Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
300 Level First Semester Examination – Dec./Jan. 2017
SCT 333-2 Computational Chemistry

Uva Wellassa University

Instructions to candidates
Answer all questions.
Duration: Two (02) hours
Number of questions: Four (04)
Point allocation: 100 marks

1.
   a. Write an expression for the **electronic** Hamiltonian for the carbon atom (use atomic units). (10 marks)
   b. Classify the various terms that are included in the above Hamiltonian as electronic kinetic energy, nuclear-electronic attraction, and electron repulsion. (7 marks)
   c. Which energy contributions are not included in the electronic Hamiltonian that are included in the full Hamiltonian? (8 marks)

2.
   a. Explain what basis functions are as used in electronic structure calculations. (5 marks)
   b. State the Gaussian product rule? (5 marks)
   c. Discuss the pros and cons in the usage of Slater-Type Orbitals (STOs) and Gaussian-type orbitals (GTOs)? (7 marks)
   d. What is the difference between STO-1G and STO-3G basis sets? (8 marks)

3.
   a. What is meant by a potential energy surface (PES)? (5 marks)
   b. State the Born-Oppenheimer (BO) approximation? (5 marks)
   c. Describe the variational theorem. (5 marks)
   d. What was the drawback of the wavefunction proposed by the Hartree approach? (5 marks)
   e. How does the Hartree – Fock approach overcome the above-mentioned drawback? (Explain using an example) (5 marks)

4.
   a. What is a "functional" as opposed to a "function" in mathematics? (Describe using an apropriate example) (5 marks)
   b. Briefly describe the Kohn-Sham (KS) approach to Density Functional Theory (DFT). (5 marks)
   c. According to the mathematical formulation of KS approach to DFT, what are the terms that combine to produce the "exchange correlation functional" ? (5 marks)
   d. Describe the following different approaches for approximating exchange-correlation potential.
      i. Local density approximation (LDA) (5 marks)
      ii. Local spin density approximation (LSDA) (5 marks)