R-302
(2)

2023

CHEMISTRY — HONOURS

Paper : DSE-A-1 and DSE-A-2

The figures in the margin indicate full marks.

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

Paper : DSE-A-1

(Molecular Modelling and Drug Design)

Full Marks : 50

Answer ***question no.*** **1** and ***any eight*** questions from the rest (***Q.*** **2** to ***Q.*** **12**).

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

(a) What are the internal coordinates of a molecule?

(b) What are non-covalent interactions?

(c) Write an expression to estimate the bond-angle distortion energy identifying the parameters used in the expression.

(d) What are local and global minima of a molecule?

(e) Write an expression for Coulomb interaction energy between two point charges, identifying the parameters used in the expression.

(f) What is the significance of 'time step' in a Molecular Dynamics simulation?

(g) While running a molecular dynamics simulation, what are most commonly stored in the computer?

(h) What is a ligand?

(i) In a Molecular Dynamics simulation how the kinetic energy of a molecule is calculated?

(j) What is the criterion for selection of a successful step in Monte Carlo method?

(k) What is meant by 'stable conformation' of a molecule?

2. What is a potential energy surface? For a molecule containing N atoms comment on the dimensionality of its potential energy surface. What does the slope at a particular point on the surface signify? 2+1+2

3. Write a short note on Steepest Descent method for energy minimization. 5

4. What is a scoring function? How are they used in molecular docking? 2+3

5. Write a function that can be used to estimate the potential energy of a molecule. Explain all the terms and parameters used in it. 1+4

6. What is Molecular Dynamics simulation? Briefly outline the steps. 2+3

7. What is the significance of 'Velocities' in a Molecular Dynamics simulation? Suggest a method of assigning it to different atoms of the system. 2+3

8. Write a short note on Lennard-Jones potential. 5

9. What is QSAR? Suggest a suitable utility of this relationship. 1+4

10. Write an expression for Morse potential explaining the parameters and their units. Draw a suitable graphical representation of it. 3+2

11. What is in Molecular Docking? Briefly explain how it can be used in drug design. 3+2

12. Show with a sketch why it is not correct to say that a transition state is not a maximum on a potential energy surface. 5

Paper : DSE-A-2

(Applications of Computers in Chemistry)

Full Marks : 50

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

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

(a) Give appropriate statement(s) in Fortran for evaluating value of 11 divided by 2.

(b) Translate the following algebraic expression to Fortran :

$$\left(3+\frac{a}{b}\right)^{m-1}$$

(c) Distinguish between a function subprogram and a subroutine subprogram (at least 2 points of difference).

(d) Translate the following Fortran expression to algebraic form :

ABS(SQRT(X – Y**3) – Z**3/COS(A + B))

(e) Atomic masses of the following elements are typed into cells given in parenthesis: Hydrogen (B2), Phosphorus (C2), Oxygen (D2). The molar mass of phosphoric acid is to be calculated in D5. What formula is to be typed in cell D5?

(f) In the following Excel spreadsheet:

	A	B	C	D
1	1	5	4	?

Cell C1 has been generated using formula = B1 – A1. The cell C1 has been copied and simply pasted in cell D1. Find out the value in cell D1.

(g) For a set of data points (x, y), typed in column A and B in a spreadsheet, mention two methods using inbuilt Excel function to find the slope and intercept of the best fit line.

(h) Give syntax for the library function MMULT in Excel. What does it perform?

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

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

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

(l) Consider the following spreadsheet :

1.	A	B	C
2.	x	$f(x)$	$f'(x)$
3.	0	12	
4.	5	15	
5.	10	16	

Find the derivative $f'(x)$ at $x = 5$ by using a suitable formula for differentiation.

2. (a) Give appropriate statement to open an output file 'OUTPUT.DAT'. Also give the write statement in the Fortran program.

(b) A first-order reaction proceeds with rate constant k_1. Reading the value of k_1, write a Fortran program to find out the time of completion of 80% of the reaction. 2+3

3. (a) Write a program using DO LOOP to find the sum of first 10 positive integers.

(b) Find the output of the following program :

```
INTEGER  A(10)
DO  I = 1,10,2
A(I) = 2*I - 3
A(I + 1) = I**2 - 5
END DO
WRITE  (*,*)  (A(I),I = 1,10)
END
```

2+3

4. Read the following matrices A and B from the input file :

$$A = \begin{pmatrix} 1.0 & 2.5 & 3.2 \\ 3.1 & -2.4 & 1.9 \end{pmatrix} \quad B = \begin{pmatrix} 3.0 & 2.1 \\ 1.0 & -1.2 \\ 1.2 & 0.9 \end{pmatrix}$$

Write a Fortran program to multiply the above two matrices and write the product matrix $AB = C$ to an output file. 5

5. (a) Write a program to identify the largest 5 numbers read into an one-dimensional array.

(b) Write a program which calculates the sum of the following series : $\frac{1}{2}+\frac{2}{3}+\frac{3}{4}+...+\frac{99}{100}$.

3+2

6. (a) For titrating 10 ml of a 0.1(N) solution with a 0.1(N) titrant, the following volume of titrant were obtained by the analyst :

Analyst A : 9.8, 9.91, 9.85, 10.08, 10.25 (ml)

Analyst B : 10.09, 10.12, 10.10, 10.12, 10.08 (ml)

Calculate the mean and standard deviation for the above two sets of results and hence comment on the accuracy and precision of the results.

(b) How can we represent the above calculation in Excel spreadsheet? 3+2

7. (a) Consider a fourth order polynomial of the form $ax^4 + bx^3 + cx^2 + dx + e = 0$, where a, b, c, d, e are known quantities. Describe a step by step Excel procedure to find out the maxima or minima of the function using GOALSEEK.

(b) Mention the syntax of the LINEST function and its corresponding arguments. 3+2

8. The following table shows the value of the acceleration due to gravity 'g' obtained through experiment.

$g(m/s^2)$	9.68	9.85	9.73	9.76	9.74

(a) Is the mean of the values significantly different statistically from a hypothesised value of $g = 9.81$ m/s^2?

(b) Test the hypothesis at the $\alpha = 0.05$ level of significance given t_{crit} with $\alpha = 0.05$ and $\gamma = 4$ is 2.776. 3+2

9. In thermodynamics, it is known that the entropy change of a system that is heated at constant pressure from temperature T_1 to temperature T_2 is given by $\Delta S = \int_{T_1}^{T_2} \left({}^{C_P}/_{T} \right) dT$, where C_p is the constant-pressure molar heat capacity and T is the temperature on the Kelvin scale. Calculate ΔS for the heating of 1.00 mol of solid zinc from 20.0 K to 100.0 K by carrying out a five-point integration using Trapezoidal Rule. The C_p values corresponding to different temperatures are given below. Determine the different Excel quantities using calculator.

T (Kelvin)	C_p (J/mol/K)
20	1.7
40	8.171
60	13.6
80	16.87
100	19.15

5

10. The water-gas reaction shown below has an equilibrium constant value of 0.106 at 700 K. The reaction was started using 0.150(M) each of hydrogen and carbon dioxide, respectively. Make a rough sketch of an Excel Spreadsheet and describe step by step how you would find the equilibrium composition of all chemical species using SOLVER.

$$H_2(g) + CO_2(g) \rightleftharpoons H_2O(g) + CO(g)$$ 5

11 (a) For the titration of weak mono-protic acid HA with a strong base MOH, deduce the following explicit expression for the titration curve :

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

where,

C_a is the concentrations of acid HA

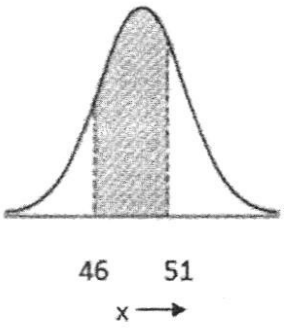
C_b is the concentrations of base MOH

V_a and V_b are the volumes of the acid and base respectively.

(b) Describe the step by step Excel procedure to generate the pH-metric titration curve using SOLVER function. 3+2

12. Why do we use t-test in chemical analysis? For the two-sample t-test whose 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. (a) How will you use Excel to calculate the area under the curve between x = 46 and x = 51 for normally distributed data with mean = 50 and standard deviation = 4?



(b) What is the difference between population standard deviation and sample standard deviation? Give mathematical formula for them. 3+2