Quantum Cluster Equilibrium Prediction of Liquid Ethanol

Alhadji Malloum[†,◇,*] and Jeanet Conradie[†]

[†] Department of Chemistry, University of the Free State, PO BOX 339, Bloemfontein 9300, South Africa.

[◇] Department of Physics, Faculty of Science, University of Maroua, PO BOX 46, Maroua, Cameroon.

ABSTRACT: Quantum cluster equilibrium theory (QCE) has been widely used to determine the properties of pure and binary mixture of liquids [1,2]. The main limitation of the application of QCE is the exploration of different possible clusters formed by the solvent molecules. Therefore, in this study, we applied the QCE theory to predict liquid properties of ethanol after thorough exploration of the potential energy surfaces (PESs) of the ethanol clusters from dimer to hexamer. The exploration started by generating possible structures using classical molecular dynamics followed by optimizations at the MP2/aug-cc-pVDZ level of theory. 484 different configurations of the ethanol clusters have been finally used in the QCE theory. The results show that the population of liquid ethanol is constituted from the contribution of hexamer, pentamer, and tetramer (see Figure 1). In addition, we noted that the ethanol monomer, dimer and trimer do not contribute to the population of liquid ethanol. Furthermore, based on the predicted population of the liquid ethanol, we calculated its infrared spectrum at different temperatures. The calculated infrared spectrum is found to be in qualitative agreement with experiment. Some thermodynamic properties, such as the heat capacity, are also predicted to be in good agreement with experiment.

KEYWORDS: Liquid ethanol, ethanol clusters, quantum cluster equilibrium, liquid thermodynamic properties

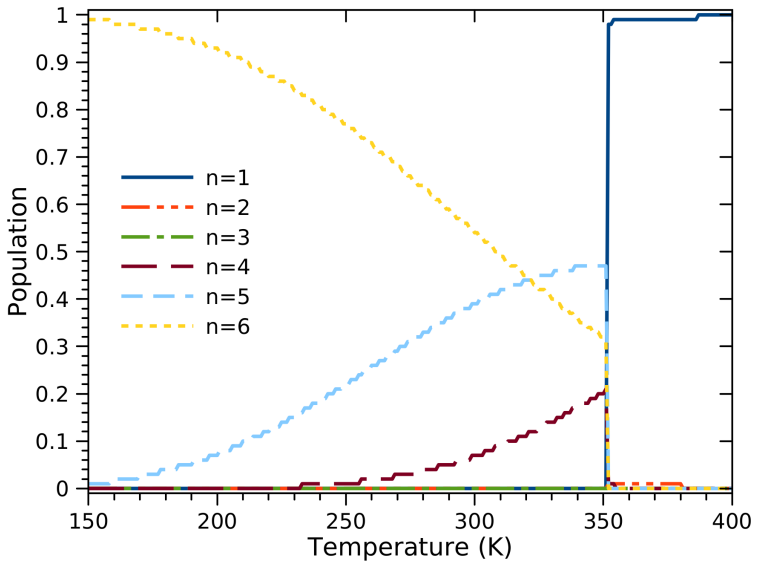

Figure 1 QCE predicted population of liquid ethanol as a function of temperature from 150 to 400 K. For each cluster size *n*, the reported population is the sum of the population of different configurations of the considered cluster.

References

1 Weinhold, F. Quantum cluster equilibrium theory of liquids: General theory and computer implementation. *J. Chem. Phys.* **1998**, *109*, 367–372.

2 Ludwig, R.; Weinhold, F.; Farrar, T. Quantum cluster equilibrium theory of liquids part I: Molecular clusters and thermodynamics of liquid ammonia. *Ber. Bunsen. Phys. Chem.* **1998**, *102*, 197–204.

* *E-mail: MalloumA@ufs.ac.za; Tel: +237 695 15 10 56*