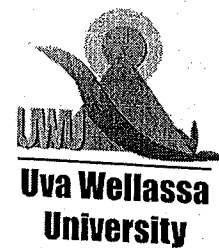


Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
3rd Year 2nd Semester Examination – August/September 2014
Repeat Exam
SCT 333-2 Computational Chemistry



Number of Questions : Four (04)

Answer all questions

Time allocation: Two (02) hours

Total marks allocated: 100

1. a. What is a computational model?
b. List three basic parameters that need to be considered when conducting a computational project.
c. What are the three basic types of calculations conducted in computational chemistry?
(25 Marks)
2. Briefly discuss advantages and disadvantages of following levels of theory used in computational chemistry.
 - a. Molecular mechanics
 - b. Semi empirical molecular orbital methods
 - c. Ab-initio molecular orbital method(25 Marks)
3. a. Indicate the most suitable level of theory to conduct following computational projects. Give reasons for your choice.
 - i. Dynamics of protein folding
 - ii. Simulate UV-visible spectra of $[\text{Cu}(\text{NH}_3)_4\text{H}_2\text{O}]^{2+}$ complexb. What is meant by “relative computational cost”? Explain using molecular mechanics calculations and *ab-initio* calculations as examples.
(25 Marks)
4. a. Following equation states the Hamiltonian for a molecule.

$$\hat{H} = \sum_i^{\text{electrons}} \frac{-\hbar^2}{2m_e} \nabla_i^2 + \sum_A^{\text{nuclei}} \frac{-\hbar^2}{2m_A} \nabla_A^2 + \sum_i^{\text{electrons}} \sum_A^{\text{nuclei}} \frac{-e^2 Z_A}{r_{iA}} + \sum_{i>j}^{\text{electrons}} \frac{e^2}{r_{ij}} + \sum_{A>B}^{\text{nuclei}} \frac{e^2 Z_A Z_B}{r_{AB}}$$

Identify terms used for

- i. electrostatic interactions between nuclei
 - ii. electrostatic interactions between electrons
 - iii. electrostatic interactions between nuclei and electrons
 - iv. Kinetic energy of nuclei
 - v. Kinetic energy of electrons.
- b. State Born-Oppenheimer approximation. According to this approximation, which term cancels out from the Hamiltonian?
 - c. What do you mean by a potential energy diagram?
(25 Marks)