RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. (Honors) Degree in Chemistry / B.Sc. (Join Major) Degree in Chemistry and Physics / B.Sc (4 year) Degree in Applied Sciences
Fourth Year – Semester- I Examination – July/August 2018

CHE 4201 – Applied Molecular Chemistry / Computational Chemistry

Time: Two (2) hours

Answer all **Four Questions**

1. (a) Describe the following terms

   I. Molecular Dynamics and Monte Carlo Methods
   II. Quantum and Classical Models

   (20 marks)

   (b) In classical simulations, the potential function that describes the interaction between molecules is the most important. The interaction potential between two inert gas atoms is given by the equation.

$$U = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} + \left(\frac{\sigma}{r}\right)^{6} \right]$$

   Where σ is the collision diameter, ε is the well depth and the r is the separation between two atoms. Derive the equation for the force acting on each particle.

   (40 marks)

(c) Two spherical particles are at the positions A and B with coordinates (x_1,y_1,z_1) and (x_2,y_2,z_2) respectively. The dispersion interaction of these particles is represented by a Lennard-Jones (12-6) potential function,

$$U(r) = 4\varepsilon\left[\frac{\sigma^{12}}{r_{12}^{12}} - \frac{\sigma^{6}}{r_{12}^{6}}\right]$$

where r_{12} is the distance between two particles.

Evaluate an expression for the force acting on the particle 2 in the X-direction.

$$\left[r_{12} = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}\right]$$

(40 marks)

2. (a) Write down the main steps of Monte Carlo simulations of a molecular system

(20 marks)

(b) Briefly explain the features of the acceptance ratio in a Monte Carlo simulation consideration the significance of the step size (Δ) of the simulation.

(30 marks)

(c) You are constructing a new molecular mechanics force field for molecules used in the preparation of the Group 13/Group 15 semiconductor indium phosphide; such precursor molecules are composed of H, C, In, and P. Discuss what parameters you will need to include in your force field definition and how you might go about determining optimal values. You need not define a full potential energy function (although you are welcome to do so if you want to) but you should be reasonably specific about the nature of the various parameters.

(50 marks)

3. (a) The Schrodinger equation has the form; $\hat{A}\psi = a\psi$. Briefly describe the terms $\hat{A}$,ψ and a in the above equation.

(10 marks)

(b)

I. The Hamiltonian for a multi electron system composed of several nuclei consists of various parts. Write equations for the following terms in the Hamiltonian.

i. The kinetic energy of the electrons
ii. The kinetic energy of the nuclei
iii. The Coulombic interaction between the nuclei and the electrons
iv. The Coulombic interaction between the electrons
v. The Coulombic interaction between the nuclei

Write down the full Hamiltonian for the multi electron system.

(30 marks)

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

(25 marks)

(c) Briefly explain the following terms using a potential energy surface. Saddle point, gradient point, and global minimum.

(15 marks)

(d) Assume that you work in a project for determination of the five lowest energy conformers of the human melanocyte stimulating hormone (MSH) polypeptide. You are provided with the following computational methods
MM(molecular mechanics) HF/UHF/6-31G** HF/RHF/6-31G**

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

(20 marks)

4 (a)

I. What are basis sets

(15 marks)

II. The basis set terminology was introduced by Pople and coworkers and the general form is given as M-ijk…G. Explain the meaning of M,i,j,k.

(15 marks)

III. Compare the Slater type orbital (STO) and Gaussian type orbital(GTO)

(10 marks)

(b) Explain four properties of a molecule that can be calculated using Ab initio method

(20 marks)

(c)

I. You wish to carry out a computer simulation study of CO_2 gas. Towards this end you are required to construct a Z- matrix. Write down the Z matrix for this molecule.

(10 marks)

II. Z matrix is a molecular representation method which adopting in GAUSSIAN computational chemistry software. Briefly overview another two molecular representation methods commonly using in computational chemistry software.

(30 marks)

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