Crystal structure of 1,10-di(1H-1,2,4-triazol-1-yl)decane hydrate, C_{28}H_{48}N_{12}·H_{2}O

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Abstract

C_{28}H_{48}N_{12}O, monoclinic, C12/c1 (no. 15), \(a = 29.470(2)\) Å, \(b = 5.4438(2)\) Å, \(c = 21.508(2)\) Å, \(\beta = 113.803(8)^\circ\), \(V = 3157.0\) Å\(^3\), \(Z = 4\), \(R_{wp} (F) = 0.037\), \(wR_{wp} (F^2) = 0.111\), \(T = 293\) K.

Source of material

Starting materials and solvents for synthesis were purchased commercially and used as received, except for 1,10-di(1H-1,2,4-triazol-1-yl)decane which was prepared according to reported procedures [1]. A mixture of 1,10-di(1H-1,2,4-triazol-1-yl)decane (0.28 g, 1 mmol), methanol (5 mL) and water (1 mL) was stirred at room temperature for 1 hour, and was filtrated. The filtrate was left to afford colourless single crystals after ca. one week in a 38 % yield.

Experimental details

All H atoms on C atoms were generated geometrically and refined as riding atoms with \(U_{iso} (H) = 1.2\) \(U_{eq}(C)\). The water H atoms were located from difference Fourier map and refined with \(d(O-H) = 0.871\) Å, and \(U_{iso}(H) = 1.5\) \(U_{eq}(O)\). During refinement of the crystal structure of the title compound, we realized that, owing to inherently poor crystal quality, the \(N_{eq}/N_{param}\) ratio is relatively low.

Discussion

In the past decades, much attention has been focused on the design and synthesis of metal-organic coordination networks. 1,2,4-Triazole and, in particular, its derivatives are very interesting bridging ligands to construct coordination networks [2]. 1,10-di(1H-1,2,4-triazol-1-yl)decane, with a flexible long carbon chain, is a good candidate for construction of multi-dimensional coordination polymers.

The asymmetric unit of the title crystal structure contains one 1,10-di(1H-1,2,4-triazol-1-yl)decane molecule and a lattice water molecule. In the crystal structure, there are hydrogen bonds between OW and N3 (the distance OW—N3 is 2.918 Å and the angle OW—HW—N3 is 174.95°), which interlink molecules to stabilize the structure.
### Table 3. Atomic coordinates and displacement parameters (in Å²).

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References