Name:

Enrolment No:

UPES

End Semester Examination, December 2024

Course: Introduction to Computational Chemistry **Semester: III**

Program: MSc Chemistry **Time : 03 hrs.**

Course Code: CHEM8048 **Max. Marks: 100**

Instructions:

- **Read all questions carefully.**
- **Use of scientific calculator is allowed.**
- **Q 7 and Q 11 have internal choice questions.**

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	Define algorithm and provide an example in C programming language.	**4**	**CO1**
Q 2	Can the following matrices be multiplied? Defend your answer. $A = \begin{bmatrix} 1 & 4 \\ 2 & 3 \end{bmatrix}$ $B = \begin{bmatrix} 1 & 5 \\ 2 & 4 \\ 4 & 1 \end{bmatrix}$	**4**	**CO2**
Q 3	Discuss Bisection method to find the roots of a function.	**4**	**CO1**
Q 4	What is an identity matrix? Give examples of it for a 2×2, 3×3, and 4×4 matrix.	**4**	**CO2**
Q 5	Explain interpolation and curve fitting.	**4**	**CO1**
	SECTION B **(4Qx10M= 40 Marks)**		
Q 6	How is computational chemistry important in the field of research?	**10**	**CO1**
Q 7	As per Runge-Kutta method, express the equation for y_{k+1}. **OR** Describe Trapezoidal and Simpson's 1/3 rules for solving numerical integrations.	**10**	**CO1**
Q 8	What do the following equations represent? Elaborate: $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{f'''(\xi_1)}{6}$ $f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{f'''(\xi_2)}{6}$	**10**	**CO1**

Q 9	Solve the following system of equations using Gaussian elimination method: $2x + 4y + 6z = 22$ $3x + 8y + 5z = 27$ $-x + y + 2z = 2$	**10**	**CO2**
SECTION-C (2Qx20M=40 Marks)			
Q 10	For the following matrices, prove that AB + AC = A(B+C). $A = \begin{bmatrix} 8 & 9 & 1 \\ 2 & 5 & 1 \\ 1 & 0 & 1 \end{bmatrix}$ $B = \begin{bmatrix} 7 & 4 & 1 \\ 7 & 1 & 0 \\ 1 & 7 & 1 \end{bmatrix}$ $C = \begin{bmatrix} 0 & 0 & 4 \\ 0 & 5 & 4 \\ 1 & 1 & 0 \end{bmatrix}$	**20**	**CO2**
Q 11	Compute the value of A^{-1} for the following 2×2 matrices. In the case A^{-1} cannot be calculated for the given A, explain why? i) $A = \begin{bmatrix} -1 & -1 \\ 2 & 9 \end{bmatrix}$ ii) $A = \begin{bmatrix} 3 & 1 \\ -1 & 5 \end{bmatrix}$ iii) $A = \begin{bmatrix} 4 & 1 \\ 1 & 1 \end{bmatrix}$ iv) $A = \begin{bmatrix} -6 & -1 \\ 8 & 1 \end{bmatrix}$ **OR** Calculate the value of A^{-1} for the following 3×3 matrix. $A = \begin{bmatrix} 2 & 3 & 3 \\ 1 & 1 & 2 \\ 2 & 1 & 1 \end{bmatrix}$	**5×4** **OR** **20**	**CO2**