6-6-24

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63/1 (SEM–6) DSE3/CHMHE 6036

2024

CHEMISTRY

Paper : CHMHE 6036

(Application of Computers in Chemistry)

Full Marks : 60

Pass Marks : 24

Time : Three hours

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

1. Choose the correct answer from the following : ***(any five)*** 1×5=5

   (a) What is stored in RAM?

   (i) The BIOS

   (ii) Data and instructions for use by CPU

   (iii) The operating system

   (iv) Save files for games

Contd.

(b) Which of the following is an output device ?

(i) Keyboard

(ii) Mouse

(iii) Printer

(iv) Floppy

(c) BASIC stands for

(i) Beginner's All-purpose Systematic Instruction Codes

(ii) Beginner's All-purpose Symbolic Instruction Codes

(iii) Beginner's All-purpose Systematic Information Codes

(iv) Beginner's All-purpose Symbolic Information Codes

(d) Which of the following is invalid basic variable ?

(i) PRESS 1

(ii) FRA≠

(iii) GAS$

(iv) GTHIONS

(e) Identify the valid numeric constant.

(i) 15,328

(ii) $350

(iii) 32.5E-40

(iv) 2.58E5

(f) The roots of the equation $x^2 - 7x + 10 = 0$ using the quadratic formula are

(i) $x = 2, x = 7$

(ii) $x = 3, x = 7$

(iii) $x = 2, x = 5$

(iv) $x = 3, x = 5$

(g) A program that translates a high level language program into a machine level language program is called

(i) complier

(ii) interpreter

(iii) hacker

(iv) assembler

(h) The process of finding the best fitting curve is called

(i) iteration method

(ii) least square method

(iii) extrapolation method

(iv) false position method

(i) Newton-Raphson method can be considered as

(i) chord method

(ii) diameter method

(iii) tangent method

(iv) secant method

(j) _____ shape is generally preferred in case of application of Simpson's rule.

(i) Square

(ii) Rectangle

(iii) Trapezoid

(iv) Triangle

2. Answer the following questions : ***(any five)*** 2×5=10

(a) What are library functions? Give examples. 1+1=2

(b) State the use of REM statement in BASIC program.

(c) Convert the binary number 01101000 into decimal number.

(d) Differentiate between the following : 1+1=2

(i) BIT and BYTE

(ii) Flowchart and Program

(e) Express the following in BASIC expression : 1+1=2

(i) $P = \frac{RT}{v-b} - \frac{a}{v^2}$

(ii) $N = (2J+1)e^{-BJ(J+1)hc/kT}$

(f) What do you mean by programming language? What are different types of programming language? 1+1=2

(g) Draw a flowchart to print the square of first 100 natural numbers.

3. Answer the following questions : ***(any five)*** 5×5=25

(a) Explain the following : 2½+2½=5

(i) ASCII code

(ii) Debugging

(b) Write a BASIC program to compute and print the roots of a quadratic equation.

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

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

(e) Find the roots of the equation $2x = \cos x + 3$ by iterative method up to three decimal places.

(f) A gardener planted a tomato plant and kept track of the growth of the plant every other day as shown below :

Day	1	3	5	7	9
Height (mm)	0	4	8	10	12

What will be the height of the plant on the 4^{th} day ?

(g) Explain the following : 2½+2½=5

(i) String

(ii) Graphics

(h) What do you mean by numerical integration ? Explain the trapezoidal rule of numerical integration. 1+4=5

(i) What is constant in C++ ? How many types of constants are allowed in C++ ? Write the rules to construct different types of constants. 1+1+3=5

4. Answer the following questions : ***(any two)*** 10×2=20

(a) What do you mean by false position method ? Find the root for the equation $x^3 - 3x + 1 = 0$ using the Regula-Falsi method and correct it to three decimal places with three iterations. 2+8=10

(b) Consider the time series data given below :

x_i	8	3	2	10	11	3	6	5	6	8
y_i	4	12	1	12	9	4	9	6	1	14

Use the least square method to determine the equation of best fit line for the data and also plot the line. 8+2=10

(c) Solve the following system of equation by Gauss-Siedal method :

$$5x - 2y + z = -4$$

$$x + 6y - 2z = -1$$

$$3x + y + 5z = 13$$

(d) Derive Simpson's 'one-third' rule. Evaluate the following integral by using Simpson's $\frac{1}{3}$rd and $\frac{3}{8}$th rules :

5+5=10

$$\int_0^1 \frac{1}{1+x^2}\,dx \qquad \left(\text{Take } h = \frac{1}{6}\right)$$
