A GLOBAL POTENTIAL ENERGY SURFACE FOR HNO₃

MYCHEL E. VARNER, JOHN F. STANTON, Institute for Theoretical Chemistry, Department of Chemistry, University of Texas at Austin, Austin, TX 78712; BASTIAAN J. BRAAMS, Cherry L. Emerson Center of Scientific Computation and Department of Chemistry, Emory University, Atlanta, Georgia 30322.

A potential energy surface has been fit to the energy and energy gradient for thousands of configurations of HNO₃. Prior to explicit inclusion of data for the cis,perp-HOONO conformation, this isomer was predicted to be a local minimum on the fitted surface. The status of cis,perp-HOONO as a minimum was later confirmed through ab initio frequency calculations. Molecular dynamics simulations were carried out on the fitted surface to investigate the cis/trans isomerization of the HOONO structure.