BSc

2024

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.*** **13**).

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

(a) Distinguish between conformation and configuration of a molecule.

(b) For a linear tetra-atomic molecule draw the potential energy versus torsion angle graph.

(c) What is the coordinate system one can use to describe the three-dimensional structure of a molecule?

(d) What is the importance of 'time step' in a Molecular Dynamics simulation?

(e) Suggest a non-derivative method for energy minimization.

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

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

(h) What is meant by sequence alignment?

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

(j) What are covalent and non-covalent interactions?

(k) What are the units of length and energy commonly used in molecular mechanics?

(l) What is a ligand?

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

3. What is Molecular Dynamics simulation? Briefly outline the steps. What is meant by the length of the simulation? 2+2+1

4. What is energy minimization? What is the significance of the gradient calculated in the derivative methods? 3+2

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5. Name a second-order energy minimization method and briefly outline the steps. 1+4

6. What is QSAR? Briefly explain its use in drug design. 1+4

7. What is the significance of Temperature in a Molecular Dynamics simulation? Suggest a method to keep it constant during the simulation. 2+3

8. What is meant by *de novo* drug design? Briefly outline the steps. 2+3

9. From a molecular dynamics trajectory of liquid water explain how you can calculate the diffusion coefficient of the water molecules. 5

10. What is Monte Carlo simulation? Briefly outline the major steps involved. 2+3

11. 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

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

13. Write short notes on Lennard-Jones potential along with its graphical representation. 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) Translate the following FORTRAN expression to its algebraic form :

ASIN (X) / LOG 10(X).

(b) Find the value of an integer variable 'J' in the following FORTRAN expression :

J = MOD (9, 3).

(c) Calculate the expected output from the following :

```
A = 0
B = 3
  DO J = 1, B
      A = A + J**2
  END DO
WRITE (*, *) A
```

(d) Find logical result (True or False) for the given values :

X = 2.0

Y = –2.0

Z = 10.0

X. EQ. Y. OR. ((X/Y) + Z). EQ. 9.0. OR. Z. LE. Y

(e) What are the limitations of using Goal Seek in Excel?

(f) What is excel function TINV used for?

(g) In Excel, what does $ B $ 3 mean? How is it different from B $ 3?

(h) What does NORM DIST (75, 50, 5, TRUE) signify in Excel?

(i) What does FDIST (X, Deg. freedom 1, Deg. freedom 2) mean in Excel?

(j) What is central limit theorem?

(k) What is the difference between paired and unpaired t test?

(l) What do you understand by central divided difference in connection with numerical differentiation?

2. (a) Write a FORTRAN program to calculate the area of a trapezium, where the inputs are the lengths of the two parallel sides (a and b) and the perpendicular distance (h) between them.

Given, $\Delta = \frac{1}{2}(a+b).h$.

(b) Find the values of the outputs of the following program :

```
DIMENSION J(5)
      DO K = 1, 5
            J = 2*K
      END DO
J(2) = J(2) + J(3)
J(5) = J(5) – J(4)
WRITE (*,*) (J(L), L = 1,5)
```

2+3

3. (a) What is logical IF statement in programming? With any suitable example of a FORTRAN program of your choice discuss how logical IF can be used for conditional transfer of control in a program.

(b) Translate the following mathematical expression into FORTRAN statements :

(i) $\dfrac{e^{x+y}}{x+y}$

(ii) $\sqrt{|\cos(a-nb)|}$.

3+2

4. (a) Write a FORTRAN program to calculate the factorial of an integer.

(b) Write a FORTRAN code to transpose a (2×2) matrix and check whether the matrix is symmetric or not. 2+3

5. (a) Write a FORTRAN program to calculate the sum of the following series :

$$1 + X + X^2 + \ldots + X^N;\ X = 2.0,\ N = 10$$

(b) Give the statement to declare a two-dimensional array P containing real variables. What is the maximum number of elements it can store? 3+2

6. (a) Describe, step-by-step, the procedure to solve the given set of equations with Excel using Goal Seek :

$$7x - 2y = 45$$

$$5x + y = 37.$$

(b) Mention two limitations of Solver. 3+2

7. The equilibrium $N_2O_4(g) \rightleftharpoons 2NO_2(g)$ has an equilibrium constant $K_p = 0.12$ at 300 K. The reaction started with 0.02 mol of N_2O_4 and total pressure is 1 bar. Describe the step-by-step procedure to find the equilibrium composition using SOLVER in Excel. Also find K_c if the volume of the reaction container is 500 cm^3, using appropriate formulae in Excel. 4+1

8. You are required to find a second order polynomial fit for a set of data (x_i, y_i). For this purpose, write down the step-by-step EXCEL procedure for finding out the coefficient of the equation. 5

9. Using Trapezoidal rule, evaluate the following definite integral in Excel :

$$\int_1^5 \frac{1}{x} dx .$$

What will be the value of the same integral using Simpson's 1/3rd Rule? Using five point calculation for both cases, determine different Excel quantities using calculator. 5

10. Calculate the molar solubility of calcium oxalate in a solution that has been buffered so that its pH is constant and equal to 4.00. For the solubility of calcium oxalate the following equilibrium reactions can be written :

$$Ca(C_2O_4) \rightleftharpoons Ca^{2+} + (C_2O_4)^{2-}$$
$$H_2(C_2O_4) + H_2O \rightleftharpoons H(C_2O_4)^- + H_3O^+$$
$$H(C_2O_4)^- + H_2O \rightleftharpoons (C_2O_4)^{2-} + H_3O^+$$
$$2H_2O \rightleftharpoons H_3O^+ + OH^-.$$

Write down the Mass balance equation if,

$$K_{sp} = 1{,}70E - 09$$
$$K_1 = 5.60E - 02$$
$$K_2 = 5.42E - 05$$
$$K_w = 1E - 14.$$

Use Solver to find the equilibrium concentrations of Ca^{2+}, $(C_2O_4)^{2-}$, $H(C_2O_4)^-$ and $H_2(C_2O_4)$, where K_{sp}, K_1, K_2 and K_w have their usual significance. 1+4

11. How will you find the values of a and b for the non-linear equation $y = ax/(1 + bx)$ corresponding to the following set of data using linear regression? Mention stepwise the Excel procedure for your calculation.

x_j	y_j
0.1	3.032
0.3	3.66
0.5	4.288
0.8	5.23
1	5.858

5

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12. The table represents the mass fraction of fluoride in a toothpaste sample examined by an analyst in different time using a new method. The true value is 0.033. Is his measurement free of systematic error? Given $\sigma = 0.00509$ and $t_{crit} = 2.306$

Fluoride content	0.042	0.04	0.028	0.035	0.044	0.035	0.041	0.043	0.04

5

13. (a) From the following table :

	Machine - 1	**Machine - 2**
Mean production time	23.00	20.00
Standard deviation	2.71	2.79
Sample size	10	10

calculate the t-value corresponding to the two samples assuming equal variances (that allows to determine a pooled estimate from the given standard deviation values in table) that tests which machine works faster.

(b) Explain the Syntax : TTEST (array1, array 2, 2, 1) in Excel worksheet. 3+2