



Proton distribution in KHCO_3 from *ab initio* molecular dynamics simulation.

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The proton distribution in the $(\text{HCO}_3)_2$ - dimer of KHCO_3 at 298 K has been studied with the Car–Parrinello molecular dynamics (CPMD) and path integrals molecular dynamics (PIMD) simulations. According to earlier neutron studies hydrogen is disordered and occupies two positions with an occupancy ratio of 0.804/0.196. CPMD results with four cells reproduce experimental data with high accuracy. The occupancy ratio from the CPMD simulation after 35 ps run is 0.783/0.217. Present results support a mechanism for the disorder which involves proton transfer from donor to acceptor and not orientational disordering of the entire dimer. The question of simultaneous or successive proton transfer in the two hydrogen bonds in the dimer is ambiguous. In present CPMD simulations the observed time lag between proton transfers within one dimer was in the range of 1–20 fs.

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