

Total number of printed pages-7

63 (FY)SEM-5/MAJ/CHMMAJ3044

2025

CHEMISTRY

(Major)

Paper : CHMMAJ3044

(Computers in Chemistry)

Full Marks : 50

Pass Marks : 20

Time : Two hours

The figures in the margin indicate full marks for the questions.

1. Answer the following questions : 1×5=5

(a) Which of the following is not a valid string constant ?

(i) TEMP\$

(ii) \$GAS

(iii) PRESS1\$

(iv) MESSAGE\$

- (b) Which of the following is not a high level programming language ?
- (i) C++
 - (ii) Python
 - (iii) Assembly language
 - (iv) Java
- (c) What is the full form of ASCII ?
- (i) American Standard Code-II
 - (ii) Asian Standard Code-II
 - (iii) Asian Standard Code for Information Interchange
 - (iv) American Standard Code for Information Interchange
- (d) What is the purpose of REM statement in BASIC ?
- (i) To execute a command repeatedly
 - (ii) To perform a calculation
 - (iii) To insert a comment or remark
 - (iv) To stop a program

(e) Newton-Raphson method can be considered as

(i) Chord method

(ii) Diameter method

(iii) Tangent method

(iv) Secant method

2. Answer the following : **(any five)** $2 \times 5 = 10$

(a) Convert the binary number 11001001 into a decimal number.

(b) Draw a flow chart to print the squares of first 100 natural numbers.

(c) Explain the following :

(i) Graphics

(ii) Debugging

(d) Differentiate Operating system and Programming language.

(e) What do you mean by compiled and interpreted language ?

(f) Express the following statements as in the BASIC language :

(i) $(A + B) \times (C + D) / (A^2 \times B^2)$

(ii) $(A + B) \times (C + D) / \{ \exp(2) \}$

(g) Find the value of a , b , c and d , if

$$\begin{bmatrix} a - b & 2a + c \\ 2a - b & 3c + d \end{bmatrix} = \begin{bmatrix} -1 & 5 \\ 0 & 13 \end{bmatrix}$$

3. Answer the following : **(any five)**

5×5=25

(a) Draw a flow chart to implement the

kinetic gas equation, $PV = \frac{1}{3}mNC^2$ and

write the BASIC program to calculate the pressure.

2+3=5

(b) System of simultaneous are given as :

$$A_1x + B_1Y = C_1$$

$$A_2X + B_2Y = C_2$$

Write a BASIC program to compute the values of X and Y .

(c) What is linear interpolation? Given that :

x	2	4	6
y	4	?	7

Use the linear Interpolation formula to find the value of y when $x = 4$.

$$2+3=5$$

(d) Using Newton-Raphson method, find the cube root of 12 assuming $x_0 = 2.5$.

(e) Solve $x^2 - 3 = 0$ for $x \in [1, 2]$, by using the bisection method.

(f) What do you mean by numerical integratgion? Explain the Trapezoidal rule of numerical integration.

1+4=5

(g) Derive the Simpson's 'One-Third' rule.

(h) Write a BASIC program to determine the emperical formula of hydrocarbons.

4. Answer the following : (**any one**) 10

(a) Write a BASIC program to determine the electronegativity of an atom from bond energy data using Pauling's relation—

$$|\chi_A - \chi_B| = 0.208 \times \sqrt{D_{AB} - \sqrt{D_{AA} \times D_{BB}}}$$

where, D_{AB} = Bond energy of A - B bond (in eV) D_{AA} and D_{BB} = Bond energies of A - A and B - B bonds (in eV) and the constant 0.208 converts energy difference into electronegativity scale.

(b) What do you mean by False Position method? Find the root for the equation $x^3 - 3x + 1 = 0$ using Regula-Falsi method and correct it to three decimal places with three iterations.

2+8=10
