

Influence of methyl and nitro group substitutions on the structure and vibrational characteristics of the hydrazo-bridge in 6,6'-dimethyl-3,3',5,5'-tetranitro-2,2'-hydrazobipyridine.

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Streszczenie

The crystal and molecular structures of 6,6'-dimethyl-3,3',5,5'-tetranitro-2,2'-hydrazobipyridine have been determined by X-ray diffraction and DFT quantum chemical methods. The B3LYP/6-311G(2d,2p) approach has been used in the theoretical calculations. The studied compound crystallizes in the monoclinic $P2(1)/n$ space group ($Z=2$) with one-half molecule in the asymmetric unit. In the molecular structure of the studied compound the intramolecular N-H center dot center dot center dot O hydrogen bonds play a crucial role. These molecules also interact in the unit cell by means of weak intermolecular C-H center dot center dot center dot O contacts. IR and Raman spectra have been measured and simulated from the optimized geometry. In the calculations the monomeric unit has been taken into account because the intermolecular interactions between the components of the unit cell are weak and the factor group splitting is not observed in the experimental spectra. The structural and vibrational properties of the hydrazo bonds have been described with their relation to the intramolecular N-H center dot center dot center dot O interaction existing in the structure of the monomeric form.

Słowa kluczowe

6,6'-dimethyl-3,3',5,5'-tetranitro-2,2'-hydrazobipyridine, Hydrazo group, X-ray studies, Vibrational spectra, density functional calculations

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