

Molecular conformation *versus* C-H...Ph weak hydrogen bonds in 4-(4-*H*-1,2,4-triazol-4-yl)-2-X-phenylmethanimine (X=CH₃,Cl,Br) crystals.

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Streszczenie

Three 4-(4-*H*-1,2,4-triazol-4-yl)-2-X-phenylmethanimines where X=CH₃ (**1**), Cl (**2**), and Br (**3**) have been synthesised and characterised by spectroscopic, theoretical, and single crystal X-ray methods. Crystallographic analysis showed that conformation of **1** is non-planar whereas of **2** and **3** are planar. In the studied crystals the C-H groups in triazole residues participate in the C-H...N hydrogen bonds and additionally in the C-H...O (water) hydrogen bond in **2**. The aromatic phenyl ring is an acceptor of two intermolecular C-H...Ph hydrogen bonds only in **1**. Observed non-planar conformation of **1** and results of optimisation of molecular geometry by DFT method suggest that conformation of **1** is highly influenced by very weak the C-H...Ph hydrogen bonds in studied crystals.

Słowa kluczowe

4-Substituted-1, molecule, 4-triazoles, Crystal structure, DFT calculations, Hydrogen bond

Adres publiczny

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