Uva Wellassa University, Sri Lanka

End Semester Examination – Jan 2010

SCT 333-2 Computational Chemistry

Time: Two (02) hours

This examination consists of two parts: **Part A** and **Part B**

Part B

Answer three (03) questions only

1.

(a) Define the following:

(i) Basis function

(ii) Primitive Gaussian

(iii) Basis set

Suppose you are performing electronic structure calculations on the ethanol molecule.

(b) Describe a minimal basis set for ethanol, including the total number of atomic orbitals.

(c) Describe the 6-31G basis set for ethanol, including the total number of atomic orbitals.

(d) Describe the 6-311G** basis set for ethanol, including the total number of atomic orbitals.

2.

(a) State the approximations made in

(i) Hartree method,

(ii) Hartree – Fock (HF) Method.

State a key difference between these methods.

(b) State HF equation for a single electron in a many electron system. Identify all operators therein.

(c) How electron-electron correlation is taken into account in Hartree method and HF method.

(d) Hartree-Fock calculations that employ basis sets consisting of 8, 25, 50, and 100 basis functions, respectively, are carried out on the ammonia molecule. Sketch a plot of how you would expect the total electronic energy of the ammonia molecule to vary as a function of basis set size. Explain the theoretical principle behind the shape of the plot.

3.

(a) Describe the major energy components of a molecular mechanics force field.

(b) Give an equation for the stretching energy of a bond in a molecular mechanics force field. Make sure that you define any symbols that you use. Sketch a plot of the shape of the stretching energy as a function of the bond length.

(c) Consider the hydrogen peroxide molecule, HOOH. Provide an explicit account of the terms that would be required in a molecular mechanics force field to describe this molecule. Also include a listing of the force field parameters that would be needed for HOOH, including force constants and equilibrium geometrical parameters.

4. 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 kcal mol^{-1} $Å^{-2}$.

(b) Plot the stretching energy as a function of bond length for this system.

(c) What happens to the plot from question (b) if the stretching force constant is doubled?

(d) What happens to the plot from question (b) if the stretching force constant is halved?