

CHEM 802: ADVANCED COMPUTER APPLICATIONS IN CHEMISTRY

INSTRUCTIONS: ANSWER ALL QUESTIONS

QUESTION ONE (20 MARKS)

- a) Discuss three main tools of computational chemistry (6mks)
- b) Discuss Hartree-Fock theory (2mks)
- c) Using the H₂ molecule discuss the LCAO approximation (3mks)
- d) Discuss:
 - i) Minimal basis sets (3mks)
 - ii) Polarization functions (3mks)
 - iii) Split valence functions (3mks)

QUESTION TWO (20 MARKS)

- a) Give three advantages and three disadvantages of the Unrestricted Hartree-Fock Theory (3mks)
- b) Discuss
 - i) Effective core potentials (3mks)
 - ii) Electron correlation energy (3mks)
 - iii) Electronic energy decomposition and define the terms (3mks)
- c) Using a suitable equation, discuss the Moller-Plesset perturbation theory (4 mks)
- d) Explain the term electron density in quantum mechanics using an equation (4mks)

QUESTION THREE (20 MARKS)

- a) Using a suitable equation, discuss a density functional (3mks)
- b) Give three advantages and three disadvantages in the DFT method (3mks)
- c) Briefly discuss
 - i) Diffuse functions (3mks)
 - ii) Gaussian basis functions (3mks)
 - iii) Basis functions (3mks)
- d) Explain the Pauli Principle in quantum mechanics (1 mk)
- e) Write the equation showing that the Hartree wave function is not antisymmetric (2mks)
- f) Using an equation show the symmetric wavefunction can be made antisymmetric (2mks)