

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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(0630+0505)

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 :

$$\text{ASIN}(X) / \text{LOG } 10(X).$$

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

$$J = \text{MOD}(9, 3).$$

- (c) Calculate the expected output from the following :

$$A = 0$$

$$B = 3$$

$$\text{DO } J = 1, B$$

$$A = A + J^{**}2$$

END DO

WRITE (*, *) A

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

$$X = 2.0$$

$$Y = -2.0$$

$$Z = 10.0$$

$$X. \text{ EQ. } Y. \text{ OR. } ((X/Y) + Z). \text{ EQ. } 9.0. \text{ OR. } Z. \text{ LE. } Y$$

- (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?

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(0630+0505)

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.

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

- (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) $\frac{e^{x+y}}{x+y}$

(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 :

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

- (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 $\text{N}_2\text{O}_4(\text{g}) \rightleftharpoons 2\text{NO}_2(\text{g})$ 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.

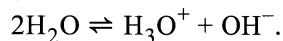
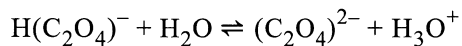
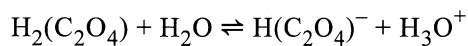
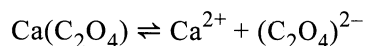
4+1

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 :



Write down the Mass balance equation if,

$$K_{\text{sp}} = 1,70\text{E} - 09$$

$$K_1 = 5.60\text{E} - 02$$

$$K_2 = 5.42\text{E} - 05$$

$$K_{\text{w}} = 1\text{E} - 14.$$

Use Solver to find the equilibrium concentrations of Ca^{2+} , $(\text{C}_2\text{O}_4)^{2-}$, $\text{H}(\text{C}_2\text{O}_4)^-$ and $\text{H}_2(\text{C}_2\text{O}_4)$, 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 $t_{\text{crit}} = 2.306$

Fluoride content	0.042	0.04	0.028	0.035	0.044	0.035	0.041	0.043	0.04
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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