ELSEVIER

Chemical Physics 199 (1995) 73–82

Chemical Physics

Statistical mechanical simulations on properties of liquid pyridine

Kritsana Sagarik [a,*], Eckhard Spohr [b]

[a] *School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand*
[b] *Abteilung für Theoretische Chemie, Universität Ulm, D-7900 Ulm, Germany*

Received April 13, 1995

Abstract

An intermolecular potential describing the interaction between pyridine molecules was constructed using the test-particle model (T-model). The computed T-model potential was used in the investigation of the equilibrium structures and binding energies of pyridine dimers. It was found that a herringbone structure is the most stable dimer in the gas phase. The results of the statistical mechanical simulations revealed that this dimer structure may not be present in an appreciable amount in the liquid phase. The molecular dynamics (MD) simulations confirmed that the molecular motions of pyridine in the liquid phase are rather anisotropic, as can be seen from the computed rotational diffusion constants. This finding is in good agreement with the experimental investigation on reorientational motions of pyridine reported by Kintzinger and Lehn.