Uva Wellassa University of Sri Lanka
Faculty of Science & Technology
Science & Technology Degree Program
2nd Semester Examination – September/October 2013

Uva Wellassa University

SCT 333-2 Computational Chemistry

Part B - ESSAY TYPE QUESTIONS

(Answer All Questions)

1.

a. Discuss the advantages of Hartree Fock method when compared to Hatree method. (25 marks)

b. The electron – electron repulsion term cannot be accounted for exactly. Why? Comment briefly. (25 marks)

c. How the electron-electron interaction term is accounted for in Hartree-Fock method stating any new operators used. (25 marks)

d. State the Slater determinant for C (Z = 6) atom. (25 marks)

2.

a. State the approximations made in Zero Differential Overlap method of semi-empirical modelling. (20 marks)

b. What is the main advantage of NDDO approximation over ZDO? (20 marks)

c. A section of the output file generated from an energy minimization calculation carried out for HCHO using molecular modelling method is annexed. Answer following questions. (60 marks)

i. What is the level of theory employed in the calculation?

ii. Write the wave functions that correspond to HOMO and LUMO orbitals.

iii. Calculate the energy difference between HOMO and LUMO.

iv. Is the HOMO molecular wave function is normalized?