Infrared spectra and X-ray structure of (tetrazol-5-yl)acetic acid.

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The (tetrazol-5-yl)acetic acid crystal was characterized by the X-ray diffraction and FTIR spectroscopic methods. The analysis of the crystal structure reveals that the compound exists in the solid state as 1H-tautomer. The molecules are linked by two types of the intermolecular hydrogen bonds forming an infinite two-dimensional network in the (101) plane. Intramolecular N-H···O hydrogen bonds are also formed in the crystal. The analysis of the FTIR spectra of the crystalline sample and its deuterated analogue, based on the B3LYP/6-311++G(2d,2p) frequency calculations of two model tetramers, has been performed in relation to the obtained crystal structure data.

Słowa kluczowe

azoles, Molecular structure, Hydrogen bond, DFT calculations

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