Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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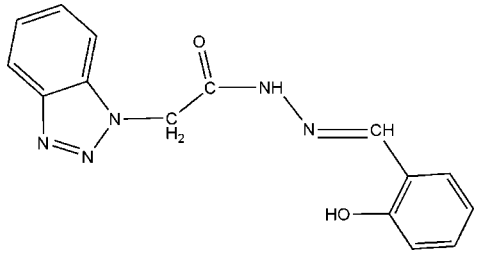
Received 5 November 2007; accepted 6 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.045; wR factor = 0.095; data-to-parameter ratio = 6.4.

The title compound, $C_{15}H_{13}N_5O_2$, was synthesized by the reaction of 2-(1*H*-benzotriazol-1-yl)acetohydrazide with 2-hydroxybenzaldehyde. In the crystal structure, molecules are linked into infinite chains by N—H···N hydrogen bonds. There is also an intramolecular O—H···N hydrogen bond.

Related literature

For related literature, see: Allen *et al.* (1987); Anderson *et al.* (1997); Garnovski *et al.* (1993); Musie *et al.* (2001); Paul *et al.* (2002); Xu *et al.* (2002); Yang (2006).



Experimental

Crystal data

$C_{15}H_{13}N_5O_2$
M_r = 295.30
Monoclinic, *Pc*
a = 10.644 (3) Å
b = 4.4834 (12) Å
c = 15.807 (4) Å
β = 105.672 (6)°
V = 726.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.987, T_{max} = 0.991
3578 measured reflections
1291 independent reflections
752 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.095
S = 1.00
1291 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 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
N2—H2···N5^{i}	0.86	2.07	2.927 (5)	172
O1—H1···N1	0.82	1.92	2.638 (6)	145

Symmetry code: (i) $x, -y-1, z-\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This project was supported by the Postgraduate Foundation of Taishan University (No. Y04–2-08).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2170).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, S1–19.
Anderson, O. P., Cour, A. L., Findeisen, M., Hennig, L., Simonsen, O., Taylor, L. & Toflund, H. (1997). *J. Chem. Soc. Dalton Trans.* pp. 111–120.
Garnovski, A. D., Nivorozhkin, A. L. & Minki, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Musie, G. T., Wei, M., Subramaniam, B. & Busch, D. H. (2001). *Inorg. Chem.* **40**, 3336–3341.
Paul, S., Barik, A. K., Peng, S. M. & Kar, S. K. (2002). *Inorg. Chem.* **41**, 5803–5809.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Xu, L.-Z., Zhang, S.-S., Li, H.-J. & Jiao, K. (2002). *Chem. Res. Chin. Univ.*, **18**, 284–286.
Yang, D.-S. (2006). *Acta Cryst.* E**62**, o1591–o1592.

  doi:10.1107/S1600536807056206

supplementary materials

Acta Cryst. (2007). E**63**, o4642 [**doi:10.1107/S1600536807056206**]

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

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Comment

Recently, a number of Schiff bases have been investigated in terms of their coordination chemistry (Garnovski *et al.*, 1993; Musie *et al.*, 2001; Paul *et al.*, 2002; Yang, 2006) and biological applications (Anderson *et al.*, 1997). Schiff bases containing the triazole group have attracted much interest because their potential bioactivities (Xu *et al.*, 2002). In order to search for new triazole compounds with higher bioactivity, the title compound, (I), was synthesized and its crystal structure determined. In (I) (Fig. 1), the bond lengths are in good agreement with the expected values (Allen *et al.*, 1987). The dihedral angle formed by the triazole ring and the 2-hydroxybenzylidene group is 78.99 (2)°. In the crystal structure (Fig. 2), the molecules are linked into infinite chains by N—H···N hydrogen bonds. There is also an intramolecular O—H···N hydrogen bond.

Experimental

The title compound was synthesized by the reaction of 2-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)acetohydrazide (1 mmol, 191.2 mg) with 2-hydroxybenzaldehyde (1 mmol, 122.1 mg) in ethanol (20 ml) under reflux conditions (348 K) for 2 h. The solvent was removed and the solid product recrystallized from tetrahydrofuran. After five days colorless crystals suitable for X-ray diffraction study were obtained. Yield, 248.1 mg, 84%. m.p. 239–241 K.

Analysis calculated for $C_{15}H_{13}N_5O_2$: C 61.01, H 4.44, N 23.72%; found: C 60.58, H 4.48, N 23.68%.

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). In the absence of significant anomalous scattering, Friedel pairs were merged.

Figures

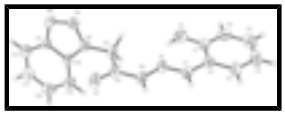

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

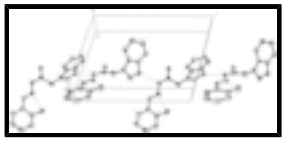

Fig. 2. The structure of the infinite chains formed *via* hydrogen bonds (dashed lines). H atoms have been omitted for clarity.

2-(1*H*-Benzotriazol-1-yl)-*N*′-(2-hydroxybenzylidene)acetohydrazide

Crystal data

$C_{15}H_{13}N_5O_2$	F_{000} = 308
M_r = 295.30	D_x = 1.350 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 328 reflections
a = 10.644 (3) Å	θ = 2.9–15.7º
b = 4.4834 (12) Å	μ = 0.10 mm^{-1}
c = 15.807 (4) Å	*T* = 298 (2) K
β = 105.672 (6)º	Block, colorless
V = 726.3 (3) Å^3	0.14 × 0.12 × 0.10 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	1291 independent reflections
Radiation source: fine-focus sealed tube	752 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 298(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −12→12
T_{min} = 0.987, T_{max} = 0.991	*k* = −5→5
3578 measured reflections	*l* = −18→17

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.095	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
1291 reflections	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
201 parameters	Extinction coefficient: 0.016 (3)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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	1.2445 (4)	0.3630 (10)	0.8367 (3)	0.0847 (14)
H1	1.1824	0.2477	0.8248	0.127*
O2	0.8341 (4)	−0.4778 (9)	0.7704 (2)	0.0702 (12)
N1	1.0742 (4)	−0.0033 (9)	0.7359 (3)	0.0506 (12)
N2	0.9753 (4)	−0.2095 (9)	0.7182 (2)	0.0543 (12)
H2	0.9487	−0.2873	0.6667	0.065*
N3	0.9099 (4)	−0.2348 (9)	0.9340 (3)	0.0538 (12)
N4	0.9687 (4)	−0.4372 (10)	0.9947 (3)	0.0570 (12)
N5	0.8977 (4)	−0.4742 (10)	1.0501 (3)	0.0555 (12)
C1	1.2886 (6)	0.4036 (12)	0.7645 (4)	0.0625 (16)
C2	1.2334 (5)	0.2633 (11)	0.6851 (4)	0.0532 (14)
C3	1.2857 (6)	0.3228 (14)	0.6156 (4)	0.078 (2)
H3	1.2493	0.2328	0.5616	0.093*
C4	1.3899 (7)	0.5109 (15)	0.6246 (6)	0.091 (2)
H4	1.4241	0.5459	0.5773	0.109*
C5	1.4441 (7)	0.6491 (15)	0.7048 (6)	0.097 (2)
H5	1.5152	0.7761	0.7114	0.117*
C6	1.3929 (7)	0.5985 (14)	0.7742 (5)	0.088 (2)
H6	1.4279	0.6943	0.8276	0.105*
C7	1.1280 (5)	0.0542 (11)	0.6743 (3)	0.0509 (14)
H7	1.0977	−0.0431	0.6207	0.061*
C8	0.9199 (6)	−0.2896 (12)	0.7823 (3)	0.0515 (14)
C9	0.9742 (6)	−0.1365 (12)	0.8690 (3)	0.0614 (16)
H9A	1.0668	−0.1778	0.8900	0.074*
H9B	0.9633	0.0774	0.8610	0.074*
C10	0.7975 (5)	−0.1396 (11)	0.9496 (3)	0.0489 (14)
C11	0.7912 (5)	−0.2888 (12)	1.0249 (3)	0.0498 (14)
C12	0.6873 (6)	−0.2467 (13)	1.0622 (4)	0.0640 (16)
H12	0.6822	−0.3468	1.1127	0.077*
C13	0.5944 (6)	−0.0500 (14)	1.0198 (4)	0.0745 (18)
H13	0.5244	−0.0122	1.0430	0.089*
C14	0.5995 (6)	0.0970 (13)	0.9435 (4)	0.0768 (19)
H14	0.5313	0.2234	0.9161	0.092*

C15	0.7021 (6)	0.0612 (12)	0.9073 (4)	0.0648 (16)
H15	0.7073	0.1653	0.8575	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.101 (4)	0.080 (3)	0.066 (3)	−0.025 (3)	0.011 (3)	−0.002 (2)
O2	0.089 (3)	0.069 (3)	0.058 (2)	−0.032 (2)	0.029 (2)	−0.011 (2)
N1	0.062 (3)	0.042 (3)	0.052 (3)	−0.008 (2)	0.023 (2)	−0.001 (2)
N2	0.070 (3)	0.055 (3)	0.043 (3)	−0.013 (3)	0.023 (3)	−0.004 (2)
N3	0.064 (3)	0.058 (3)	0.042 (3)	−0.006 (3)	0.019 (2)	0.003 (2)
N4	0.060 (3)	0.062 (3)	0.051 (3)	−0.002 (2)	0.018 (3)	0.000 (2)
N5	0.066 (3)	0.060 (3)	0.042 (3)	0.000 (3)	0.018 (2)	0.007 (2)
C1	0.064 (4)	0.050 (4)	0.072 (5)	−0.003 (3)	0.016 (4)	0.010 (4)
C2	0.054 (4)	0.043 (3)	0.065 (4)	0.003 (3)	0.021 (3)	0.009 (3)
C3	0.067 (4)	0.079 (5)	0.099 (5)	0.003 (4)	0.043 (4)	0.019 (4)
C4	0.085 (6)	0.074 (5)	0.132 (7)	−0.004 (4)	0.059 (5)	0.024 (5)
C5	0.070 (5)	0.067 (5)	0.154 (8)	−0.007 (4)	0.029 (6)	0.026 (6)
C6	0.079 (5)	0.066 (5)	0.103 (6)	−0.015 (4)	−0.004 (4)	0.027 (4)
C7	0.063 (4)	0.046 (3)	0.047 (3)	0.004 (3)	0.021 (3)	0.002 (3)
C8	0.074 (4)	0.042 (3)	0.041 (3)	−0.012 (3)	0.021 (3)	−0.006 (3)
C9	0.083 (4)	0.058 (4)	0.053 (4)	−0.018 (3)	0.036 (3)	−0.002 (3)
C10	0.066 (4)	0.044 (3)	0.036 (3)	−0.009 (3)	0.012 (3)	−0.004 (3)
C11	0.056 (4)	0.049 (4)	0.044 (3)	−0.002 (3)	0.012 (3)	0.002 (3)
C12	0.073 (4)	0.063 (4)	0.062 (4)	−0.004 (4)	0.027 (3)	−0.002 (4)
C13	0.080 (5)	0.068 (5)	0.078 (4)	0.000 (4)	0.025 (4)	−0.006 (4)
C14	0.073 (5)	0.063 (5)	0.085 (5)	0.014 (4)	0.005 (4)	0.002 (4)
C15	0.088 (5)	0.043 (3)	0.058 (4)	−0.007 (3)	0.009 (4)	0.004 (3)

Geometric parameters (Å, °)

O1—C1	1.358 (6)	C4—H4	0.930
O1—H1	0.820	C5—C6	1.369 (9)
O2—C8	1.220 (6)	C5—H5	0.930
N1—C7	1.282 (6)	C6—H6	0.930
N1—N2	1.372 (5)	C7—H7	0.930
N2—C8	1.351 (6)	C8—C9	1.502 (7)
N2—H2	0.860	C9—H9A	0.970
N3—N4	1.345 (6)	C9—H9B	0.970
N3—C10	1.354 (6)	C10—C11	1.382 (6)
N3—C9	1.449 (5)	C10—C15	1.387 (7)
N4—N5	1.312 (5)	C11—C12	1.400 (7)
N5—C11	1.375 (6)	C12—C13	1.359 (7)
C1—C2	1.385 (7)	C12—H12	0.930
C1—C6	1.389 (7)	C13—C14	1.389 (8)
C2—C3	1.385 (7)	C13—H13	0.930
C2—C7	1.436 (7)	C14—C15	1.373 (8)
C3—C4	1.369 (8)	C14—H14	0.930
C3—H3	0.930	C15—H15	0.930

C4—C5	1.389 (9)		
C1—O1—H1	109.5	N1—C7—H7	118.8
C7—N1—N2	117.1 (4)	C2—C7—H7	118.8
C8—N2—N1	119.5 (4)	O2—C8—N2	121.9 (5)
C8—N2—H2	120.3	O2—C8—C9	123.0 (5)
N1—N2—H2	120.3	N2—C8—C9	115.1 (5)
N4—N3—C10	110.3 (4)	N3—C9—C8	111.7 (4)
N4—N3—C9	119.6 (5)	N3—C9—H9A	109.3
C10—N3—C9	130.0 (5)	C8—C9—H9A	109.3
N5—N4—N3	108.7 (4)	N3—C9—H9B	109.3
N4—N5—C11	107.9 (4)	C8—C9—H9B	109.3
O1—C1—C2	122.8 (5)	H9A—C9—H9B	107.9
O1—C1—C6	116.1 (6)	N3—C10—C11	104.8 (4)
C2—C1—C6	121.1 (6)	N3—C10—C15	133.2 (5)
C1—C2—C3	117.9 (6)	C11—C10—C15	122.0 (5)
C1—C2—C7	122.1 (5)	N5—C11—C10	108.3 (4)
C3—C2—C7	120.0 (6)	N5—C11—C12	130.0 (5)
C4—C3—C2	121.6 (7)	C10—C11—C12	121.7 (5)
C4—C3—H3	119.2	C13—C12—C11	115.6 (5)
C2—C3—H3	119.2	C13—C12—H12	122.2
C3—C4—C5	119.6 (7)	C11—C12—H12	122.2
C3—C4—H4	120.2	C12—C13—C14	122.9 (6)
C5—C4—H4	120.2	C12—C13—H13	118.6
C6—C5—C4	120.0 (7)	C14—C13—H13	118.6
C6—C5—H5	120.0	C15—C14—C13	121.9 (6)
C4—C5—H5	120.0	C15—C14—H14	119.0
C5—C6—C1	119.7 (7)	C13—C14—H14	119.0
C5—C6—H6	120.2	C14—C15—C10	115.9 (5)
C1—C6—H6	120.2	C14—C15—H15	122.1
N1—C7—C2	122.4 (5)	C10—C15—H15	122.1
C7—N1—N2—C8	176.6 (5)	C10—N3—C9—C8	−84.5 (6)
C10—N3—N4—N5	−0.6 (5)	O2—C8—C9—N3	−1.5 (8)
C9—N3—N4—N5	175.2 (4)	N2—C8—C9—N3	−179.9 (5)
N3—N4—N5—C11	−0.5 (6)	N4—N3—C10—C11	1.5 (5)
O1—C1—C2—C3	179.5 (6)	C9—N3—C10—C11	−173.8 (5)
C6—C1—C2—C3	0.3 (8)	N4—N3—C10—C15	−179.4 (5)
O1—C1—C2—C7	−2.6 (8)	C9—N3—C10—C15	5.4 (8)
C6—C1—C2—C7	178.1 (5)	N4—N5—C11—C10	1.4 (6)
C1—C2—C3—C4	0.8 (9)	N4—N5—C11—C12	179.8 (5)
C7—C2—C3—C4	−177.1 (5)	N3—C10—C11—N5	−1.8 (5)
C2—C3—C4—C5	−0.7 (10)	C15—C10—C11—N5	179.0 (5)
C3—C4—C5—C6	−0.4 (10)	N3—C10—C11—C12	179.7 (5)
C4—C5—C6—C1	1.4 (10)	C15—C10—C11—C12	0.4 (7)
O1—C1—C6—C5	179.3 (6)	N5—C11—C12—C13	−178.4 (5)
C2—C1—C6—C5	−1.4 (9)	C10—C11—C12—C13	−0.2 (8)
N2—N1—C7—C2	−179.3 (4)	C11—C12—C13—C14	1.2 (9)
C1—C2—C7—N1	3.8 (8)	C12—C13—C14—C15	−2.5 (10)
C3—C2—C7—N1	−178.3 (5)	C13—C14—C15—C10	2.5 (8)

N1—N2—C8—O2	−178.0 (5)	N3—C10—C15—C14	179.4 (5)
N1—N2—C8—C9	0.4 (7)	C11—C10—C15—C14	−1.5 (7)
N4—N3—C9—C8	100.7 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N5^{i}	0.86	2.07	2.927 (5)	172
O1—H1···N1	0.82	1.92	2.638 (6)	145

Symmetry codes: (i) *x*, −*y*−1, *z*−1/2.

Fig. 1

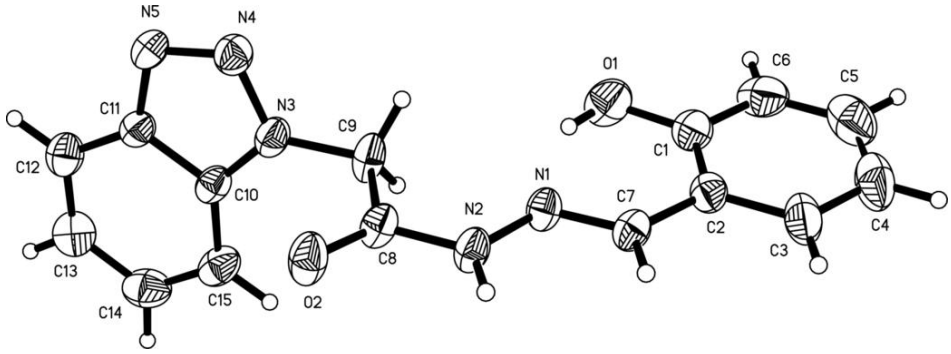
N5
N4
C11
N3
C9
C12
C10
C13
C14
C15
O2
C8
N2
N1
C7
O1
C6
C5
C1
C2
C3
C4

Fig. 2