Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Department of Science and Technology
400 Level First Semester Examination – May/July 2017
SCT 433-1 Multi Scale Modelling Techniques

Uva Wellassa University

Instructions to candidates

Duration: One (01) hour

Number of questions: Three (03)

Answer All Questions

All symbols carry standard meanings. Graph sheets will be provided

---

1. (a) In molecular mechanics, what are the advantages and disadvantages of having multiple atom types for a single element? Use at least one example in the context of your answer.

   (b) 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.

   (i). porphyrin

   (ii). $Fe(CO)_4$

   (iii). a small protein such as crambin

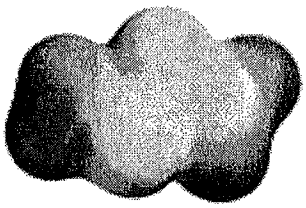
   (iv). the water dimer, $(H_2O)_2$ (100 marks)

2. A student investigates the bond in the A-B diatomic molecule using a software package for molecular mechanics. The student measures the bond length as 1.25 Å. When the single point energy of the molecule is calculated, the student gets a value of 30.0 kcal/mol. The equilibrium A-B bond length is 1.00 Å.

   (a) Using the information obtained above, determine the force constant for bond stretching. Use units of $kcalmol^{-1}$ $Å^{-2}$.
   (b) Plot the stretching energy as a function of bond length for this system (100 marks)

3. (a) Define following terms
   (i) Basis set (ii) electron density (iii) electrostatic potential maps
   (b) Electrostatic potential map of alanine is shown below. Comment on resonance structure of alanine.

   $H_3N^+CH_2CH_2CO_2^-$



   Blue Green Red

   (c) Explain important steps involved in Hatree-Fock method. (100 marks)