2021

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) Assuming mixed mode expressions, find the value of the expressions :

   (i) `2*6/5` (ii) `7./(4*2.)`

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

   X is greater than 20 or is equal to 5.

   (c) Locate error in the following IF-THEN construct :

   ```
   If (a > b) PRINT*,  'a > b'
      END  IF
   ```

   (d) Correct the following invalid logical statement :

   ```
   IF(I==J)THEN
   P=Q+R
   IF(K==M)THEN
   S=V+T
   ```

   (e) State TRUE or FALSE :

   (i) .NOT. is a binary logical operator in FORTRAN.

   (ii) .NEQV. is a binary logical operator in FORTRAN.

   (f) If a = 15.0, c = 6.0, d = 4.0, x = 3.0 and y = 4.0, evaluate the following as TRUE or FALSE :

   a – 5.5 >= 9.5 .OR. c < d .AND. x >= y

   (g) Formulas in Excel always begins with _____ sign.

   (h) What is the syntax in Excel for finding the cumulative distribution function using standard normal distribution?

   (i) What are Type - I and Type - II error in Hypothesis testing?

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(j) When do you need to include subprogram in your program?

(k) In F-statistics, $F = s_1^2/s_2^2$, where the terms have their usual significance. What is the relation between s_1 and s_2.

(l) How will the nature of normal distribution change if we increase standard deviation keeping mean constant?

2. (a) The following are mathematical expressions and corresponding incorrect FORTRAN expressions. Write the correct FORTRAN expressions :

(i) $\left(\dfrac{a}{b+c}\right)^2$ A/(B+C)**2

(ii) $\left(\dfrac{x}{y}\right)^{n+1}$ (X/Y)**N+1

(iii) $\sqrt{\left(\dfrac{a^2}{b+c}\right)}$ SQRT(A**2/(B+C))

(b) Use built-in or Library FUNCTION in the following translation into FORTRAN :

(i) $\dfrac{\sin x}{|y|+\cos z}$ (ii) $\dfrac{e^{x+y}}{x+y}$ 3+2

3. (a) Suppose A, B, J and K contain the following values : A = 2.7, B = 3.5, J = 3 and K = –2. Find the values of X and L after each pair of statements :

(i) X = A + J*K**2 + B

   L = A + J*K**2 + B

(ii) X = ABS(A–J*B)/5

   L = ABS(A–J*B)/5

(b) Suppose A and B have the following values : A = 2.5 and B = 3.5. Find the values of A and B as a result of the following program segments :
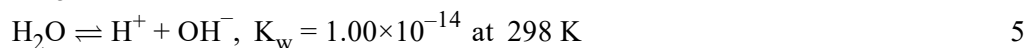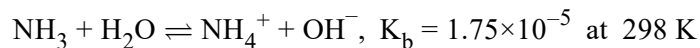
(i) A = B

   B = A

(ii) T = A

   A = B

   B = T   3+2

4. How can you determine the concentration of species in an aqueous solution containing 0.010 mole NH_3 in 1.000 L using the Solver function of Microsoft Excel. Give stepwise procedure. Given;

The binary equilibrium is,

$$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-, \ K_b = 1.75 \times 10^{-5} \text{ at } 298 \text{ K}$$

$$H_2O \rightleftharpoons H^+ + OH^-, \ K_w = 1.00 \times 10^{-14} \text{ at } 298 \text{ K}$$ 5

5. (a) What is Excel's NORM.DIST ( ) function. Write down the syntax of this function including arguments. How is it different from NORM.S.DIST ( ) function?

   (b) Calculate the values of PDF and CDF when $x = 33$ for normally distributed data with mean $= 35$ and standard deviation $= 2$.   3+2

6. In a titration of a weak acid, let 'x' denotes the volume of the base and 'y' the second derivate of the volume of the acid with respect to pH. Then in the vicinity of $y = 0$ (the equivalence point), 'y' should be a linear function of 'x'. Now for the following 10 experimental data, give the stepwise procedure (Excel) for determination of 95% confidence limit for the equivalent volume of base.

x, ml →	30·64	30·68	30·75	30·79	30·82	30·89	30·96	31·00	31·07	31·13
y, ml →	−1·486	−1·137	−0·781	−0·262	−0·180	0·080	0·383	0·393	0·623	1·202

Given : $t_{0.95,8} = 2\cdot306$

M = infinity because $y = 0$ is a theoretical point.   5

7. The CdSe content (g/L) of six different samples of nanocrystals was measured by 2 different methods. Check whether the two methods differ significantly at the 95% confidence level or, not. Provide the step by step excel procedure. (Given : $t_{0.95, 5} = 2\cdot57$)   5

Sample	Method 1 (Anodic Stripping)	Method 2 (Atomic Absorption)
A	0·88	0·83
B	1·15	1·04
C	1·22	1·39
D	0·93	0·91
E	1·17	1·08
F	1·51	1·31

8. A certain steel is graded according to the results of three tests. The tests are :

   (a) Carbon content $< 0\cdot7\%$

   (b) Rockwell hardness > 50

   (c) Tensile strength $> 30,000$ kilos/cm

   The steel is graded 10 if it passes all three tests, 9 if it passes only tests 1 and 2, 8 if it passes only test 1, and 7 if it passes none of the tests. Obtain a flowchart corresponding to this statement of the problem. Write a FORTRAN program corresponding to this flowchart.   5

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9. You are required to find a polynomial fit of the type $y = ax^2 + bx + c$ for a set of data (x_i, y_i). For this purpose, find the following :

   (a) sum of squared residuals

   (b) conditions to be obeyed by the best fit line

   (c) using the above conditions we arrive at three equations

   $$a\Sigma x_i^4 + b\Sigma x_i^3 + c\Sigma x_i^2 = \Sigma x_i^2 y_i$$
   $$a\Sigma x_i^3 + b\Sigma x_i^2 + c\Sigma x_i = \Sigma x_i y_i$$
   $$a\Sigma x_i^2 + b\Sigma x_i + nc = \Sigma y_i$$

   Arrange these equations in matrix form and write down the step by step EXCEL procedure for finding out a, b and c.　　　　　　　　　　　　　　　　1+1+3

10. (a) Write a FORTRAN program to read two one-dimensional arrays of integers and print a third array which is the union of the two arrays and the intersection of the arrays.

    (b) Write a FORTRAN program to find the sum of squares of elements on the diagonal of a square matrix.　　　　　　　　　　　　　　　　3+2

11. Using Trapezoidal rule in Microsoft Excel, evaluate the definite integral $\int_1^2 \dfrac{dx}{1+x}$. What will be the value of the same integral using Simpson's $\frac{1}{3}$ rd rule? Using five point calculation for both cases, determine different Excel quantities using calculator.　　　　　　　　　　　　　　　5

12. (a) The force f due to gravity between two bodies of masses m_1, m_2 is given by

    $$f = Gm_1 m_2 / r^2$$

    where $G = 6 \cdot 673E - 11$, r is the real distance (in meters) between the two bodies and m_1 and m_2 are in kg. Write a REAL function in FORTRAN to evaluate f. G should be defined as a parameter.

    (b) Write a FORTRAN function which calculates and returns the distance between any two points whose coordinates are (x_1, y_1), (x_2, y_2).　　　　　　　　　　　3+2

13. (a) Write a FORTRAN program to check whether 2 matrix commute with each other, i.e., whether $AB = BA$ or not.

    (b) What does the following program segment execute?

    ```
    T = A(1)
    DO 100 K = 1, N – 1
    A(K) = A(K + 1)
    A(K + 1) = T
    100 CONTINUE
    A(N) = T
    ```
    　　　　　　　　　　　　　　　　2+3