Proton transfer dynamics in the propionic acid dimer from path integral molecular dynamics calculations.

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The double proton transfer process in the cyclic dimer of propionic acid in the gas phase was studied using a path integral molecular dynamics method. Structures, energies and proton trajectories were determined. Very large amplitude motions of the skeleton of a propionic acid molecule were observed during the simulations, and almost free rotation of the C(2)H(5) group around the C(α)-C bond. A double-well symmetric potential with a very small energy barrier was determined from the free energy profile for the proton motions. Infrared spectra for different isotopomers were calculated, and comparative vibrational analysis was performed. The vibrational results from CPMD appear to be in qualitative agreement with the experimental ones.

Adres publiczny

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http://link.springer.com