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Theoretical studies on hydrogen bonding in hydroxylamine clusters and liquid

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Abstract

Structures and interaction energies of dimers and trimers of hydroxylamine (NH_2OH) were investigated using an intermolecular potential derived from the test-particle model (T-model). The T-model results were examined using ab initio calculations at various levels of accuracy, ranging from MP2/6-311G(d,p) to MP2/6-311++G(2d,2p) for the dimers, as well as from MP2/6-31G(d,p) to MP2/6-311++G(2d,2p) for the trimers. Both T-model and MP2 calculations confirmed that a cyclic arrangement of O–H \cdots N hydrogen bonds (H-bonds) represents the absolute minimum energy geometry of the dimers. Several local minimum energy geometries were suggested based on the T-model and MP2 results. For the trimers, the T-model and MP2 predicted a slightly different absolute minimum energy geometry. The T-model preferred a compact H-bonded structure, whereas MP2 with the largest basis set preferred a stacked H-bond arrangement. Ab initio calculations at the SCF/6-311++G(2d,2p) level showed that the effects of electron correlation play an important role in the association of compact H-bonded clusters. Some properties of liquid NH_2OH were investigated based on the T-model potential. Molecular Dynamics (MD) simulations were performed for the liquid at 318 and 329 K. MD results suggested a slightly higher possibility of finding the O–H \cdots O H–bond, compared to the O–H \cdots N H–bond in the liquid. There was no direct evidence showing the existence of cyclic dimers in the liquid. © 1999 Elsevier Science B.V. All rights reserved.

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