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 (1*H*-Benzimidazol-1-yl)methanol

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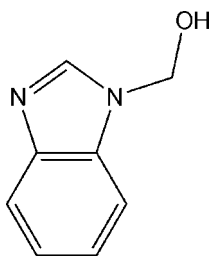
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 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.105; data-to-parameter ratio = 12.1.

In the title compound, $\text{C}_8\text{H}_8\text{N}_2\text{O}$, the $\text{N}-\text{CH}_2$ and CH_2-O bond lengths can be correlated to the manifestation of an anomeric effect in the $\text{N}-\text{CH}_2-\text{O}$ moiety. In the crystal, intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into zigzag chains, with graph-set motif $C(6)$, parallel to $[001]$. These chains are further linked into sheets by weak nonclassical $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For a related structure, see: Shi *et al.* (2011). For bond-length data, see: Allen *et al.* (1987). For chemical background on the synthesis and uses of the title compound, see: Milata *et al.* (2001). For graph-set analysis, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_8\text{H}_8\text{N}_2\text{O}$
 $M_r = 148.2$
 Monoclinic, $P2_1/c$
 $a = 13.3181$ (10) Å
 $b = 4.2677$ (3) Å
 $c = 12.4795$ (10) Å
 $\beta = 95.143$ (6)°

 $V = 706.45$ (9) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 0.78$ mm⁻¹
 $T = 120$ K
 $0.41 \times 0.30 \times 0.23$ mm

Data collection

 Agilent Xcalibur diffractometer with an Atlas (Gemini Ultra Cu) detector
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\min} = 0.744$, $T_{\max} = 1$

 4736 measured reflections
 1248 independent reflections
 1086 reflections with $I > 3\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.105$
 $S = 1.78$
 1248 reflections
 103 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\text{o}\cdots\text{N2}^{\text{i}}$	0.894 (19)	1.85 (2)	2.7355 (16)	173.8 (17)
$\text{C1}-\text{H1}\cdots\text{O1}^{\text{ii}}$	0.96	2.41	3.2887 (17)	152

 Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2398).

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supporting information

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(1*H*-Benzimidazol-1-yl)methanol

Augusto Rivera, Mauricio Maldonado, Jaime Ríos-Motta, Karla Fejfarová and Michal Dušek

S1. Comment

Benzimidazole derivatives are compounds that have received much attention because of their applications in several areas. Although the synthesis of title compound had been reported in the literature (Milata *et al.*, 2001), we have developed an alternative route to prepare this compound starting from the synthetically available benzoaminal 6*H*,13*H*-5:12,7:14-dimethanedibenzo[*d,i*][1,3,6,8]tetraazecine (DMDBTA).

In the title compound, C₈H₈N₂O, (Fig.1) the benzimidazole ring is essentially planar, with a maximum deviation for N1 of 0.0089 (12) Å from the least-squares plane defined by the nine constituent atoms. The sum of bond angles around this nitrogen atom was 359.90 (11)°, which is consistent with the planarization of the heterocyclic ring. The distances within the benzimidazole ring of the title compound are very similar to those found in bis(1*H*-benzimidazol-1-yl)methane monohydrate (Shi *et al.*, 2011). However, the observed N—CH₂ bond length [N1—C8, 1.4638 (17) Å] is longer in relation to the mentioned mean value observed in related structure [N—CH₂, 1.452 (4) Å] (Shi *et al.*, 2011). Moreover, the CH₂—O bonds in the residue tend to be shorter than the normal values by 0.033 Å (Allen *et al.*, 1987). This fact can be correlated to the manifestation of an anomeric effect in N—CH₂—O moiety, but it operates in the opposite direction. In the crystal structure, intermolecular O—H⋯N hydrogen bonds link the molecules into *zigzag* chains with graph-set motif C(6) parallel to [001], (Bernstein *et al.*, 1995) (Fig. 2). These chains are further linked into sheet by weak non-classical C—H⋯O hydrogen bonds between H atom of the benzimidazole ring and the O atom of a neighbouring molecule.

S2. Experimental

A solution of 6*H*,13*H*-5:12,7:14-dimethanedibenzo[*d,i*][1,3,6,8] tetraazecine (DMDBTA) (0.25 mmol) and *p*-nitrophenol (0.5 mmol) in propan-2-ol (15 ml) was placed in a round-bottomed flask equipped with a water-cooled condenser. The reaction mixture was heated at 347 K for 3 h. giving a white precipitate which was filtered off, and the mother liquor was then concentrated by a rotary evaporator to give an oil accompanied by precipitates, which was removed by filtration. Single crystal of the precipitate (title compound), suitable for X-ray crystallography, was grown by slow evaporation from water:propan-2-ol solution at room temperature after several days. Melting point 407 K.

The NMR spectra were acquired at room temperature on a Bruker AMX 400 Avance spectrometer. ¹H NMR (δ, 400 MHz, CDCl₃): 5.60, 6.78, 7.23, 7.29, 7.66, 8.28. ¹³C NMR (δ, 100 MHz, CDCl₃): 67.8, 111.4, 119.8, 122.3, 122.9, 133.7, 144.1, 144.8.

S3. Refinement

The hydroxyl hydrogen atom was found in difference Fourier maps and its coordinates were refined freely. All other H atoms were positioned geometrically and treated as riding on their parent atoms. The isotropic atomic displacement parameters of hydrogen atoms were evaluated as 1.2×*U*_{eq} of the parent atom.

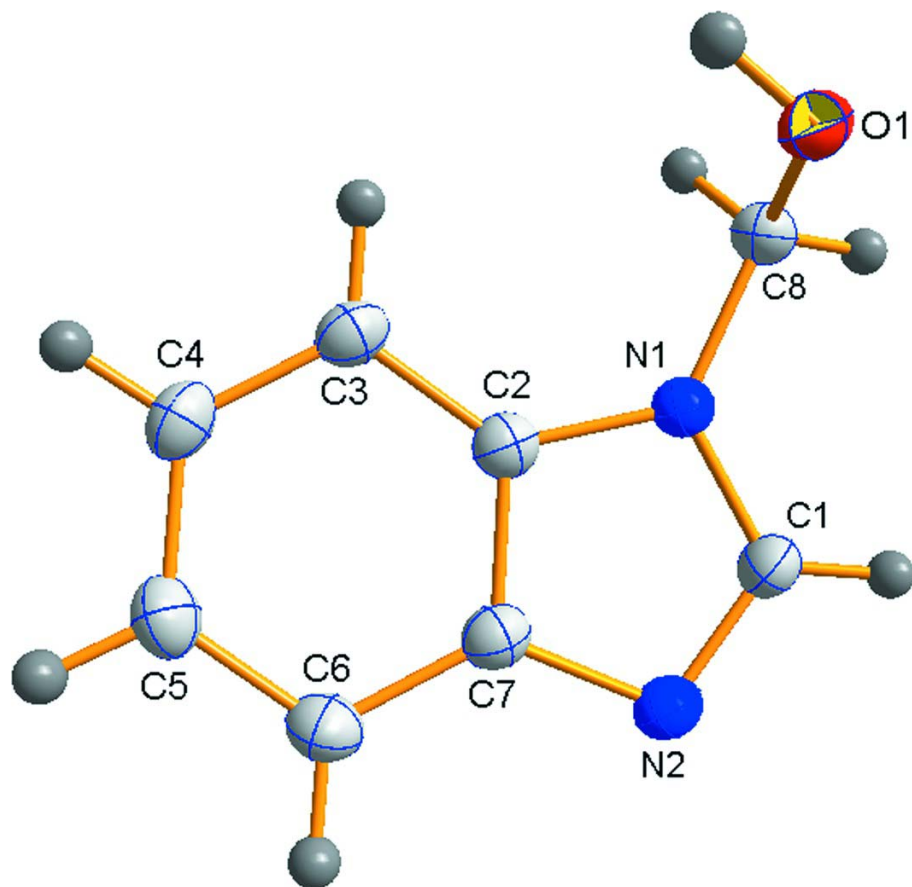
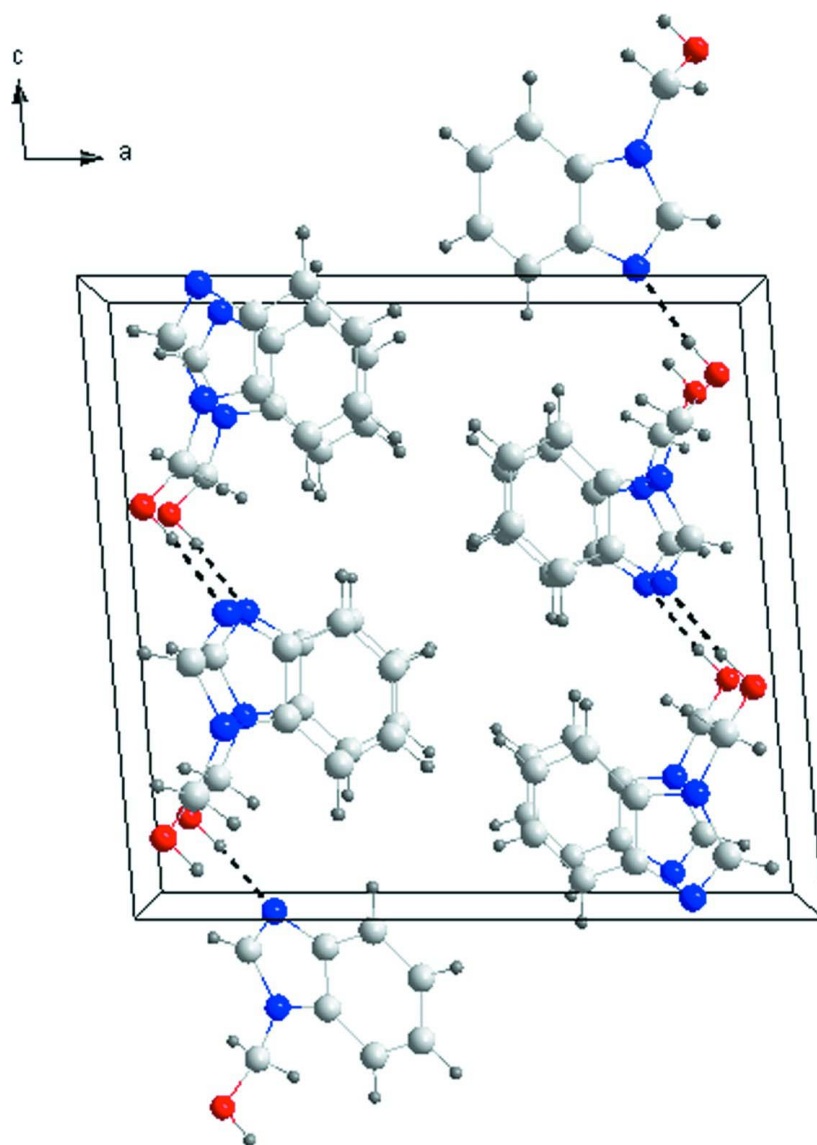


Figure 1

A view of the title molecule. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

Packing of the molecules of the title compound view along the *b* axis. Dashed lines indicate the intermolecular hydrogen bonds.

(1*H*-Benzimidazol-1-yl)methanol

Crystal data

$C_8H_8N_2O$

$M_r = 148.2$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 13.3181\ (10)\ \text{\AA}$

$b = 4.2677\ (3)\ \text{\AA}$

$c = 12.4795\ (10)\ \text{\AA}$

$\beta = 95.143\ (6)^\circ$

$V = 706.45\ (9)\ \text{\AA}^3$

$Z = 4$

$F(000) = 312$

$D_x = 1.393\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.5418\ \text{\AA}$

Cell parameters from 2690 reflections

$\theta = 3.3\text{--}66.8^\circ$

$\mu = 0.78\ \text{mm}^{-1}$

$T = 120\ \text{K}$

Block, colourless

$0.41 \times 0.30 \times 0.23\ \text{mm}$

Data collection

Agilent Xcalibur
diffractometer with an Atlas (Gemini ultra Cu)
detector
Radiation source: Enhance Ultra (Cu) X-ray
Source
Mirror monochromator
Detector resolution: 10.3784 pixels mm⁻¹
rotation method data acquisition using ω scans
Absorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.744$, $T_{\max} = 1$
4736 measured reflections
1248 independent reflections
1086 reflections with $I > 3\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\max} = 67.1^\circ$, $\theta_{\min} = 3.3^\circ$
 $h = -15 \rightarrow 15$
 $k = -5 \rightarrow 5$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.105$
 $S = 1.78$
1248 reflections
103 parameters
0 restraints
29 constraints

H atoms treated by a mixture of independent
and constrained refinement
Weighting scheme based on measured s.u.'s $w =$
 $1/[\sigma^2(I) + 0.0016I^2]$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.18 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. *CrysAlisPro* (Agilent, 2010) Empirical absorption correction using spherical harmonics, implemented in *SCALE3 ABSPACK* scaling algorithm.

Refinement. The refinement was carried out against all reflections. The conventional R -factor is always based on F . The goodness of fit as well as the weighted R -factor are based on F and F^2 for refinement carried out on F and F^2 , respectively. The threshold expression is used only for calculating R -factors *etc.* and it is not relevant to the choice of reflections for refinement.

The program used for refinement, *Jana2006*, uses the weighting scheme based on the experimental expectations, see `_refine_ls_weighting_details`, that does not force S to be one. Therefore the values of S are usually larger than the ones from the *SHELX* program.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.93101 (7)	0.3994 (2)	0.86004 (8)	0.0311 (3)
N1	0.83140 (8)	0.4446 (3)	0.69371 (9)	0.0247 (3)
N2	0.81868 (9)	0.2744 (3)	0.52326 (9)	0.0291 (4)
C1	0.86934 (10)	0.4481 (3)	0.59626 (11)	0.0277 (4)
C2	0.74835 (9)	0.2487 (3)	0.68347 (10)	0.0243 (4)
C3	0.68095 (10)	0.1551 (3)	0.75625 (11)	0.0268 (4)
C4	0.60448 (10)	-0.0444 (3)	0.71773 (11)	0.0289 (4)
C5	0.59534 (10)	-0.1479 (3)	0.61064 (12)	0.0308 (4)
C6	0.66286 (10)	-0.0572 (3)	0.53902 (11)	0.0296 (4)
C7	0.74087 (9)	0.1443 (3)	0.57631 (10)	0.0255 (4)
C8	0.87514 (9)	0.6034 (3)	0.79091 (10)	0.0271 (4)
H1	0.927903	0.566907	0.582034	0.0333*
H3	0.687318	0.225735	0.829577	0.0322*
H4	0.556364	-0.114071	0.765431	0.0347*
H5	0.540778	-0.285048	0.586627	0.037*
H6	0.656443	-0.13025	0.465963	0.0356*

H8a	0.91753	0.77186	0.771157	0.0325*
H8b	0.822274	0.695733	0.827835	0.0325*
H1o	0.8905 (14)	0.341 (4)	0.9098 (15)	0.0373*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0258 (5)	0.0439 (6)	0.0239 (5)	0.0053 (4)	0.0035 (4)	0.0043 (4)
N1	0.0236 (6)	0.0287 (6)	0.0218 (6)	-0.0009 (4)	0.0024 (4)	-0.0001 (4)
N2	0.0285 (6)	0.0358 (7)	0.0235 (6)	-0.0006 (4)	0.0053 (4)	-0.0005 (5)
C1	0.0253 (7)	0.0338 (8)	0.0248 (7)	-0.0016 (5)	0.0056 (5)	0.0012 (5)
C2	0.0235 (6)	0.0249 (7)	0.0244 (7)	0.0038 (5)	0.0017 (5)	0.0013 (5)
C3	0.0272 (7)	0.0287 (7)	0.0250 (7)	0.0048 (5)	0.0052 (5)	0.0014 (5)
C4	0.0252 (7)	0.0297 (7)	0.0327 (8)	0.0028 (5)	0.0070 (6)	0.0055 (5)
C5	0.0261 (7)	0.0300 (7)	0.0355 (8)	-0.0017 (5)	-0.0014 (6)	0.0024 (6)
C6	0.0323 (7)	0.0305 (7)	0.0255 (7)	0.0005 (5)	-0.0008 (6)	-0.0002 (5)
C7	0.0254 (7)	0.0267 (7)	0.0243 (7)	0.0030 (5)	0.0029 (5)	0.0008 (5)
C8	0.0268 (7)	0.0309 (7)	0.0234 (7)	-0.0002 (5)	0.0015 (5)	-0.0010 (5)

Geometric parameters (Å, °)

O1—C8	1.3932 (16)	C3—C4	1.3804 (18)
O1—H1o	0.894 (19)	C3—H3	0.96
N1—C1	1.3581 (18)	C4—C5	1.402 (2)
N1—C2	1.3834 (16)	C4—H4	0.96
N1—C8	1.4638 (17)	C5—C6	1.379 (2)
N2—C1	1.3133 (17)	C5—H5	0.96
N2—C7	1.3941 (18)	C6—C7	1.3961 (18)
C1—H1	0.96	C6—H6	0.96
C2—C3	1.3916 (19)	C8—H8a	0.96
C2—C7	1.4045 (18)	C8—H8b	0.96
C8—O1—H1o	106.4 (11)	C5—C4—H4	119.1913
C1—N1—C2	106.41 (11)	C4—C5—C6	121.57 (12)
C1—N1—C8	125.77 (11)	C4—C5—H5	119.2139
C2—N1—C8	127.72 (11)	C6—C5—H5	119.2142
C1—N2—C7	104.65 (11)	C5—C6—C7	117.76 (13)
N1—C1—N2	113.94 (12)	C5—C6—H6	121.1194
N1—C1—H1	123.0293	C7—C6—H6	121.1187
N2—C1—H1	123.0296	N2—C7—C2	109.49 (11)
N1—C2—C3	132.10 (12)	N2—C7—C6	130.52 (12)
N1—C2—C7	105.52 (11)	C2—C7—C6	119.99 (12)
C3—C2—C7	122.38 (11)	O1—C8—N1	112.01 (11)
C2—C3—C4	116.66 (12)	O1—C8—H8a	109.4718
C2—C3—H3	121.6681	O1—C8—H8b	109.4708
C4—C3—H3	121.6689	N1—C8—H8a	109.4717
C3—C4—C5	121.62 (13)	N1—C8—H8b	109.4709
C3—C4—H4	119.1906	H8a—C8—H8b	106.8062

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots N2 ⁱ	0.894 (19)	1.85 (2)	2.7355 (16)	173.8 (17)
C1—H1 \cdots O1 ⁱⁱ	0.96	2.41	3.2887 (17)	152

Symmetry codes: (i) $x, -y+1/2, z+1/2$; (ii) $-x+2, y+1/2, -z+3/2$.