

(Annexure H-2)

# **FACULTY OF COMPUTER SCIENCE & IT**

**SYLLABUS**

**of**

**COMPUTER FOR CHEMISTS**

**for**

**Master of Science (Chemistry) Semester-I**

**Under Credit Based Continuous Evaluation Grading System**

**(CBCEGS)**

**Session: 2023-24**



**The Heritage Institution**

**KANYA MAHA VIDYALAYA  
JALANDHAR**

**(Autonomous)**  
**Kanya Maha Vidyalaya, Jalandhar (Autonomous)**

CURRICULUM AND SCHEME OF EXAMINATIONS OF TWO YEAR MASTER DEGREE  
PROGRAMME

**Master of Science (Chemistry)**

Session 2023-24

<b>Master of Science (Chemistry) Semester I</b>										
<b>Course Code</b>	<b>Course Title</b>	<b>Course Type</b>	<b>Hours per week</b>	<b>Credit</b>		<b>Marks</b>			<b>Examination Time (in Hours)</b>	
			<b>L-T-P</b>	<b>L-T-P</b>	<b>Total</b>	<b>Total</b>	<b>Ext.</b>			<b>CA</b>
							<b>L</b>	<b>P</b>		
MCHM-1135	Computer for Chemists	C	1-0-2	1-0-1	2	50	20	20	10	3+3

**Master of Science (Chemistry) Semester - I  
Session 2023-24**

**COMPUTER FOR CHEMISTS  
Course code: MCHM – 1135**

**COURSE OUTCOME**

**After passing this course the student will be able to:**

CO1: Comprehend various programming constructs like variables, data-types, operators, etc of C programming language.

CO2: Apply various control statements of C Programming Language for designing solutions to different real-world problems.

CO3: Comprehend signature, declaration, definition and calling of functions in C for modularization of problem.

CO4: Implement single and multidimensional arrays for representing complex data collections.

**Master of Science (Chemistry) Semester - I**  
**Session 2023-24**

**COMPUTER FOR CHEMISTS**  
**COURSE CODE: MCHM - 1135**

**Examination Time: (3+3) Hours**

**Max. Marks: 50**

**L-T-P: 1-0-1**

**Theory: 20**

**Credits: 2**

**Practical: 20**

**CA: 10**

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

**Instructions for Paper Setter -**

Eight questions of equal marks (4 marks each) 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**

Introduction to programming, algorithms and flowcharts.

Elementary programming, a typical C program, print function.

Introduction of declarations, assignments and variables: concept of an integer, concept of a variable, rules for naming variables, Data Types, assignment statement, arithmetic operators.

Integer arithmetic expressions, relative priority of arithmetic operators, use of parenthesis, modulus operator.

**UNIT-II**

Input/Output Functions, Decision making in C, relational operators, logical operators, if statement, if else statement, 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 one parameters.

#### **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 (15 Hrs.)**

**(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 quadratic equation.
3. Calculation of linear regression.
4. Calculation of curve linear regression.

#### **UNIT - II**

5. Calculation of Bohr orbit from de Broglie Lambda for electron.
6. Calculation of wave number and frequency from value of wavelength.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Determination
11. Calculation of lattice energy using Born Lande equation.

#### **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 of molecular 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 and S.
15. Calculation of reduced mass of diatomic molecule.

16. Calculate the RMS and most probable velocity of agas.

#### UNIT - IV

17. Calculate the ionic mobility from ionic conductance values.

18. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.

19. Calculation of value of g- factor from value of J and S.

20. Calculate the bond length and bond angles using crystal structure data.

#### References / Textbooks:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
2. Henry Mullish, Herbert L. Cooper, The Spirit of C: An Introduction to Modern Programming, Jaico Publications, 1987.
3. Anshuman Sharma, Learn Programming in C, Lakhanpal Publishers,7th Edition.
4. E Balagurusamy, Programming in ANSI C, Tata McGraw-Hill, 2002.
5. Yashvant Kanetkar, Let Us C, BPB Publications, 2016.
6. Byron Gottfried, Schaum's Outline Programming with C, McGraw Hill, 1996.

Note: The latest editions of the books should be followed.