A GLOBAL POTENTIAL ENERGY SURFACE FOR HNO_3

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A potential energy surface has been fit to the energy and energy gradient for thousands of configurations of HNO_3. 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.