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1.

i. Briefly state main functions of following methods in computational chemistry.
   a. Molecular mechanics
   b. Molecular dynamics
   c. Hatree Fock method
   d. Semi empirical methods

ii. Explain how the potential energy surfaces are defined within the Born Oppenheimer framework.

iii. State the meaning of Schrodinger Cat concept.

iv. Write expressions for following operators in atomic units:
   a. Kinetic energy
   b. Electron-electron repulsion
   c. Explain Electron – nuclear interactions

2.

i. Define a force field and force field parameters as applied in MM methods

ii. Suggest a possible force field for $H_2O_2$. Justify your selection.

iii. Indicate whether it would be appropriate to carry out a molecular mechanics calculation using a typical force field (such as MMFF or Amber) to determine the minimized energy for the molecular systems listed below.
   a. porphyrin
   b. $Fe(CO)_4$
   c. a small protein such as crambin
   d. the water dimer, $(H_2O)_2$

iv. Describe advantages and disadvantages of MM methods in chemical calculations.

3.

i. Briefly describe formulations of non-bonding interactions in molecules.
Use this information to answer parts (ii) – (iv)





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- The interaction between two non-bonded atoms is described using a function called the Lennard-Jones 6-12 potential (LJ).
- It has the form $E_{nb} = \frac{A}{r^6} - \frac{B}{r^{12}}$, where A and B are constants which depend on the two interacting atoms and r is the distance between them. For two carbon atoms interacting, A = 745 and B = 2524840.

ii. Sketch the variation of non-bonded energy as a function of distance.

iii. At what distance does the minimum energy occur for this particular non-bonded interaction?

iv. Which of the two terms in the LJ expression is responsible for the attractive part of the interaction? Which term is responsible for the repulsive part of the interaction?

4.

i. A computational chemist performed an energy minimization using the Amber force field on the lactic acid molecule found that the lowest energy conformer had an energy of 19.856 kcal/mol. Upon carrying out a literature search, the chemist found a journal article in which a study using the MM2 force field determined the global minimum for lactic acid to be 3.898 kcal/mol. Is there something wrong with the chemist's work? Explain.

ii. Explain the advantages of using following algorithms in optimizations

   a. Newton Rapson method
   b. Secant method
   c. Conjugate gradient method

5. Suppose you are performing electronic structure calculations on the CO.

   i. Describe a minimal basis set for CO, including the total number of atomic orbitals.
   ii. Describe the 6-31G basis set for CO, including the total number of atomic orbitals.
   iii. Describe the 6-311G basis set for CO, including the total number of atomic orbitals.
   iv. Approximately how would the CPU time for single point energy calculations on CO scale using these basis sets?