

COMPUTATIONAL CHEMISTRY III EXAMINATION

ATTEMPT ALL QUESTIONS IN SECTION A AND ANY OTHER TWO IN SECTION B. TIME: THREE HOURS

SECTION A

Question 1. (20 Marks)

Prove that for 64 argon atoms the edge length of the cubic simulation box is 14.4744 Å. Given, density of argon 1.40 gm/cc at 85 K, atomic weight of argon 39.948.

Question 2. (10 Marks)

What is the importance of choosing the Boltzmann factor as a representative of probabilities?

Question 3. (10 Marks)

How does the principle of detailed balance work?

Question 4. (20 Marks)

Make the topology files of another dipeptide, a tripeptide and a polypeptide (with four amino acids residues) and perform molecular dynamics simulations.

Question 5. (20 Marks)

What are the reasons for choosing a speed of 0.3 rpm of the spindle in the measurements of viscosities?

SECTION B

Question 1. (10 Marks)

PART A

What is the origin of the fast mode of stress relaxation?

PART B

What is the origin of the entropic mode of stress relaxation?

Question 2. (10 Marks)

What is the origin of the constancy of $\langle b^2 \rangle$?

Question 3. (10 Marks)

In a system with 100 chains of polyethylene (each chain is of 20 beads), do you expect variations in R^2 , R_g^2 and $\langle b^2 \rangle$? Justify with reasons

Question 4. (10 Marks)

What changes would you expect in the chain if the angle bending potential and a torsional potential were considered along with the Fraenkel potential?