



MACHAKOS UNIVERSITY

University Examinations 2021/2022

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

THIRD YEAR SUPPLEMENTARY/SPECIAL EXAMINATION FOR

BACHELOR OF SCIENCE IN ANALYTICAL CHEMISTRY

SAN 304: COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELLING

DATE: 17/03/2022

TIME: 8:30-10:30 AM

INSTRUCTIONS:

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

QUESTION ONE (COMPULSORY) (30 MARKS)

- a) Define Computational chemistry and state its two major applications. (4 marks)
- b) Explain the best approximation to the true wave function where each electron is occupying an orbital - the picture that most chemists use to rationalize chemistry. (2 marks)
- c) Define the Hartree Fock theory based on to the true many-body wavefunction. (1 mark)
- d) Explain why Computation is expensive. (2 marks)
- e) Provide three basic research areas that computational chemistry has been a useful tool. (3 marks)
- f) List the benefits of combining experiment with theory. (4 marks)
- g) Distinguish between Quantum mechanics and Molecular mechanics. (4 marks)
- h) Density functional theory (DFT) has become very popular in recent years.
- What makes Density Functional Theory (DFT) very popular? (2 marks)
 - How has DFT theory been improved over time to overcome its shortcomings (3 marks)

- iii. Given a set of nuclei and electrons, determine the properties that a theoretical chemist can attempt to calculate. (5 marks)

QUESTION TWO (20 MARKS)

- a) Provide the information can one deduce from the following calculations:
- i. Band structure (2 marks)
 - ii. DOS (2 marks)
 - iii. PDOS (2 marks)
- b) Which flavour in Monte Carlo Mainly:
- i. Is used in boson systems for path integral ground state calculations. (2 marks)
 - ii. Is the most common with high-accuracy method for electrons since it comes quite close to the exact ground-state energy fairly efficiently. (2 marks)
 - iii. Is commonly used in many sorts of quantum problems. (2 marks)
- c) Docking involves two biomolecules. What questions can one solve using the calculation. (3 marks)
- d) List the three goals during docking. (3 marks)
- e) Docking tools comprehensively utilize which search algorithms? (2 marks)

QUESTION THREE (20 MARKS)

- a) Explain the design constrains of molecular dynamics. (2 marks)
- b) Which theory is best approximation to the true wave function where each electron is occupying an orbital? (2 marks)
- c) List four tools are which are mainly used for high throughput docking simulations. (4 marks)
- d) Which are the three main components in all small molecule docking programs? (3 marks)
- e) Explain two simulation approach used in large molecules, ligand-receptor docking. (5 marks)
- f) Using molecular mechanic's approach, explain how a material is perceived and the geometry optimized. (2 marks)
- g) List one most common force field applied in each of the following: liquids, Proteins and inorganic elements. (2 marks)

QUESTION FOUR (20 MARKS)

- a) What does Hartree-Fock theory neglect by assuming a single-determinant form for the wavefunction. (2 marks)
- b) Explain two approaches used to mitigate limitations of the Hartree-Fock method by going beyond the ansatz of a single-determinant wavefunction. (2 marks)
- c) Write the equation for the foundation of the quantum mechanics approach and define the units. (3 marks)
- d) Define from the Born-Oppenheimer approximations the Hamiltonian operator three terms. (3 marks)
- e) List four examples of intermolecular interactions the Density Functional Theory was deficient in determining and how it was overcome. (4 marks)
- f) What did Thomas and Fermi first explore in improving Density Functional Theory explain their study focus. (6 marks)

QUESTION FIVE (20 MARKS)

- a) Docking simulations software predict optimized docked conformer based upon _____ of the system. (2 marks)
- b) Explain the practical considerations in computation calculations set up. (2 marks)
- c) Local density approximation is most accurate data for which application? Discuss its limitations such that care must be taken in its application. (1 mark).
- d) Explain Hohenberg and Kohn two key theorems. (5 marks)
- e) Kohn and Sham derived a coupled set of differential equations enabling the ground state density to be found. Explain the three distinct parts into which they separated the equation. (6 marks)
- f) Name the four comprehensively utilized docking tools employed in search algorithms. (4 marks)