2021

CHEMISTRY — HONOURS

Paper : DSE-A-1

(Molecular Modelling and Drug Design)

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 (**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 significance 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

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. Show with a sketch why it is not correct to say that a transition state is not a maximum on PES. 5

9. Give four applications of Molecular Mechanics. Which is the most widely used? 5

10. Molecular mechanics can calculate the values (in cm^{-1}) of vibrational frequencies, but without 'outside assistance' it cannot calculate their intensities. — Explain. 5

11. If the surface is quadratic, then Newton-Raphson method will be a good choice for energy minimization. — Explain. 5

12. What are the basic elements of the Monte-Carlo method? Write down the differences between Molecular Dynamics and Monte Carlo methods. 5

13. An important concept in computer simulation is that of the phase space. — Explain. 5

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