

The hydrazo-bond in 4,4'-dimethyl-3,3'-dinitro-2,2'-hydrazobipyridine-crystal structure, conformation and vibrational characteristics.

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The crystal and molecular structure of 4,4'-dimethyl-3,3'-dinitro-2,2'-hydrazobipyridine have been determined by X-ray diffraction and quantum chemical DFT analysis. The title compound crystallizes in *P* space group, with one-half molecule in the asymmetric unit. The molecular structure is stabilized by intramolecular NH...O hydrogen bonds. The molecules are linked by a combination of weak intermolecular CH...O interactions and also aromatic π - π stacking. The molecular structure of the studied compound has been determined using the DFT B3LYP/6-311G(2d,2p) approach and compared to that derived from X-ray studies. The IR and Raman wavenumbers have been calculated for the optimized geometry of a possible monomer structural model. The structural and vibrational properties of the intramolecular NH...O interaction are described.

Słowa kluczowe

lanthanides, 4'-dimethyl-3, 3'-dinitro-2, 2'-hydrazobipyridine, Hydrazo bond, IR and Raman spectra, X-ray study, Quantum chemical calculations

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