



KENYATTA UNIVERSITY

UNIVERSITY EXAMINATIONS 2011/2012

SECOND SEMESTER EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE

SCH 207: INTRODUCTION TO COMPUTATIONAL CHEMISTRY

DATE: THURSDAY 29TH MARCH 2012

TIME: 11.00 A.M. – 1.00 P.M.

INSTRUCTIONS

Answer ALL the questions

- 1
- a) i) Describe briefly Computational Chemistry (4marks)
 - iii) Distinguish between Computer-Aided Molecular Modeling (CAMP) and Computer-aided molecular design (CAMD) (2 marks)
 - b) Explain briefly the term basis set (3 marks)
 - c) Consider the 6-31G(d) basis set.
 - i) Explain the meaning of all the numbers and letters. (3 marks)
 - ii) Why is choice of basis set important in computation? (2 marks)
 - d) State the capabilities and limitations of PHREEQC software used in Hydrogeochemical simulations (5 marks)
 - Total (19 marks)**
- 2
- a) State briefly the steps involved in developing a simulation model (6 marks)
 - b) What makes a problem suitable for simulation modeling and analysis? (5 marks)
 - c) State benefits of simulation modeling and analysis (3 marks)
 - d) What are some pitfalls to guard against in simulation? (4 marks)
 - Total (18 marks)**
- 3.
- (a) i) What is Molecular Mechanics? (2 marks)
 - ii) State three components of a force field (3 marks)
 - iii) In MM, the potential energy V is given as:
$$V = V_{str} + V_{\phi} + V_{vdW} + V_{es} + V_{\omega}$$
Define these terms (4 marks)
 - (b) What are some advantages and disadvantages of MM? (2 marks)
 - ii) Briefly describe the term QSAR? (2 marks)
 - (c) What two factors determine how accurate an *ab initio* quantum mechanical calculation will be? (2 marks)

- (d) i) Briefly describe the Born-Oppenheimer approximation to the Schrodinger equation which results in the concept of a potential energy surface, (3 mark)
Total (18 marks)

- 4 a) Use the Gaussian input file below to answer the question

```
%chk=Test.chk
%mem=500mb
%nproc=1
# hf/6-31g(d) opt freq
```

Test Calculation

```
0 1
O
H      1      B1
H      1      B2  2      A1

B1      0.96000000
B2      0.96000000
A1      109.47122063
```

- i) State the: I) theory and basis set used (4 marks)
 II) Type of calculation(s) used (2 marks)
 ii) Identify the molecule and explain the meaning of the value B1, B2 & A1 (3 marks)
- b) Describe briefly the term speciation chemistry (6 marks)
- Total (15 marks)**