CHEMISTS

COURSE OUTCOMES:

After passing this course the student will be able to:

CO1: design algorithms and flowcharts for various programming problems.

CO2: make use of I/O statements, Control statements, Loopingand arrays in programming.

CO3: understand various character code notations.

CO4: write code involving simple formulae in Chemistry.

M.Sc. Chemistry (Semester-I)

(Session 2018-19)

Course code: MCHM - 1135

COMPUTER FOR CHEMISTS

Time: (3+3) Hours **Max. Marks: 75**

Theory: 40

Practical: 20

CA: 15

Note: The students are allowed to use Non-Programmable Calculator.

Instructions for Paper Setter -

Eight questions of equal marks are to set, two in each of the four sections (A-D). Questions of Sections A-D should be set from Units I-IV of the syllabus respectively. Questions may be divided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any section.

1. Computer Programming in C language (30 Hrs.)

UNIT-I

Principles of programming, algorithms and flowcharts.

Elementary programming, a typical C program, printf unction.

Introduction of declarations, assignments and variables: concept of an integer, concept of avariable, rules for naming variables, assignment statement, arithmetic operators.

Integer arithmetic expressions, truncation effects, relative priority of arithmetic operators, use ofparenthesis, modulus operator.

UNIT-II

Floating point numbers, scientific notation, converting integers to floating point and vice versa ,coercion and cast operator, type char.

Decision making in C, scanf function, relational operators, logical operators, if statement, if elsestatement, nesting of if statement

UNIT-III

The while loop, do while loop, for loop, nesting of for loop.

Type char and ASCII code, character strings and how to print them, octal and hexadecimal Notation. User defined functions, returning value from a function, functions with more than oneparameters.

UNIT-IV

Arrays, declaring an array, initializing an array, break statement, strings and character arrays,sorting an array, finding maximum and minimum in an array, multidimensional arrays.Input and output.

2.Computer programs in Chemistry (15Hrs.)

(These are to be done in the practical class)

Development of small computer codes involving simple formulae in chemistry:

UNIT - I

1. Calculation of mean, median,mode.
2. Solution of a quadraticequation.
3. Calculation of linearregression.
4. Calculation of curve linearregression.

UNIT - II

5. Calculation of Bohr orbit from de Broglie Lambda forelectron.
6. Calculation of wave number and frequency from value of wavelength.
7. Calculation of van der Waalsradii.
8. Radioactivedecay.
9. Rate constant of a 1st order reaction, 2nd orderreaction.
10. Determination
11. Calculation of lattice energy using Born Landeequation.

UNIT - III

12. Addition, multiplication and solution of inverse of 3 X 3matrix.
13. Calculation of average molecular weight of a polymer containing n1 molecules ofmolecular weight m1, n2 molecules of molecular weight M2 and soon.
14. Program for calculation of molecular weight of organic compound containing C, H, N, O andS.
15. Calculation of reduced mass of diatomicmolecule.
16. Calculate the RMS and most probable velocity of agas.

UNIT - IV

17. Calculate the ionic mobility from ionic conductancevalues.
18. Determine the thermodynamic parameters for isothermal expansion of monoatomic idealgas.
19. Calculation of value of g- factor from value of J andS.
20. Calculate the bond length and bond angles using crystal structuredata.

Recommended Books:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
2. Mullish Cooper, The spirit of c, An Introduction to Modern Programming.
3. Learn Programming in C, Anshuman Sharma
4. Programming in ANSI C, Balaguruswamy
5. Let Us C, Yashwant Kanetkar
6. C Programming, Schaum series