MACHAKOS UNIVERSITY

University Examinations 2022/2023

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

THIRD YEAR FIRST SEMESTER EXAMINATION FOR
BACHELOR OF SCIENCE (ANALYTICAL CHEMISTRY)

SAN 304: COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELLING

DATE: **TIME:**

INSTRUCTIONS:

- The paper consists of **two** sections.
- Section **A** is **compulsory** (30 marks).
- Answer any **two** questions from section **B** (each 20 marks).

SECTION A

QUESTION ONE (COMPULSORY) (30 MARKS)

a) Explain why the words ``exact'' and ``perfect'' do not appear in definition of computational chemistry. (2 marks)

b) The primary focus of computational chemistry is solving chemically related problems by calculations. For the newcomer in the field, discuss three main problems they encounter. (6 marks)

c) Define a model as applied in calculations and state why it is useful in computation. (4 marks)

d) Molecular mechanics method has the capabilities of computing large protein molecules in a short time. Describe how the materials geometry is optimised and treated in the above method. (5 marks)

e) Give two examples of basis set used in Hartree-Fock techniques to make it more accurate. (2 marks)

f) Define semi–empirical and *ab initio* methods and state how they differ in their applications. (5 marks)

g) i. State the advantage of using electron density in density functional theory. (DFT) (2 marks)

ii. Discuss what can be attributed to heavy usage of DFT's recent calculations. (2 marks)

iii. Which is the simplest DFT approximation to the complete problem-based solution that rely only on the electron density for approximation of high-spin systems (2 marks)

SECTION B

QUESTION TWO (20 MARKS)

a) Quantum Monte Carlo (QMC) has several flavors of variational, diffusion among other functions. These calculations can be very time consuming, but they could yield extremely accurate results. Discuss the following citing their application areas.

i. Variational Monte Carlo (2 marks)

ii. Diffusion Monte Carlo (2 marks)

iii. Reptation Monte Carlo (2 marks)

iv. Gaussian quantum Monte Carlo (2 marks)

b) Atomic simulation is applied at the level of electrons and atoms. What materials properties can one work on given an atom. (3 marks)

c) Distinguish between conduction band and valence band. (3 marks)

d) Define a band gap of a semiconductor (TiO_2). (3 marks)

e) List six applications areas of computation chemistry in materials analysis. (3 marks)

QUESTION THREE (20 MARKS)

a) Write the Schrödinger equation and explain the terms in the equation. (2 marks)

b) What does each of the following reveal in computational analysis:

i. Geometry (2 marks)

ii. Band structures (2 marks)

iii. DOS (2 marks)

iv. Electron and spin density (2 marks)

c) Discuss the three-paradigm used during ligands / proteins docking calculations of biological systems. (5 marks)

d) Explain the challenges a computational analyst faces as they sequence more genomes and get more structural information when docking. (5 marks)

QUESTION FOUR (20 MARKS)

a) Discuss how drug companies use computational chemistry methods. (2 marks)

b) Define docking and provide the questions it solves? (5 arks)

c) Autodock uses pre-calculated affinity maps for each atom type in the substrate molecule. List three atoms usually used together with an electrostatic map. (3 marks)

d) Distinguish between bound and unbound Docking (4 marks)

e) Describe the following linkage criterion. (6 marks)

i. Simple linkage

ii. Complete linkage

iii. Group average approaches

QUESTION FIVE (20 MARKS)

a) State the scientific problem faced by computational analyst in adapting the configuration interaction (CI) method and make it more practical. (2 marks)

b) Explain how Quantum Monte Carlo (QMC) avoid making the Hartree-Fock mistakes. (3 marks).

c) Common approximation methods are used in computation software to reproduce experimental results. List two approaches used in the choice of the approximations. (2 marks)

d) From the Born-Oppenheimer approximations, define the Hamiltonian operator three terms. (3 marks)

e) The exchange-correlation energy functionals can be classified into non-empirical and empirical-based on their complexity. Explain the exchanges (ii-iv) with an example and give the functionals strengths and failures.

i. Distinguish between non-empirical and empirical methods (1 mark)
ii. Local Density Approximation Functional (LDA) (3 marks)
iii. Dependence on Gradient of Density Functionals (GGAs) (3 marks)
iv. Dependence on Kinetic Energy Density (meta-GGAs) (3 marks)