QUANTUM DYNAMICS STUDIES OF THE VIBRATIONAL STATES OF $HO_3(X^2A'')$

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We have explored the ground-state potential energy surface for HO_3 using the HCTH/aug-cc-pVTZ DFT method. Results show that there are two stable isomers, trans-HO_3 and cis-HO_3, with respect to the OH + O_2 dissociation limit. The binding energies are predicted to be 6.68 kcal/mole (D_0) for trans-HO_3 and 5.62 kcal/mole for cis-HO_3. 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_3 or 1.5958 Å in cis-HO_3. 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.[a]

[a]The work at Brookhaven National Laboratory was performed under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.