DSE-5
Chemistry

[This question paper contains 6 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 1259 **A**

Unique Paper Code : 32177905

Name of the Paper : Molecular Modelling and Drug Design

Name of the Course : **B.Sc. (Hons.)**

Semester : VI

Duration : 3.5 Hours Maximum Marks : 75

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Answer **Six** questions in all.
3. Each question carries **12.5** marks.
4. **First** part of the question carries **4.5** marks.
5. Remaining parts of each question carry **4** marks.
6. Attempt all parts of a question together.

P.T.O.

1. (a) What do you mean by occupied and virtual molecular orbitals. Taking CH_2 (carbene) as example calculate the total number of basis functions using 6-31G* basis set. Give the total number of occupied and virtual orbitals considering it to be a closed shell species.

(b) Using the Hiickel theory write down the secular determinant for 1, 3 butadiene. Using this calculate the energies of π molecular orbitals and its delocalization energy.

(c) The Lennard-Jones potential is represented by

$$v(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Explain each term and prove that $r_m = 2^{1/6}\sigma$.

2. (a) Match the following and explain the symbols used in each expression on the right hand side

1. Split valence basis set	a) 6-31+G*
2. Minimal basis Set	b) 3-21G
3. Split valence basis set with polarization	c) 3-21G
4. Basis set with diffuse function	d) STO-3G

(b) Distinguish between the following pairs :

(i) STOs and GTOs

(ii) Spin wave function and Spatial wave function

(c) Write the expression for a molecular mechanics force field used for macromolecular simulations. Describe what each energy term represents. Give the number of bond- stretching terms, bond-bending terms, bond-torsion terms and non-bonded interactions in a force field for propane molecule.

3. (a) The energies of Highest Occupied Molecular Orbital and Lowest Unoccupied Molecular Orbital of a molecule AB are -0.3502 eV and -0.1113 eV respectively. Comment on the Ionization energy of the molecule. State the theorem involved. Why doesn't it work for calculations of electron affinities? Justify.

(b) In context with molecular mechanics force field what do you understand by the terms transferability and atom-type.

(c) How is temperature controlled in molecular dynamics and Monte Carlo simulations? Write all steps involved in setting up a molecular dynamics simulation.

4. (a) What do you understand by the term interatomic potential? Explain any two in brief.

(b) Using Newton Raphson method find the root of the equation $x^3 - 2x - 5 = 0$. Show each step.

(c) Name the model used for simulation of pure water. Draw the pair distribution function plots for O-O, H-H, O-H for water.

5. (a) Differentiate between ab-initio and DFT methods.

(b) How does the Leap frog algorithm used in molecular dynamics simulation works? Give its advantages and drawbacks. How is it different from Verlet algorithm?

(c) The geometry of a molecule corresponds to a negative curvature in one direction and positive curvature in all other directions on Potential energy surface. What does this correspond to? What would be the value of Hessian for the same? How is it different from a stationary point?

6. (a) Distinguish between the following :

(i) Microcanonical and grandcanonical ensemble

(ii) MM3 and PM3

(b) What is the significance of using periodic boundary conditions in molecular dynamics simulations? How is it different from the calculations done in vacuum?

(c) How do internal coordinates differ from cartesian coordinates? Write z-matrix for ethyne molecule.

7. (a) De-abbreviate the following and briefly explain

(i) AMBER

(ii) OPLS

(b) Calculations based on random sampling falls under which type of simulations. Briefly explain the method and its algorithm.

(c) Define a molecular descriptor. Explain with the help of any two examples.

P.T.O.

8. (a) Differentiate between proper torsion and an improper torsion angle. How does this concept aid in Conformational Analysis?

(b) Ethanol has an LD_{50} of 7060 mg/kg. What would be the lethal dosage for an individual weighing 42 kg? How is LD_{50} different from ED_{50}?

(c) Explain the terms ZDO, CNDO, INDO and NDDO, showing why the latter three represent a progressive conceptual improvement.

9. Write down the short notes **(Any three)** :

(i) Ergodic hypothesis

(ii) Periodic Box

(iii) PDB

(iv) Hansch Analysis