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Author

Vener, MV (Vener, Mikhail V.); Medvedev, AG (Medvedev, Alexander G.); Churakov, AV (Churakov, Andrei V.); Prikhodchenko, PV (Prikhodchenko, Petr V.); Tripol'skaya, TA (Tripol'skaya, Tatiana A.); Lev, O (Lev, Ovadia)

Title

H-Bond Network in Amino Acid Cocrystals with H(2)O or H(2)O(2). The DFT Study of Serine-H(2)O and Serine-H(2)O(2)

Source

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Abstract

The structure, IR spectrum, and H-bond network in the serine-H(2)O and serine-H(2)O(2) crystals were studied using DFT computations with periodic boundary conditions. Two different basis sets were used: the all-electron Gaussian-type orbital basis set and the plane wave basis set. Computed frequencies of the IR-active vibrations of the titled crystals are quite different in the range of 10-100 cm(-1). Harmonic approximation fails to reproduce IR active bands in the 2500-2800 frequency region of serine-H(2)O and serine-H(2)O(2). The bands around 2500 and 2700 cm(-1) do exist in the anharmonic IR spectra and are caused by the first overtone of the OH bending vibrations of H(2)O and a combination vibration of the symmetric and asymmetric bendings of H(2)O(2). The quantum-topological analysis of the crystalline electron density enables us to describe quantitatively the H-bond network. It is much more complex in the title crystals than in a serine crystal. Appearance of water leads to an increase of the energy of the amino acid-amino acid interactions, up to similar to 50 kJ/mol. The energy of the amino acid-water H-bonds is similar to 30 kJ/mol. The H(2)O/H(2)O(2) substitution does not change the H-bond network; however, the energy of the amino acid-H(2)O(2) contacts increases up to 60 kJ/mol. This is caused by the fact that H(2)O(2) is a much better proton donor than H(2)O in the title crystals.