

Ab initio molecular dynamics study of the very short O–H...O hydrogen bonds in the condensed phases.

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Streszczenie

In this paper are presented the results of theoretical studies of the structure and proton motion in very short O...O intramolecular hydrogen bonds in two molecular crystals. A comparison was conducted between 3-cyano-2,4-pentanedione (I) and 4-cyano-2,2,6,6-tetramethyl-3,5-heptanedione (II) in the solid state. The dynamics of proton motion in the O–H...O hydrogen bond were investigated in the NVT ensemble at 298 and 50 K, respectively, for crystals I and II using Car-Parrinello and path integral molecular dynamics. Very large delocalization of the bridging proton was noted especially in the path integral simulation where quantum effects are taken into account. The infrared spectrum was calculated, and a comparative vibrational analysis was performed. CPMD vibrational results appear to be in qualitative agreement with the experimental ones.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>