

## QUANTUM DYNAMICS STUDIES OF THE VIBRATIONAL STATES OF HO<sub>3</sub>(X<sup>2</sup>A'')

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We have explored the ground-state potential energy surface for HO<sub>3</sub> using the HCTH/aug-cc-pVTZ DFT method. Results show that there are two stable isomers, trans-HO<sub>3</sub> and cis-HO<sub>3</sub>, with respect to the OH + O<sub>2</sub> dissociation limit. The binding energies are predicted to be 6.68 kcal/mole (D<sub>0</sub>) for trans-HO<sub>3</sub> and 5.62 kcal/mole for cis-HO<sub>3</sub>. The isomerisation barrier height is only 2.02 kcal/mole from the trans- isomer to the cis- one. The central O-O bond length is obtained as 1.6299 Å in trans-HO<sub>3</sub> or 1.5958 Å in cis-HO<sub>3</sub>. A global potential energy surface has been constructed from thousands of ab initio energy points. Based on this surface, we have carried out a full dimensional quantum dynamics study. Results are used to compare with the FTIR experimental observations.<sup>a</sup>

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