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Crystallographic and spectroscopic studies as well as DFT quantum chemical calculations of hydrazo-bond conformation in 4,4′-dimethyl-3,3′,5,5′-tetranitro-2,2-hydrazobipyridine.

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Streszczenie

The crystal and molecular structures of 4,4′-dimethyl-3,3′,5,5′-tetranitro-2,2′-hydrazobipyridine have been determined by X-ray diffraction studies and DFT quantum chemical calculations. The 6-311G (2d, 2p) basis set with the B3LYP functional has been used to discuss the optimised structure and vibrational dynamics of the studied compound. It crystallizes in the monoclinic *C*2/*c* space group with one-half molecule in the asymmetric unit. The intramolecular NH···O hydrogen bonds and weak intermolecular CH···O contacts play an important role in stabilization of the structure. Structural and vibrational properties of the studied compound have been compared to those of other similar compounds. The conformation of the hydrazo bridge has been analysed in relation to the intramolecular NH···O interactions inside the monomeric form. Low temperature behavior of the studied compound has been discussed.

Słowa kluczowe

4,4′-dimethyl-3,3′,5,5′-tetranitro-2,2′-hydrazobipyridine, Hydrazo group, X-ray diffraction, Vibrational spectra, DFT analysis

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