Crystal structure of 1-(1*H*-benzimidazole)methyl-1*H*-benztriazole dihydrate, $C_{14}H_{11}N_5 \cdot 2H_2O$

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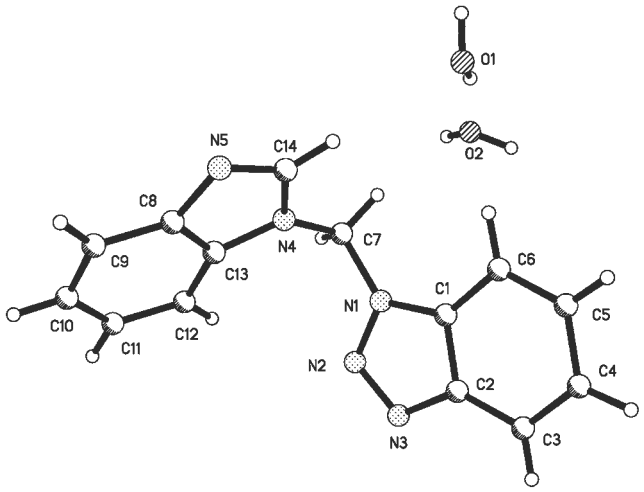

Abstract

$C_{14}H_{15}N_5O_2$, monoclinic, $P2_1/n$ (no. 14), a = 12.437 Å, b = 7.146 Å, c = 15.922 Å, β = 97.03°, V = 1404.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.041, $wR_{ref}(F^2)$ = 0.092, T = 293 K.

Source of material

The title compound was obtained by reacting benzimidazole (1.18 g, 0.01 mol) with 1-chloromethylbenzotriazole (1.67 g, 0.01 mol) [1] and potassium carbonate (1.38 g, 0.01 mol) in acetone (100 ml). The reaction mixture was refluxed for 10 h. After removal of the solvents, the residue was dispersed in water and filtered to obtain the brown crude product. Then the crude product was recrystallized from ethanol/water (1:1) and the target crystals were subjected to X-ray diffraction analysis.

Discussion

Benzimidazole and related heterocycle compounds have been extensively investigated because of their applications as intermediate for the synthesis of chemiluminescent compounds [2] and as cytomegalovirus inhibitors and anthelmintic agents [3].

The asymmetric unit of the title crystal structure consists of one 1-(1*H*-benzimidazole)methyl-1*H*-benzotriazole and two water molecules. In the crystal structure, the bond lengths and angles are in normal range. The bond angle N1–C7–N4 is 113.1(1)°, which is very close to those of 1-benzyl-1*H*-benzimidazole (114.12(8)°) [4] and 1-[6-(9*H*-carbazol-9-yl)hexyl]-2-phenyl-1*H*-benzimidazole (113.9(1)°) [5], respectively. There are three classical intermolecular hydrogen bonds linking the molecules into chains. The crystal packing of the title sturcture is further interlinked by the non-classical hydrogen bond and π-π stacking into the 3D supramolecular architecture.

Table 1. Data collection and handling.

Crystal:	brown block, size 0.15 × 0.18 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.95 cm^{-1}
Diffractometer, scan mode:	Xcalibur Eos Gemini, φ/ω
$2\theta_{max}$:	52.74°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6546, 2859
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1670
$N(param)_{refined}$:	250
Programs:	SHELXS-97, SHELXL-97, SHELXTL [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(7B)	4*e*	0.677(1)	–0.327(2)	0.525(1)	0.047(4)
H(14)	4*e*	0.642(1)	0.014(2)	0.368(1)	0.058(5)
H(4)	4*e*	1.167(2)	–0.240(2)	0.370(1)	0.060(5)
H(12)	4*e*	0.686(1)	–0.141(3)	0.665(1)	0.048(5)
H(6)	4*e*	0.833(1)	–0.215(2)	0.331(1)	0.058(5)
H(7A)	4*e*	0.690(1)	–0.301(2)	0.429(1)	0.058(5)
H(2B)	4*e*	0.732(1)	–0.585(3)	0.311(1)	0.081(7)
H(10)	4*e*	0.574(1)	0.372(3)	0.721(1)	0.070(6)
H(9)	4*e*	0.550(1)	0.458(3)	0.574(1)	0.056(5)
H(5)	4*e*	1.008(1)	–0.207(2)	0.283(1)	0.071(6)
H(2A)	4*e*	0.648(2)	–0.591(3)	0.361(1)	0.12(1)
H(1B)	4*e*	0.653(2)	–0.309(2)	0.252(1)	0.091(8)
H(3)	4*e*	1.163(2)	–0.265(3)	0.516(1)	0.075(6)
H(11)	4*e*	0.641(1)	0.084(3)	0.764(1)	0.077(6)
H(1A)	4*e*	0.593(2)	–0.199(4)	0.194(1)	0.15(1)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.6465(1)	–0.1998(2)	0.23105(9)	0.0579(8)	0.082(1)	0.0608(9)	–0.0130(8)	–0.0107(7)	0.0175(8)
N(5)	4*e*	0.5990(1)	0.2187(2)	0.44680(9)	0.0441(8)	0.067(1)	0.0491(9)	0.0019(8)	0.0042(6)	0.0065(8)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.9031(1)	–0.2423(2)	0.45565(9)	0.0409(8)	0.0371(9)	0.0395(9)	–0.0021(8)	–0.0004(7)	0.0006(8)
O(2)	4*e*	0.6779(1)	–0.5268(2)	0.32589(8)	0.078(1)	0.0632(9)	0.0515(8)	0.0081(8)	0.0112(7)	0.0023(7)
N(4)	4*e*	0.66264(9)	–0.0626(2)	0.48980(7)	0.0386(7)	0.0523(9)	0.0349(7)	–0.0027(7)	0.0017(5)	–0.0019(7)
C(13)	4*e*	0.6444(1)	0.0330(2)	0.56235(9)	0.0315(8)	0.053(1)	0.0383(9)	–0.0056(8)	0.0050(6)	–0.0046(8)
N(3)	4*e*	0.9712(1)	–0.2753(2)	0.59189(8)	0.062(1)	0.059(1)	0.0428(9)	0.0064(8)	–0.0102(7)	–0.0023(7)
C(3)	4*e*	1.0984(1)	–0.2556(3)	0.4805(1)	0.040(1)	0.054(1)	0.073(1)	–0.005(1)	–0.0116(9)	–0.007(1)
C(7)	4*e*	0.7065(1)	–0.2478(3)	0.4853(1)	0.046(1)	0.053(1)	0.045(1)	–0.0096(9)	0.0080(8)	–0.006(1)
C(2)	4*e*	0.9988(1)	–0.2569(2)	0.5110(1)	0.0449(9)	0.041(1)	0.046(1)	0.0002(8)	–0.0087(7)	–0.0037(8)
C(6)	4*e*	0.9034(1)	–0.2238(3)	0.3684(1)	0.046(1)	0.061(1)	0.041(1)	–0.0044(9)	–0.0020(8)	0.0051(9)
N(2)	4*e*	0.8665(1)	–0.2740(2)	0.58866(8)	0.071(1)	0.060(1)	0.0350(8)	0.0048(8)	–0.0021(7)	0.0005(7)
C(8)	4*e*	0.6047(1)	0.2067(3)	0.5349(1)	0.0317(8)	0.059(1)	0.046(1)	–0.0035(8)	0.0054(7)	–0.0006(9)
C(14)	4*e*	0.6334(1)	0.0566(3)	0.4239(1)	0.0405(9)	0.071(1)	0.037(1)	–0.004(1)	0.0022(7)	0.001(1)
C(4)	4*e*	1.0995(2)	–0.2397(3)	0.3953(1)	0.043(1)	0.067(1)	0.078(2)	–0.010(1)	0.009(1)	–0.004(1)
C(12)	4*e*	0.6587(1)	–0.0187(3)	0.6472(1)	0.052(1)	0.063(1)	0.038(1)	–0.003(1)	0.0082(8)	0.0010(9)
C(10)	4*e*	0.5927(2)	0.2878(3)	0.6779(1)	0.062(1)	0.072(2)	0.061(1)	–0.008(1)	0.022(1)	–0.020(1)
C(9)	4*e*	0.5778(1)	0.3383(3)	0.5940(1)	0.044(1)	0.056(1)	0.072(1)	–0.002(1)	0.0146(9)	–0.003(1)
C(5)	4*e*	1.0020(2)	–0.2238(3)	0.3403(1)	0.057(1)	0.074(1)	0.052(1)	–0.010(1)	0.0127(9)	0.006(1)
C(11)	4*e*	0.6324(2)	0.1131(3)	0.7039(1)	0.067(1)	0.082(2)	0.041(1)	–0.005(1)	0.0141(9)	–0.006(1)
N(1)	4*e*	0.8233(1)	–0.2542(2)	0.50677(8)	0.0461(8)	0.0493(9)	0.0335(7)	–0.0003(7)	–0.0004(6)	0.0004(7)

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