The X-ray revision of the structure of bis(4-hydroxybenzhydrazide) copper(II) sulfate (VI) dihydrate and its vibrational spectroscopy.

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Streszczenie

The structure of known copper(II) complex with4-hydroxybenzoic acid hydrazide has been corrected on thebasis of a new X-ray analysis. It has been found, that thesulfate(VI) ion is bonded in apical position of Cu(II) coor-dination pyramid having two organic ligands at the base.Two water molecules are not coordinated as has been pos-tulated before, but stabilizes the sulfate(VI) group orienta-tion and link the layers of complex molecules by stronghydrogen bonds. The detailed interpretation of the measuredIR and Raman spectra has been performed with aid of both:quantum calculations as well as H/D and63Cu–65Cu isotopesubstitution.

Słowa kluczowe

4-Hydroxybenzhydrazide, 4-Hydroxybenzoic hydrazide , Copper(II) complex, crystal structure, IR Raman spectra, TD DFT calculations, Deuteration

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