Comparison of Proton Acceptor and Proton Donor Properties of H_2O and H_2O_2 in Organic Crystals of Drug-Like Compounds: Peroxosolvates vs. Crystallohydrates

Autorzy

Mikhail V. Vener

Andrei V. Churakov

Alexander P. Voronin

Olga D. Parashchuk

Sergei V. Artobolevskii

Oleg A. Alatortsev

Denis E. Makhrov

Alexander G. Medvedev

Aleksander Filarowski

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Two new peroxosolvates of drug-like compounds were synthesized and studied by a combination of X-ray crystallographic, Raman spectroscopic methods, and periodic DFT computations. The enthalpies of H-bonds formed by hydrogen peroxide (H_2O_2) as a donor and an acceptor of protons were compared with the enthalpies of analogous H-bonds formed by water (H_2O) in isomorphic (isostructural) hydrates. The enthalpies of H-bonds formed by H_2O_2 as a proton donor turned out to be higher than the values of the corresponding H-bonds formed by H_2O. In the case of H_2O_2 as a proton acceptor in H-bonds, the ratio appeared reversed. The neutral O···H-O/O···H-N bonds formed by the lone electron pair of the oxygen atom of water were the strongest H-bonds in the considered crystals. In the paper, it was found out that the low-frequency Raman spectra of isomorphous crystalline hydrate and peroxosolvate of N-(5-Nitro-2-furfurylidene)-1-aminohydantoin are similar. As for the isostructural hydrate and peroxosolvate of the salt of protonated 2-amino-nicotinic acid and maleic acid monoanion, the Raman spectra are different.

Słowa kluczowe

bifurcate hydrogen bonds, crystal packing, hydrogen bond enthalpy, low-frequency Raman spectroscopy, periodic DFT computations