RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. (Hons) Degree in Chemistry/ B.Sc. (Join Major) Degree in Chemistry and Physics

Fourth Year - Semester I Examination — September / October 2019

CHE 4201 –COMPUTATIONAL CHEMISTRY

Time: Two (2) hours

Answer all Questions

1. a) Describe the following terms:

   i. Periodic boundary condition
   ii. Minimum image convention
   iii. Quantum and Classical models

(30 marks)

b) For a given intermolecular potential function, U(r), $\left(\frac{dU(r)}{dr}\right)_{r=r_e} = 0$. Show that $r_e = \left(\frac{n}{6}\right)^{\frac{1}{n-6}} \sigma$ for Lennard-Jones (n-6) potential function. If Lennard-Jones (12-6) potential parameters for element A are 281 K and 0.379 nm respectively, calculate r_e for A-A interaction.

(40 marks)

c) "Scientists prefer functional form, C/r^n, (n is an even number) over more accurate exponential term, Ae^{-Br}, to model short range repulsion energy in molecular simulation studies". Explain the above statement.

(30 marks)

2. a) Molecular dynamics simulation yields structural and dynamical properties of the system while Monte Carlo simulation yields only structural properties of the system. Explain.

(30 marks)

b) Explain the use of molecular simulation methods to refine potential parameters?

(50 marks)

c) Write down the main steps of a Monte Carlo simulation in a molecular system

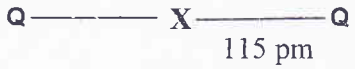
(20 marks)

3. a) i. Compare the slater type orbital and Gaussian type orbital

ii. What is LCAO approximation

(30 marks)

b) i. The structure of XQ_2 molecule is given below. XQ_2 is a linear molecule. Write down the Z matrix for this molecule.



(20 marks)

ii. Explain the following terms using a potential energy surface. Saddle point, local minimum and global minimum

(30 marks)

iii. Explain four properties of a molecule that can be calculated using Ab initio method

(20 marks)

4. a) Assume that you work in a project on the determination of the five lowest energy conformers of the corticoid steroid binding globulin (CBG). You are provided with the following computational methods

i. Molecular dynamics

ii. HF/UHF/6-31G**
iii. HF/RHF/6-31G**

State which computational method best fits the problem at hand, explain your choice.

(25 marks)

b) i. Both He and H_2 are two electron systems.Write Hamiltonian operators for both systems.

(50 marks)

ii. State the Born-Oppenheimer approximation and indicate the important parts of the electronic Hamiltonian after the approximation.

(25 marks)

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