Weak hydrogen and dihydrogen bonds instead of strong N-H···O bonds of a tricyclic [1,2,4,5]-tetrazine derivative. Single-crystal X-ray diffraction, theoretical calculations and Hirshfeld surface analysis.

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Octahydro-1*H*,6*H*-bis[1,4]oxazino[4,3-b:4′,3′-e][1,2,4,5]tetrazine, **1**, and its monohydrated analog, **2**, were obtained by an oxidation process of *N*-aminomorpholine with iodine. Both compounds crystallize in monoclinic space groups $P2_1/c$ and $C2/c$ for **1** and **2**, respectively. Despite the presence of a strong hydrogen bond donor – the NH group – the crystal packing of **1** is determined by weak C–H···O and C–H···N hydrogen bonds. In order to explore more precisely this intriguing fact, the theory of Atoms In Molecules (AIM) was used to examine intermolecular interactions in a crystal. An analysis of the topological properties of electron density with the determination of bond critical point revealed a set of contacts which were carefully scrutinized to determine whether they fulfill the criteria of hydrogen and dihydrogen bond existence in the AIM method. Their stability was checked by DFT calculations. In the case of **2**, the crystal packing is realized by strong O1w–H1w···N and N–H···O1w hydrogen bonds with water. The possibility of accepting more than one hydrogen atom by each lone electron pair of water is discussed based on the AIM method and Natural Bond Orbital (NBO) analysis. Hirshfeld surfaces were employed to confirm the existence of intermolecular interactions in **1** and **2**.

Adres publiczny

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