2022

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*** from the rest.

1. Answer ***any ten*** questions : 1×10

(a) Name a parameter that is an indicator of 'goodness of fit' that is complementary to the correlation coefficient. Give a brief reason.

(b) What is the limitation of solver in Excel?

(c) A correlation coefficient with magnitude (for linear regression) close to ± 1 is no guarantee that x-y data are linearly correlated. — Justify or criticise.

(d) What does '`=F.INV.RT(0.05,5,7)`' signify?

(e) What does '`=LINEST(array 1,array 2,False,True)`' signify?

(f) Predict the value of x (a real variable) from the following Fortran expression :

$x = \text{mod}\ (4, 3) + 4/3$

(g) Explain the use of 'implicit none statement' in Fortran programing.

(h) Correct the error, if any, in the following expression : Real A, B, C

```
IF (A.LT.B.LT.C) THEN
PRINT *, 'A<B<C'
END IF
```

(i) Write a Fortran expression of the following mathematical one : $\left(\cos^{-1} x\right) \Big/ e^{|5-2x|}$

(j) Write program statement to accomplish the following :
Determine the average of the ten elements of an array Y.

(k) What Excel function will be used to calculate a two tailed student t-value for a 95% confidence limit?

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

2. (a) Write a Fortran program for the multiplication of the two matrices A(2, 3) and B(3, 3).

   (b) Write a Fortran program to transpose a matrix K(3, 3). 3+2

3. Write a main Fortran program to read in a value x. Then create a function subprogram to compute the number x raised to nth power. Then using this function, write another function that computes the repeated fraction : 5

$$\cfrac{1}{x^4+\cfrac{1}{x^3+\cfrac{1}{x^2+\cfrac{1}{x^1}}}}$$

4. (a) Write a Fortran program to find the sum of the following series (upto 16 terms) : $1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+....$

   (b) Calculate the value of n count at the end of the two loops :

```
n count = 0
Do m = 1, 2
Do n = 1, 2
n count = n count + (m * n)
END DO
END DO
```

   3+2

5. (a) Write a FORTRAN program to verify whether a matrix is an identity matrix or not.

   (b) Write a program to determine RMS (root mean square) value of several numbers. 3+2

6. (a) A manufacturer X designed 25 shelves for fitting into a bookcase, which were needed to be put together by the customer. The variance of the shelf length was found to be 9.23 mm. Another manufacturer Y designed 27 shelves for the same purpose. The variance of the shelf length was 0.25 mm.

      (i) At 5% significance level, test the claim, using F-statistics, that the shelves sold by X was manufactured with more variation than the shelves designed by manufacturer Y.

      (ii) Mention and comment on null and alternative Hypotheses.

      (iii) Using Excel, write the syntax of the built-in function that might have given you the critical F-value— 1.946.

   (b) Make a rough sketch of an Excel Spreadsheet and describe step by step how you would have solved the equation :

   $x^2 - 3x - 40 = 0$, using Goal Seek.

   Given : x has one positive and one negative roots. 3+2

7. A study was conducted to determine the effectiveness of reducing high blood pressure (B.P.) (using medicine) of 10 patients. The table below shows the B.P. figures of the patients before and after the medicine in this program,

Patient	B.P. before medication mmHg	B.P. after medication mmHg
1	185	169
2	192	187
3	206	193
4	177	176
5	225	194
6	168	171
7	256	228
8	199	204
9	218	195
10	239	217

(a) Is this program effective for reducing blood pressure of the patients?

(b) Construct a 95% confidence interval and determine the marginal error.

(c) Write the syntax of the in-built function (Excel) to perform the paired t-test automatically.

Given : $S_d = 13.025$, $\bar{X}_d = -13.1$, Critical value of $t = 1.83$. 5

8. (a) Using the following data described in a spreadsheet, find two regression lines (x on y and y on x) using the variables.

(b) Also find the correlation coefficient.

(c) Write the syntax using the proper built-in function in excel order to determine the correlation coefficient. 5

1.	A	B	C	D	E	F	G	H	I
2.	x_i	y_i	$\sum x_i$	$\sum y_i$	$\sum x_i y_i$	$\sum x_i^2$	$\sum y_i^2$	$\bar{x}$	$\bar{y}$
3.	1	2	21	48	211	91	490	3.5	8.0
4.	2	4							
5.	3	7							
6.	4	9							
7.	5	12							
8.	6	14							

9. You are asked here to find the solubility of calcium oxalate when the pH is unknown, using Solver. The following pieces of information are given :

$2[Ca^{+2}]+[H_3O^+] = 2[C_2O_4^{-2}] + [HC_2O_4^{-1}] + [OH^-]$ – charge balance

$[Ca^{+2}] = [C_2O_4^{-2}] + [HC_2O_4^{-1}] + [H_2C_2O_4]$ – mass balance

K_{sp}, K_1, K_2 have got usual significance.

A spreadsheet (Excel) is given below with some additional information :

1.	A	B
2.	K_{sp}	1.70E–09
3.	K_1	5.60E–02
4.	K_2	5.42E–05
5.	K_w	1.00E–14
6.	Equation	
7.	$[C_2O_4^{-2}]$	
8.	$[HC_2O_4^{-1}]$	
9.	$[Ca^{+2}]$	
10.	$[H_3O^+]$	
11.	$[OH^-]$	
12.	blank	
13.	Documentation	
14.	Cell description	
15.	Cells (for solver results)	
16.	blank	
17.	blank	
18.	Constraints	
19.	Write the constraints necessary	
20.	.....	
21.	..... etc.	

Copy the spreadsheet and take liberty to extend cells if required. Now, describe briefly how you could determine the solubilities of CaC_2O_4 at different pHs. Also mention necessary assumption and initial guess, if required. 5

10. (a) Find the derivatives and fill in the spreadsheet sketched by you, using calculator :

1.	A	B	C	D	E
2.	x	$f(x)$	Backwards	Forwards	Central
3.	0	12			
4.	5	15			
5.	10	16			
6.	15	14			
7.	20	10			
8.	25	04			
9.	30	06			

(b) How would you describe stepwise in Excel to do the sum, the formula cells properly using the spreadsheet given above? 3+2

11. How can you determine the composition of a 0.01(M) solution of Sodium Acetate ($Na^+ A^-$) using the Goal Seek function of Microsoft Excel? Give stepwise procedure. Given :

The binary equilibrium is

$$A^- + H_2O \rightleftharpoons HA + OH^-,\ K_b = \frac{[HA][OH^-]}{[A^-]}$$

$$H_2O \rightleftharpoons H^+ + OH^-,\ K_w = [H^+][OH^-]$$

Given : $pK_w = 14$, $pK_b = 9.244$. 5

12. A study was made to determine the activation energy E_a for a chemical reaction. The rate constant k was determined as a function of T, and the data in the table below obtained :

1000/T	1·669449	1·589825	1·545595	1·501502	1·464124	1·428571
log k	–3·26761	–2·60206	–2·284	–1·85387	–1·60206	–1·19382

The data should fit a linear model of the form $\log k = \log A - E_a/(2.303\ RT)$, where A is the pre-exponential factor.

(a) Find the slope, intercept and standard error of the estimate using least square analysis. Provide the stepwise Excel procedure for the calculation.

(b) If the calculated and theoretical prediction of E_a are 38697 Cal mol^{-1} and 41000 cal mol^{-1}, then test the null hypothesis that E_a is the value at the 95% confidence level.

[Given $t_{(0.025,\ 4)} = 2.776$] 3+2

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13. The CdSe content (g/L) of six different samples of nanocrystals was measured by two methods. Do the two methods differ significantly at the 95% confidence level? (Given $t_{0.95,5} = 2.57$).

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

Write down the stepwise Excel calculation procedure. 3+2