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The crystal structure of bis(imidazole-1-yl) methane monohydrate, C₇H₁₀N₄O

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Abstract

C₇H₁₀N₄O, monoclinic, *I*2 (no. 5), *a* = 15.7815(13) Å, *b* = 4.3242(3) Å, *c* = 12.4658(9) Å, β = 106.301(8)°, *V* = 816.50(10) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0473, *wR*_{ref}(*F*²) = 0.1067, *T* = 113.25(10) K.

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The asymmetric unit of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

In representative experiments, 3.0 g (53.4 mmol) KOH were dissolved in 20 mL solvent, then 3.0 g (44.1 mmol) imidazole were added, 3.8 g (22.1 mmol) dibromomethane were added at 293 K. The target compound was obtained by reaction at 333 K for 5 h. The crystal of the title compound was obtained by slow evaporation at 293 K.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.45 × 0.11 × 0.03 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.10 mm ^{−1}
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	26.0°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	1634, 1239, 0.030
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1079
<i>N</i> (<i>param</i>) _{refined} :	110
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], Olex2 [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} ^a / <i>U</i> _{eq}
O1	0.27707(13)	0.3971(5)	0.32414(15)	0.0367(6)
H1A	0.2639	0.2474	0.2777	0.055*
H1B	0.2555	0.3533	0.3782	0.055*
N1	0.47702(15)	0.7137(6)	0.58374(17)	0.0253(6)
C1	0.5000	0.5228(10)	0.5000	0.0305(10)
H1C ^a	0.5496	0.3911	0.5359	0.037*
H1D ^a	0.4504	0.3911	0.4641	0.037*
N2	0.49432(16)	1.0213(6)	0.73081(18)	0.0303(6)
C3	0.40763(19)	1.0303(7)	0.6656(2)	0.0289(7)
H3	0.3635	1.1487	0.6817	0.035*
C2	0.53327(19)	0.8294(7)	0.6778(2)	0.0297(8)
H2	0.5929	0.7790	0.7023	0.036*
C4	0.39538(19)	0.8437(7)	0.5751(2)	0.0271(7)
H4	0.3431	0.8104	0.5190	0.033*
C5	0.0000	−0.2706(10)	0.5000	0.0280(10)
H5A ^a	0.0054	−0.4022	0.5646	0.034*
H5B ^a	−0.0054	−0.4022	0.4354	0.034*
N4	0.18829(16)	0.1797(6)	0.48032(19)	0.0322(7)
N3	0.07871(15)	−0.0765(5)	0.51795(17)	0.0255(6)
C7	0.18348(19)	0.2556(7)	0.5862(2)	0.0325(8)
H7	0.2207	0.3948	0.6339	0.039*
C6	0.12390(19)	−0.0199(8)	0.4424(2)	0.0284(7)
H6	0.1110	−0.1111	0.3721	0.034*
C8	0.1174(2)	0.1001(7)	0.6109(2)	0.0304(7)
H8	0.1011	0.1099	0.6770	0.036*

^aOccupancy: 0.50.

Experimental details

All H atoms were positioned geometrically and treated as riding, with O—H bond lengths constrained to

0.85 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$, N–H bond 0.88 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

Comment

A methylene-bridged two-dentate nitrogen-containing ligand is a semi-rigid ligand. *Cis-trans* conformers can rotate along methylene due to the existence of single bonds in nitrogen-containing heterocycles [5]. The synthesis of bisimidazole methane coordination polymers has attracted great interest. Many compounds with novel structures and special functions have been synthesized by self-assembly method [6–9]. The crystal structure of bis(imidazole-1-yl)methane has been reported [10].

The title compound has been reported for the first time in this paper. (*cf.* the figure) The asymmetric unit of the title structure contains one bis(imidazole-1-yl)methane (two halves of a title molecule, arranged at two-fold axes) and one water molecule in a general position. The imidazole ring is almost flat in both moieties.

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