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Structural, spectroscopic and conformational properties of 2-methyl-2(1*H*-tetrazol-1-yl)propan-1-ol experimental and theoretical approach.

Autorzy

Magdalena Pagacz-Kostrzewa

Agata Białońska

Robert Bronisz

Maria Wierzejewska

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Streszczenie

The B3LYP/6-311++G(2d,2p) calculations performed with the aim to describe the conformational landscape of the TOH molecule revealed the presence of 14 different minima (TOH1–TOH14). First two species (TOH1, TOH2) are characterized by a presence of the intramolecular hydrogen bond formed between O–H group and one of the N atoms of the tetrazole ring while the remaining 12 conformers do not contain hydrogen bonds. Comparison of the calculated geometry of the TOH conformers with that detected by the X-ray diffraction method shows that the fourth as to the energy conformer is present in the solid state. The X-ray study shows also the TOH molecules are linked to each other by the O–H⋯N intermolecular hydrogen bonds forming cyclic dimers along the [1 0 0] direction. The π⋯π stacking interactions between the tetrazole rings of consecutive molecules result in ribbons formation extended in the [1 0 0] direction. Weaker C–H⋯N hydrogen bonds link consecutive ribbons forming layers extended parallel to the (0 0 1) plane.

The calculated gas phase abundance of six most abundant TOH species at 333 K equals 37.24%, 14.85% and 29.27%, 7.52%, 2.80% and 2.52% and all these conformers were detected in the *ν*OH region of the infrared spectra of TOH isolated in argon matrices. In turn, infrared spectrum performed for the TOH crystalline sample confirms the presence of cyclic dimers consisting of two TOH4 monomers linked by two O–H⋯N hydrogen bonds. The latter spectrum was well reproduced by the B3LYP/6-311++G(2d,2p) spectrum predicted for the TOH cyclic dimer and the bands assignment was based on the potential energy distribution matrix.

Słowa kluczowe

2-Methyl-2-(1H-tetrazol-1-yl)propan-1-ol, crystal structure, infrared spectra, Matrix isolation, DFT calculations, Conformes

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