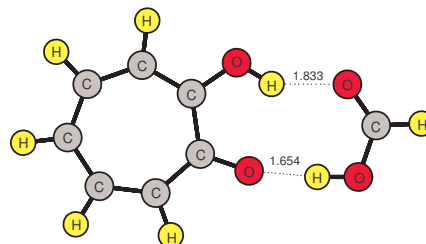


MICROWAVE MEASUREMENTS OF THE TROPOLONE-FORMIC ACID DOUBLY HYDROGEN BONDED DIMER*

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The microwave spectrum was measured for the tropolone-formic acid doubly hydrogen bonded dimer using a pulsed-beam Fourier transform microwave spectrometer in order to search for the concerted double proton tunneling motion. The tunneling motion was expected for the dimer, as the transition state of this motion exhibits C_{2V} symmetry, which has been thought to be a requirement to observe the concerted double proton tunneling. The tunneling motion was not observed for this dimer, as the transitions measured did not show observable splittings into doublets. The barrier height calculated of the dimer using B3LYP/aug-cc-pVTZ was about 15000 cm^{-1} , significantly larger than the value determined for the propiolic acid-formic acid dimer (3800 cm^{-1}),^a which showed the tunneling motion. The estimated separation of the minima in the potential energy surface is estimated to be very similar to that of propiolic acid-formic acid (about 0.8 \AA),^a so the large barrier height may be why the tunneling process was not observed.



^aDaly, A. M.; Bunker, P. R.; Kukolich, S. G. Communications: Evidence for Proton Tunneling from the Microwave Spectrum of the Formic Acid-Propiolic Acid Dimer. *J. Chem. Phys.* 132, 2010, 201101/1.

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