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2-(1*H*-Benzotriazol-1-yl)acetohydrazide

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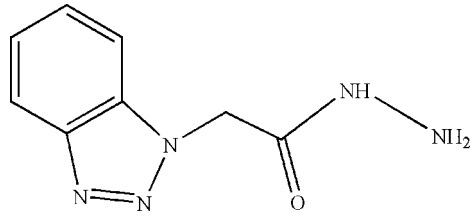
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 11.3.

The title compound, $C_8H_9N_5O$, was synthesized by the reaction of ethyl 2-(benzotriazol-1-yl)acetate with hydrazine hydrate in ethanol. In the amide group, the C—N bond is relatively short [1.3283 (16) Å], suggesting some degree of electronic delocalization in the molecule. In the crystal structure, molecules are linked into infinite chains along the *a* axis by intermolecular O—H···N hydrogen bonding.

Related literature

For general background to multiple-hydrogen-bonding *N*-heterocyclic systems as potential supramolecular reagents, see: Portalone (2007); Portalone & Colapietro (2007, 2008); For related structures, see: Shi *et al.* (2007*a*,*b*); Ji *et al.* (2008); For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_8H_9N_5O$ M_r = 191.20
Monoclinic, $P2_1/c$
a = 5.1434 (9) Å
b = 6.5885 (12) Å
c = 25.754 (5) Å
β = 94.227 (3)°
V = 870.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 295 K
0.12 × 0.10 × 0.06 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.988, T_{max} = 0.994
4367 measured reflections
1528 independent reflections
1364 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
S = 1.04
1528 reflections
135 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H1···O1^{i}	0.86	2.18	2.9977 (14)	159

Symmetry code: (i) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2267).

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supporting information

Acta Cryst. (2009). E**65**, o1538 [doi:10.1107/S1600536809021199]

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S1. Comment

In our previous papers(Shi *et al.*, 2007a; Shi *et al.*, 2007b; Ji *et al.*, 2008;), we have reported a number of Schiff-bases by the reaction of benzotriazol-1-yl-acetic acid hydrazide with relevant aldehyde or ketone. As a part of a more general study of multiple-hydrogen-bonding N-heterocyclic systems as potential supramolecular reagents (Portalone, 2007; Portalone & Colapietro, 2007, 2008), the title compound, (I), was synthesized and its crystal structure determined. The asymmetric unit of the (I) comprises one independent molecule. In (I) (Fig. 1), the bond lengths and angles are in good agreement with the expected values (Allen *et al.*, 1987). In the crystal structure (Fig. 2), the molecules are linked into infinite chains by O—H···N hydrogen bond.

S2. Experimental

The title compound was synthesized by the reaction of benzotriazol-1-yl-acetic acid ethyl ester(1 mmol) with hydrazine hydrate 85% (1.1 mmol)in ethanol (20 ml) under reflux conditions (348 K) for 24 h. The solvent was removed and the solid product recrystallized from tetrahydrofuran. After four days colorless crystals suitable for X-ray diffraction study were obtained.

S3. Refinement

All H atoms were placed in idealized positions (C—H = 0.93— 0.97 Å, N—H = 0.86 Å) and refined as riding atoms. For those bound to C, U_{iso}(H) = 1.2 or 1.5U_{eq}(C). while for those bound to N, U_{iso}(H) = 1.2 U_{eq}(N).

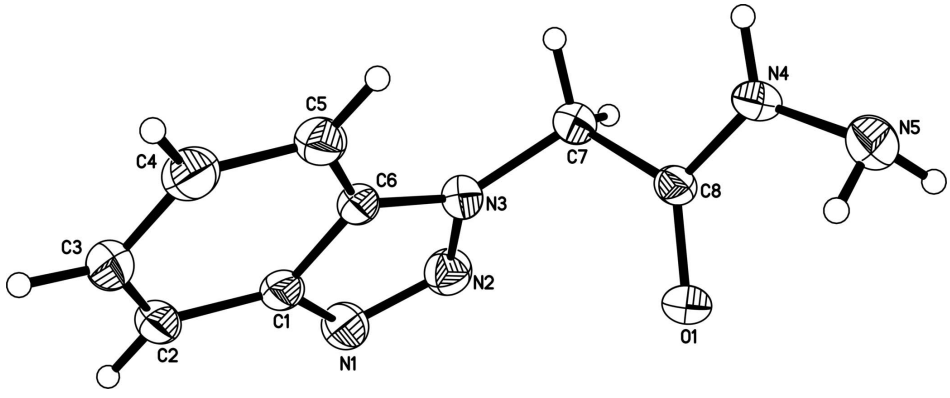

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

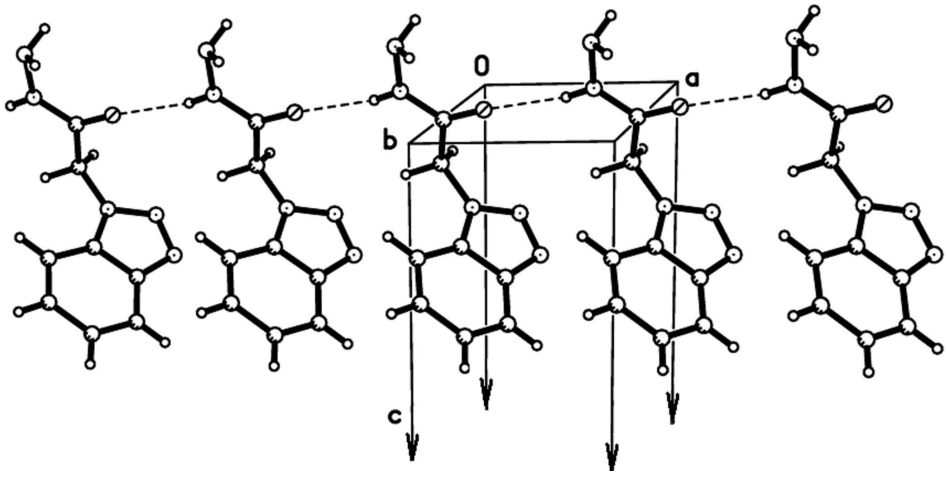

Figure 2

The structure of the infinite chains formed *via* hydrogen bonds, H atoms have been omitted for clarity. The dashed lines indicate hydrogen bonds.

2-(1*H*-Benzotriazol-1-yl)acetohydrazide

Crystal data

$C_8H_9N_5O$
$M_r = 191.20$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.1434\ (9)$ Å
$b = 6.5885\ (12)$ Å
$c = 25.754\ (5)$ Å
$\beta = 94.227\ (3)°$
$V = 870.4\ (3)$ Å^3
$Z = 4$
$F(000) = 400$
$D_x = 1.459$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2593 reflections
$\theta = 2.4–28.0°$
$\mu = 0.11$ mm^{-1}
$T = 295$ K
Block, colorless
0.12 × 0.10 × 0.06 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.988$, $T_{max} = 0.994$
4367 measured reflections
1528 independent reflections
1364 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.2°$
$h = -4\rightarrow6$
$k = -7\rightarrow7$
$l = -28\rightarrow30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.04$
1528 reflections
135 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 0.233P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.08675 (16)	0.24854 (14)	0.01128 (4)	0.0432 (3)
N1	1.3431 (2)	0.14371 (19)	0.16751 (5)	0.0505 (3)
N2	1.2038 (2)	0.05513 (19)	0.12958 (5)	0.0496 (3)
N3	0.9953 (2)	0.17411 (18)	0.11547 (4)	0.0422 (3)
N4	0.65313 (19)	0.25384 (17)	−0.00905 (4)	0.0419 (3)
H1	0.5024	0.2240	0.0012	0.050*
N5	0.6667 (2)	0.3428 (2)	−0.05866 (5)	0.0503 (3)
C1	1.2246 (2)	0.3253 (2)	0.17817 (5)	0.0406 (3)
C2	1.2914 (3)	0.4759 (2)	0.21540 (5)	0.0496 (4)
H2	1.4385	0.4637	0.2384	0.060*
C3	1.1312 (3)	0.6408 (2)	0.21632 (6)	0.0537 (4)
H3	1.1698	0.7424	0.2407	0.064*
C4	0.9094 (3)	0.6612 (2)	0.18138 (6)	0.0534 (4)
H4	0.8067	0.7768	0.1832	0.064*
C5	0.8397 (3)	0.5166 (2)	0.14492 (5)	0.0466 (3)
H5	0.6933	0.5306	0.1218	0.056*
C6	1.0018 (2)	0.3468 (2)	0.14460 (5)	0.0377 (3)
C7	0.8079 (3)	0.1139 (2)	0.07360 (5)	0.0460 (3)
H7A	0.6341	0.1507	0.0825	0.055*
H7B	0.8133	−0.0323	0.0695	0.055*
C8	0.8630 (2)	0.21429 (19)	0.02251 (5)	0.0356 (3)
H9	0.723 (3)	0.250 (2)	−0.0799 (6)	0.073 (6)*
H8	0.785 (3)	0.441 (2)	−0.0551 (8)	0.078 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0277 (5)	0.0555 (6)	0.0466 (5)	−0.0038 (4)	0.0045 (4)	−0.0023 (4)
N1	0.0450 (7)	0.0599 (8)	0.0460 (7)	0.0030 (6)	−0.0010 (5)	0.0029 (6)
N2	0.0472 (7)	0.0518 (7)	0.0500 (7)	0.0030 (6)	0.0051 (5)	0.0005 (6)
N3	0.0399 (6)	0.0508 (7)	0.0358 (6)	−0.0038 (5)	0.0024 (5)	−0.0031 (5)
N4	0.0272 (5)	0.0526 (7)	0.0457 (6)	−0.0030 (5)	0.0021 (4)	−0.0043 (5)

N5	0.0434 (7)	0.0582 (8)	0.0483 (7)	0.0013 (6)	−0.0040 (6)	0.0003 (6)
C1	0.0351 (7)	0.0530 (8)	0.0342 (7)	−0.0047 (6)	0.0054 (5)	0.0039 (6)
C2	0.0394 (7)	0.0720 (10)	0.0372 (7)	−0.0136 (7)	0.0009 (6)	−0.0029 (7)
C3	0.0515 (9)	0.0611 (10)	0.0497 (9)	−0.0159 (7)	0.0114 (7)	−0.0143 (7)
C4	0.0499 (9)	0.0521 (9)	0.0598 (9)	−0.0013 (7)	0.0145 (7)	−0.0043 (7)
C5	0.0382 (7)	0.0574 (9)	0.0441 (8)	−0.0003 (6)	0.0025 (6)	0.0020 (7)
C6	0.0346 (7)	0.0484 (8)	0.0303 (6)	−0.0061 (6)	0.0053 (5)	0.0010 (6)
C7	0.0387 (7)	0.0582 (9)	0.0412 (7)	−0.0125 (6)	0.0044 (6)	−0.0072 (6)
C8	0.0292 (6)	0.0384 (7)	0.0392 (7)	−0.0035 (5)	0.0027 (5)	−0.0110 (5)

Geometric parameters (Å, º)

O1—C8	1.2280 (14)	C1—C2	1.405 (2)
N1—N2	1.3057 (16)	C2—C3	1.365 (2)
N1—C1	1.3795 (19)	C2—H2	0.9300
N2—N3	1.3559 (16)	C3—C4	1.407 (2)
N3—C6	1.3620 (17)	C3—H3	0.9300
N3—C7	1.4478 (16)	C4—C5	1.367 (2)
N4—C8	1.3283 (16)	C4—H4	0.9300
N4—N5	1.4120 (17)	C5—C6	1.3957 (19)
N4—H1	0.8600	C5—H5	0.9300
N5—H9	0.884 (9)	C7—C8	1.5179 (18)
N5—H8	0.888 (9)	C7—H7A	0.9700
C1—C6	1.3909 (18)	C7—H7B	0.9700
N2—N1—C1	108.09 (11)	C4—C3—H3	119.1
N1—N2—N3	108.75 (11)	C5—C4—C3	122.15 (14)
N2—N3—C6	110.41 (10)	C5—C4—H4	118.9
N2—N3—C7	120.74 (12)	C3—C4—H4	118.9
C6—N3—C7	128.83 (12)	C4—C5—C6	115.87 (13)
C8—N4—N5	122.88 (10)	C4—C5—H5	122.1
C8—N4—H1	118.6	C6—C5—H5	122.1
N5—N4—H1	118.6	N3—C6—C1	104.05 (11)
N4—N5—H9	108.2 (12)	N3—C6—C5	133.05 (12)
N4—N5—H8	106.8 (13)	C1—C6—C5	122.90 (12)
H9—N5—H8	108.4 (17)	N3—C7—C8	111.69 (10)
N1—C1—C6	108.69 (12)	N3—C7—H7A	109.3
N1—C1—C2	131.22 (13)	C8—C7—H7A	109.3
C6—C1—C2	120.08 (13)	N3—C7—H7B	109.3
C3—C2—C1	117.16 (13)	C8—C7—H7B	109.3
C3—C2—H2	121.4	H7A—C7—H7B	107.9
C1—C2—H2	121.4	O1—C8—N4	123.60 (12)
C2—C3—C4	121.83 (14)	O1—C8—C7	121.49 (11)
C2—C3—H3	119.1	N4—C8—C7	114.87 (10)
C1—N1—N2—N3	−0.50 (14)	C7—N3—C6—C5	0.5 (2)
N1—N2—N3—C6	0.98 (15)	N1—C1—C6—N3	0.71 (13)
N1—N2—N3—C7	179.30 (11)	C2—C1—C6—N3	−178.58 (12)

N2—N1—C1—C6	−0.15 (14)	N1—C1—C6—C5	−179.03 (12)
N2—N1—C1—C2	179.04 (14)	C2—C1—C6—C5	1.68 (19)
N1—C1—C2—C3	−179.77 (14)	C4—C5—C6—N3	178.92 (13)
C6—C1—C2—C3	−0.66 (19)	C4—C5—C6—C1	−1.43 (19)
C1—C2—C3—C4	−0.5 (2)	N2—N3—C7—C8	−97.25 (14)
C2—C3—C4—C5	0.7 (2)	C6—N3—C7—C8	80.72 (16)
C3—C4—C5—C6	0.2 (2)	N5—N4—C8—O1	−1.0 (2)
N2—N3—C6—C1	−1.02 (13)	N5—N4—C8—C7	−178.60 (12)
C7—N3—C6—C1	−179.17 (12)	N3—C7—C8—O1	34.61 (18)
N2—N3—C6—C5	178.67 (14)	N3—C7—C8—N4	−147.76 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H1···O1^{i}	0.86	2.18	2.9977 (14)	159

Symmetry code: (i) *x*−1, *y*, *z*.