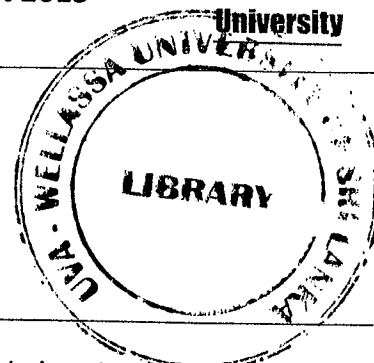


Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Department of Science and Technology
300 Level First Semester Examination – Sep/Oct 2015
SCT 333-2 Computational Chemistry



Instructions to candidates

Duration: Two (02) hours

Number of questions: Four (04)

Answer All Questions

Mark allocation: 100 mark

1. What are the three levels of calculations used in computational chemistry? Indicate which levels of theory use Schrodinger equation and which level of theory use classical mechanics. Give an example for each level of theory. (25 mark)

2. Explain how hartree fock (HF), Moller-Plessant (MP), and Density functional theory (DFT) vary in terms of electron correlation. (25 mark)

3.
 - a. What is a basis set? (5 mark)
 - b. List four different types of basis sets used in computational chemistry. (10 mark)
 - c. Give one example for each kind mentioned above (10 mark)

4. List two software used to conduct electron structure calculations (25 mark)