3 Yr. Degree/4 Yr. Honours 3rd Semester Examination, 2025 (CCFUP)

Subject : Chemistry

Course : CHEM3051 (SEC)

Time: 2 Hours **Full Marks: 40**

The figures in the margin indicate full marks.

Candidates are required to give their answers in their own words as far as practicable.

1. Answer *any five* questions from the following: 2×5=10

(a) What does the abbreviation ASCII stand for? What is the most striking difference between a binary file and an ASCII file? 1+1

(b) Five numbers are put in an Excel sheet from cells A1 to A5. Write down the Excel expression to calculate the average of these numbers. 2

(c) What will be the mean, median and mode for the data set {2,3,3,4,6}? 1+½×½

(d) Sketch the graph of the function $y = \sqrt{x+4}$. 2

(e) In a FORTRAN program with the statement implicit real *8 (a-h, o-z), the following two types of declarations are made:

(i) i = 7
j = 2
a = i/j

(ii) i = 7
j = 2
a = real (i)/real (j)

What will be the value of ä as the output in the two situations? 1+1

(f) The energy of an electron in the ground state of a hydrogen atom is –13.6 eV. What will be the corresponding energy in Joules and Calories? 1+1

(g) Convert $(25)_{10}$ and $(36)_{10}$ into binary system. 1+1

(h) For the quadratic equation $ax^2 + bx + c = 0$, write down the Excel expression to calculate the discriminant ($b^2 - 4ac$), provided a, b and c are placed in cells A1, B1 and C1 respectively in an Excel sheet. 2

2. Answer *any two* questions from the following: 5×2=10

(a) Sketch the graph of the function $f(x) = (x-1)^2 + 1$ and show that for any value p of x, $f(p) = f(2-p)$. Illustrate this result on your graph by choosing one value of p. (1+1½)+2½

(b) Write down the Excel functions / forms for the following mathematical expressions: 5

(i) $\sqrt{x}$ (ii) $2x^2 + 5x - 3$ (iii) $\log_e x$ (iv) $\log_{10} x$ (v) $(2^m 3^n)^{1/p}$

(c) The probability of finding gas molecules having speed within the range v to $v + dv$ is given by the Maxwell's speed distribution formula (in three-dimensions)

$$P(v)dv = 4\pi \left(\frac{M}{2\pi RT}\right)^{\frac{3}{2}} v^2 e^{\frac{-Mv^2}{2RT}} dv$$

where M is the molar mass of the gas, T is the temperature in Kelvin scale and R is the universal gas constant. Write down the FORTRAN statements

(i) to declare π and R as parameters,

(ii) to read (from the computer terminal) variables v, dv, M and T, and

(iii) to calculate $(M/2\pi RT)^{3/2}$ and $v^2 e^{-Mv^2/2RT}$ and store them in A and B, respectively, that may be used in a program to calculate $P(v)dv$. 1+1+1½×2

(d) What do you mean by the term standard deviation? How is variance related to the standard deviation? A biologist was interested in the average height and standard deviation of a plant species. The following data are the heights (in cm) for a sample of 20 plants:

10.0	11.0	9.5	10.0	11.0	10.0	11.5	11.0	10.5	11.5
9.0	10.0	10.5	11.5	11.0	9.5	10.5	11.0	11.0	10.5

The average height is 10.53 cm, rounded to two places. Find the standard deviation, rounded to two decimal places. 1+1+3

3. Answer *any two* questions from the following: 10×2=20

(a) (i) For the following bivariate (x_i, y_i) data, use the method of least squares to calculate the slope and intercept of the line of best fit and predict the value of y_i at $x_i = 14$.

x_i	2	4	6	8	10	12
y_i	2	4	4	5	5	7

(ii) Compute by Newton–Raphson method the positive root of the equation $3x^2+2x-9 = 0$ using initial guess $x = 1$ (show 4 iterations clearly). 5+5

(b) (i) Find the integral $I = \int_1^5 x^2 dx$ by dividing the interval into four divisions followed by using the Trapezoidal rule.

(ii) Write a FORTRAN program to evaluate the integral of log (sin x) within the limits of 0 to π using the Simpson's rule ($\pi = 3.14$ radian). 5+5

(c) (i) Given the following two square matrices A and B. Determine the product matrix C.

$$A = \begin{pmatrix} -1 & 4 \\ 2 & 3 \end{pmatrix}, B = \begin{pmatrix} 9 & -3 \\ 6 & 1 \end{pmatrix}$$

(ii) Give a description of the algorithm to carry out the matrix multiplication of a matrix A ($m \times p$) with B ($p \times n$) to produce the product matrix C ($m \times n$).

(iii) Say, you are given two 3 × 3 matrices A and B. Write down the FORTRAN statements to

(I) initialize the result (product matrix) C to zero, and

(II) perform the matrix multiplication using appropriate DO loops. 2+3+(2+3)

(d) (i) The radial wavefunction for the 2s orbital of hydrogen atom is given by

$$R_{2s}(\mathrm{r}) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}$$

where a_0 is the first Bohr radius. Draw an approximate graph of the radial distribution function for the 2s orbital and mark the location of the radial node on your graph.

(ii) Derive the formula for iteration used in the Newton–Raphson method.

(iii) Write down the expression of finding numerical differentiation by central divided difference (CDD) formula.

Given $f(x) = 2.e^{3x}$. Find $f^1(x)$ at $x = 2$ using CDD formula. 3+3+4
