Unique Paper Code	: 32177905
Name of the Paper	: DSE-Molecular Modelling and Drug Design
Name of Course	: B.Sc (H) Chemistry
Semester	: VI
Duration of Exam	: 3 Hours
Maximum Marks	: 75

Instructions for candidate

1. All questions carry equal marks.
2. Answer **four questions** in all.
3. First part of each question carries 0.75 marks.
4. Remaining parts of each question carry 6 marks.
5. Attempt all parts of a question together.

1. a. Lennard-Jones potential is_____potential. (0.75)

   b. Explain QSAR. Enlist the differences between 2-D QSAR and 3-D QSAR. (6)

   c. Explain the term "Computational Chemistry"? What are its advantages and applications over wet chemistry? What are the four basic methods used in computational chemistry? Out of these, which one is best suited for a macromolecule? (6)

   d. Explain the term "potential energy surface". Draw 2-D potential energy surface of propane and explain all stationary points. (6)

2. a. Expand MMFF. (0.75)

   b. What are the similarities and differences between first order derivative method and second order derivative method for energy optimization? Explain linear search and polynomial search. (6)

   c.(i) How do molecular mechanics method evaluate electronic properties like charge distributions?

   (ii) Plot and explain the pair distribution function for water molecule. (3,3)

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d. (i) Explain how the time step should be selected in a Molecular Dynamics simulation. What problems arise from too large or too small value of time step?
(ii) How Verlet Algorithm used in molecular dynamics simulation different from Leap Frog Algorithm? (3,3)

3. a. True or false?

Number of Cartesian coordinates is more than Internal coordinates. (0.75)

b. Write z-matrix for hydrogen peroxide. Do cartesian coordinates work better than internal coordinates? Justify your answer. (6)

c. Plot the following stationary points in a potential energy diagram:

(i) Molecule AB has energy -15.6 kcal mol^{-1}.

(ii) Molecule A--B has energy 5.1 kcal mol^{-1}.

(iii) Molecule BA has energy -9.3 kcal mol^{-1}.

How can you differentiate between AB and A--B in terms of vibrational frequencies? Apart from the stability, what information does values of vibrational frequency give?

(6)

d. What do you mean by gradient and hessian matrix? What do they represent? How can one differentiate between a stable intermediate and a transition state in terms of these matrices? (6)

4. a. What are the conditions for Grand Canonical ensemble? (0.75)

b. What is the principle, advantages and shortcomings of Semi empirical method? (6)

c. How are the biological parameters different from the structural parameter in QSAR studies? Explain with the help of at least 3 examples. (6)
d. Write down the simple Fock matrices for
(i) Cyclopropenyl radical; (ii) Cyclobutadiene (3,3)

5. a. Write any one difference between SHM and EHM. (0.75)

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b. Formulate Schrödinger's wave equation for H_2 molecule. Can it be solved? Suggest any one method to solve Schrödinger's wave equation for this system. State and apply Born-Oppenheimer approximation on H_2 molecule. (6)

c. (i) Differentiate between *ab initio* and DFT method.

(ii) Why is Hartree procedure called self-consistent field procedure? (3,3)

d. How can one mathematically define atomic orbital? Give an example. Categorize the following functions as Slater type or Gaussian type functions:

a) $\Phi = \frac{\alpha}{\pi}^{0.5} \exp(-\alpha r)$

b) $R(r)=Nr^{n-1}\exp(-\beta r)$

c) $\Phi = r^2\exp(-\alpha r^2)$

d) 3-21G (6)

6. a. What is partition coefficient (P) in QSAR studies? (0.75)

b. Write an expression for a molecular mechanics potential energy function for a standard optimization, stating clearly each and every term. Explain non-bonded interaction term in detail. (6)

c. (i) What are periodic boundary conditions in molecular dynamics simulation? What is the advantage of using a periodic box?

(ii) Differentiate between the semi-empirical methods, CNDO and PPP? (4, 2)

d. (i) Discuss the applications of Hammett's equation, with example.

(ii) What information is derived from electrostatic potential maps? (3, 3)

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