2020

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) What approximation leads to the concept of potential energy surface?

(b) What types of points on a potential energy surface are particularly relevant in understanding a molecular structure?

(c) What are the internal coordinates of a molecular system?

(d) For a linear molecule with 4 atoms (ABCD), comment on the dimensionality of the potential energy surface.

(e) Write an expression for the diatomic bond stretching energy and draw the graphical representation of the energy.

(f) Name one first-order energy minimization method. Identify the key step.

(g) What is the significance of Temperature in the context of a Molecular Dynamics simulation?

(h) What is Metropolis algorithm?

(i) Name one three-site water model and mention the features of the model.

(j) What is the active conformation of a drug molecule?

(k) What is meant by a binding site?

(l) Mention the significance of integration time-step in a classical Molecular Dynamics simulation.

2. What is meant by 'docking'? How is it used in drug design? 2+3

3. For n-Butane molecule draw a rough potential energy diagram keeping the bond lengths and bond angles fixed. Explain your diagram. 2+3

4. What is a molecular mechanics force field? Write down the term that represents torsion angle energy explaining all the variables in the expression. 2+3

5. What are non-covalent interactions? Suggest how they are important in stabilizing a glucose molecule in aqueous medium. 2+3

6. What do you mean by optimization of molecular geometry? Explain a method by which this can be achieved. 2+3

7. Mention the steps involved in a classical molecular dynamics simulation. Explain briefly how initial velocity is assigned to individual atoms. 3+2

8. From a molecular dynamics simulation of liquid water done at a particular temperature, identify two structural and / or dynamic properties of water molecules that can be estimated. Explain the process. 2+3

9. Briefly outline the steps of a Monte Carlo simulation. Which one, in your opinion, is the most critical step? 3+2

10. What are numerical errors? Suggest a possible source of such errors in a classical molecular dynamics simulation. 2+3

11. What is Lennard–Jones potential? Give an expression clearly explaining the variables used. Draw its graphical representation. 2+3

12. Name one first-order energy minimization method. Briefly outline the steps involved. 5

13. What do you mean by 'Sequence Alignment' in connection with the structure prediction of a protein? Name these general types of 'Sequence Alignment' methods. 5
