

2020

CHEMISTRY — HONOURS

Paper : DSE-A-2

(Applications of Computers in Chemistry)

Full Marks : 50

The figures in the margin indicate full marks.

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

Answer **question no. 1** and **any eight** questions from the rest.

1. Answer **any ten** questions :

1×10

(a) Write logical expression to express the following condition :

A is less than 6 or is greater than 10.

(b) Locate error in the following :

IF – THEN Construct

IF (B . NOT . 10)

WRITE (* , *) 'B is not equal to 10'.

(c) What is the result of the following operation of the intrinsic function 'MOD' in FORTRAN?

MOD(12, 5)

(d) Mention the column numbers between which statements have to be written in a Fortran program.

(e) Which arithmetic operation is signified by the symbol '* *' in Fortran?

(f) What is the result of the expression written in the formula bar of Excel : = 2⁽⁻³⁾?

(g) What Excel function returns the two-tailed inverse of *t*-distribution? Write down the syntax of the function.

(h) What Excel function will be required to calculate Interquartile range?

(i) What Excel function will calculate Fischer *F* value at 95% probability?

(j) How will you calculate mean and standard deviation of a set of data using Excel's in-built function?

(k) What is the limitation of 'Solver' in Excel?

(l) Write the algebraic expression corresponding to the following FORTRAN expression :

(A*B) + C / (D * * F + G) + A / B + C

Please Turn Over

2. (a) Write a FORTRAN program to find the sum of following series by adding n terms of the series.

$$1 + \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \dots$$

- (b) What is the use of Excel's NORM·INV () function? Write down the syntax of the function including arguments. 3+2

3. (a) Examine the following loop and determine the value of 'ires' at the end of the loop. Assume that 'ires' and 'index' variables are integer.

```
ires = 0
Do index 1 = 1, 10
    Do index 2 = 1, 10
        ires = ires + 1
    END DO
END DO
```

- (b) What is the syntax of the LINEST function in Excel, explaining each of the arguments? 3+2

4. (a) Write the subroutine program for calculation of factorial of any number n . ($n! = 1.2.3....n$).

- (b) What are the advantages and disadvantages of using Trendline in Excel (write two points for each). 3+2

5. Write only the relevant sentences which are required in a Fortran program to (a) read 3 integers (5, 97, 283) from screen in free format, (b) open a new file with name output, (c) write the given data with the format given below in the same file.

The given numbers are :

				5	
			9	7	
		2	8	3	

5

6. (a) Write a FORTRAN program to read the half-life period of a radioactive element and determine the time at which 75% of elements disintegrate.

- (b) Variables a, b, c, d, e, f and g have been initialized to the following values :

$$a = 3., \quad b = 2., \quad c = 5., \quad d = 4., \quad e = 10., \quad f = 2., \quad g = 3..$$

Evaluate the following FORTRAN assignment statements :

$$\text{Output} = a * b + c * d + e / f ** g$$

3+2

7. (a) Write a FORTRAN program to multiply the following two matrices :

$$\begin{pmatrix} 1 & 2 & 4 \\ 3 & 5 & 3 \\ 4 & 9 & 8 \end{pmatrix} \text{ and } \begin{pmatrix} 4 & 9 & 8 \\ 2 & 6 & 5 \\ 1 & 3 & 7 \end{pmatrix}$$

What will be the outcome of the program?

- (b) What values are stored in a and b after the following statements executed?

```
REAL :: a, b
INTEGER :: i, j
i = 10
j = 3
a = i / j
b = REAL (i) / j
```

3+2

8. (a) Explain the term 'Linear Correlation Coefficient r '. What is the syntax of the function ' r ' in Excel? What is the significance of the value of ' r '?
- (b) Write the FORTRAN expression for the following :

$$\left[\frac{\left(\frac{a}{b} \right)^n / (c - d^m)}{d / (b + a)^{n+m}} \right]^{\frac{1}{m^2}}$$

3+2

9. Describe the step by step Excel procedure for least square analysis (determination of slope and intercept) from the given X - Y data set :

X :	0.000	0.050	0.100	0.200	0.400
Y :	0.000	0.057	0.119	0.221	0.383

Determine different Excel quantities using calculator.

5

10. How will you determine the area under the curve in Normal or Gaussian distribution? What Excel function will you use to determine the area under the curve? Write down the syntax of the function and explain the corresponding arguments. What Excel function will you use to determine the area under the standard normal curve?

5

11. Using Simpson's rule in Microsoft Excel, show that the following two functions are orthogonal to each other.

$$P_1(x) = x ; P_2(x) = 0.5 (3x^2 - 1) \text{ where, } x = [-1, 1]$$

Use five point calculation for Simpson's rule.

Determine different Excel quantities using calculator.

5

Please Turn Over

12. Why we use t -test in chemical analysis? For the two sample t -test with standard deviations are not significantly different, state null and alternate hypothesis. Write down the mathematical expression for calculating t -statistics. What Excel function will you use to determine t -statistics? Write down the syntax of the function and explain the arguments. 5
13. Consider the titration of a weak monoprotic acid HA against a strong base MOH, and deduce the relation :

$$\frac{V_b}{V_a} = \frac{C_a \left(\frac{[A^-]}{[HA] + [A^-]} \right) - ([H^+] - [OH^-])}{C_b + \left([H^+] - \frac{[K_w]}{[H^+]} \right)}$$

where, C_a is the concentration of acid HA

C_b is the concentration of the base MOH

V_a and V_b be the volume of the acid and base respectively.

What information will be required by Microsoft Excel in order to generate values of $\left(\frac{V_b}{V_a} \right)$ for different hydrogen ion concentrations? 5
