UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Year 2005/2006

November 2005

KAA 506 – Computer in Chemistry

Time : 3 hours

Answer FIVE questions.

Only the first five questions answered by the candidate will be marked.

1. (a) Write a flowchart of a typical SCF geometry optimization procedure.

(7 marks)

(b) Give two algorithms which are normally used in a geometry optimization process. Without giving detailed mathematical descriptions, briefly describe the techniques and outline their advantages and disadvantageous.

(10 marks)

(c) Sketch a potential energy surface graph and label all the stationary points. Describe how a minima is differentiated from a transition state structure (from a computational point of view)?

(3 marks)

2. (a) Calculate the number of basis functions for sodium lactate, ($NaOOC(CH_3)$ CHOH), using;

(i) a minimal basis set,

(ii) a split valence, and

(iii) a basis set with both polarization and diffuse functions.

State the basis set used to solve the problem.

(6 marks)

(b) Based on the formal scaling for Hartree Fock procedure, estimate the time required to compute a single point calculation for $(CH_3)_4Si$ using 3-21G** basis set. Compare the time relative to SiH_4.

(4 marks)

(c) Using the appropriate method and basis set, write a complete input file for CH_3COCH_3.

(10 marks)

3. (a) For the following problems, choose the suitable molecular modeling method and state your reasons.

(i) Estimation of binding free energies of drug-like inhibitors of Chk1-kinase.

(ii) Understanding the mechanism of chromium-catalyzed ethylene trimerization.

(iii) Investigating the nitrogen dioxide sensing mechanism of tin dioxide nanoribbons.

(iv) Predicting the stability of drug–cyclodextrin inclusion complexes.

(10 marks)

(b) Write a typical expression for a molecular mechanics total energy terms. Describe each term and briefly state the physical origin of each of the energy terms.

(10 marks)

4. Design a logic gates circuit for each of the following processes:

(a) Temperature controller for the heater in a liquid tank.

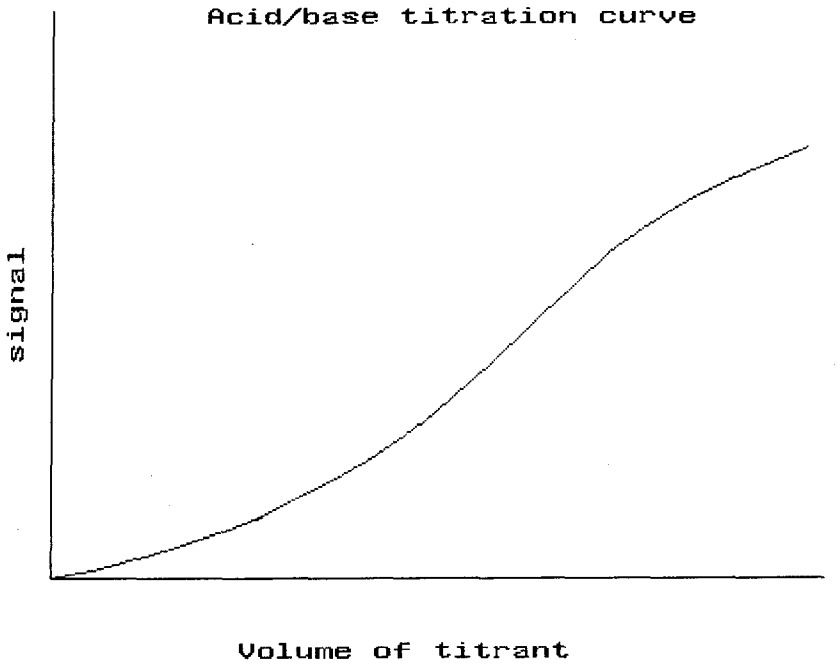
(b) pH adjustment for reagent in chemical industries.

(c) Quality control for the present of impurities in finished product.

(d) Multicomponents separation in a column chromatography.

(20 marks)

5. (a) Suggest and design an electronic technique to obtain an accurate equivalence point for the acid/base titration as the curve is shown below.



(10 marks)

(b) Draw a complete flow chart for the data acquisition and determination of the equivalence point for the above titration system.

(10 marks)

6. (a) Describe the importance of the followings with respect to the automation of analytical techniques.

(i) Operational amplifier.

(ii) Digital input and output.

(iii) Analog to digital converter.

(iv) Flow chart drawing.

(10 marks)

(b) What is the output if the input is 0111 for

(i) OR gate followed by NOR gate,

(ii) AND gate followed by NAND gate,

(iii) NOT gate followed by XOR gate,

(iv) AND gate followed by XOR gate and

(v) XOR gate followed by NAND gate.

(10 marks)

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