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3-Bromo-*N*′-(2-hydroxybenzylidene)-benzohydrazide

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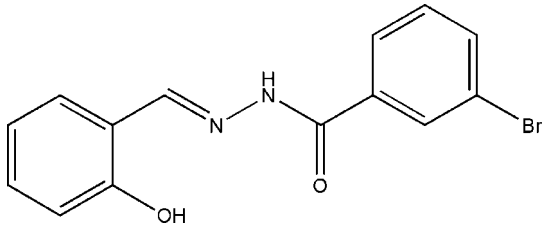
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 17.2.

The title molecule, $C_{14}H_{11}BrN_2O_2$, displays a *trans* configuration about the C=N and C—N bonds. The dihedral angle between the two benzene rings is 18.5 (3)°. An intramolecular O—H···N hydrogen bond is observed. In the crystal structure, the molecules are linked into a chain along the *c* axis by N—H···O and C—H···O hydrogen bonds.

Related literature

For related literature, see: Ali *et al.* (2002); Allen *et al.* (1987); Cukurovali *et al.* (2002); Li (2007*a*,*b*); Qian *et al.* (2006); Qiu *et al.* (2006); Tarafder *et al.* (2002); Yang (2006); Yang & Guo (2006); Zhao (2006).



Experimental

Crystal data

$C_{14}H_{11}BrN_2O_2$
M_r = 319.16
Monoclinic, $P2_1/c$
a = 10.9397 (17) Å
b = 13.672 (2) Å
c = 8.8915 (14) Å
β = 95.882 (2)°
V = 1322.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.11 mm^{-1}
T = 298 (2) K
0.32 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.436, T_{max} = 0.456
(expected range = 0.377–0.394)
7853 measured reflections
3029 independent reflections
1997 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.03
3029 reflections
176 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.93	2.639 (3)	145
N2—H2···O2^{i}	0.89 (1)	1.934 (15)	2.806 (3)	165 (4)
C7—H7···O2^{i}	0.93	2.45	3.206 (3)	139

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: CI2553).

References

Ali, M. A., Mirza, A. H., Butcher, R. J., Tarafder, M. T. H., Keat, T. B. & Ali, A. M. (2002). *J. Inorg. Biochem.* **92**, 141–148.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Cukurovali, A., Yilmaz, I., Özmen, H. & Ahmedzade, M. (2002). *Transition Met. Chem.* **27**, 171–176.
Li, H.-B. (2007*a*). *Acta Cryst.* E**63**, o972–o973.
Li, H.-B. (2007*b*). *Acta Cryst.* E**63**, o4246.
Qian, H.-Y., Yin, Z.-G., Jia, J., Liu, S.-M. & Feng, L.-Q. (2006). *Acta Cryst.* E**62**, o3623–o3624.
Qiu, X.-Y., Fang, X.-N., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2685–o2686.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tarafder, M. T. H., Jin, K. T., Crouse, K. A., Ali, A. M., Yamin, B. M. & Fun, H.-K. (2002). *Polyhedron*, **21**, 2547–2554.
Yang, D.-S. (2006). *Acta Cryst.* E**62**, o3792–o3793.
Yang, D.-S. & Guo, J.-B. (2006). *Acta Cryst.* E**62**, o4414–o4415.
Zhao, L.-F. (2006). *Acta Cryst.* E**62**, o3970–o3971.

supplementary materials

Acta Cryst. (2008). E**64**, o465 [**doi:10.1107/S1600536808001293**]

3-Bromo-*N*'-(2-hydroxybenzylidene)benzohydrazide

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Comment

The compounds derived from the condensation reaction of aromatic carbaldehydes with hydrazides exhibit a wide range of biological activities and applications (Tarafder *et al.*, 2002; Cukurovali *et al.*, 2002; Ali *et al.*, 2002). Herein the author reports the crystal structure of the title compound.

The bond lengths and bond angles in the title molecule (Fig. 1) are within normal ranges (Allen *et al.*, 1987) and comprable with those observed in similar compounds(Qiu *et al.*, 2006; Yang and Guo, 2006; Yang, 2006). The C7═N1 double bond length of 1.284 (3) Å is comparable with that in other Schiff bases (Li, 2007*b*; Qian *et al.*, 2006; Zhao, 2006). The C8—N2 bond length of 1.348 (3) Å is intermediate between a C–N single bond and a C═N double bond, because of conjugation. The dihedral angle between the C1—C6 and C9—C14 benzene rings is 18.5 (3)°. The molecule adopts a *trans* configuration about the C7═N1 and C8–N2 bonds.

There is an intramolecular O1—H1···N1 hydrogen bond (Table 1) in the title molecule, as observed in a similar compound (Li, 2007*a*). In the crystal structure, the molecules are linked into a chain along the *c* axis by N—H···O and C—H···O hydrogen bonds (Table 2 and Fig.2).

Experimental

Salicylaldehyde (0.1 mmol, 12.2 mg) and 3-bromobenzoic acid hydrazide (0.1 mmol, 21.5 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. Crystals of the title compound were formed by gradual evaporation of the solvent over 12 d at room temperature (yield 71.2%). Analysis found: C 52.45, H 3.53, N 8.86%; calculated for $C_{14}H_{11}BrN_2O_2$: C 52.69, H 3.47, N 8.78%.

Refinement

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The remaining H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å, O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Figures

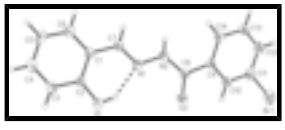

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates an intramolecular hydrogen bond.

Fig. 2. The crystal packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

3-Bromo-*N*'-(2-hydroxybenzylidene)benzohydrazide

Crystal data

$C_{14}H_{11}BrN_2O_2$	$F_{000} = 640$
$M_r = 319.16$	$D_x = 1.603$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2541 reflections
$a = 10.9397$ (17) Å	$\theta = 2.3$–25.8º
$b = 13.672$ (2) Å	$\mu = 3.11$ mm^{-1}
$c = 8.8915$ (14) Å	$T = 298$ (2) K
$\beta = 95.882$ (2)º	Block, yellow
$V = 1322.8$ (4) Å^3	0.32 × 0.30 × 0.30 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3029 independent reflections
Radiation source: fine-focus sealed tube	1997 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 298$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14 \rightarrow 11$
$T_{min} = 0.436$, $T_{max} = 0.456$	$k = -17 \rightarrow 17$
7853 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.8938P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3029 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
176 parameters	$\Delta\rho_{min} = -0.76$ e Å^{-3}
1 restraint	Extinction correction: none

Primary atom site location: structure-invariant direct methods

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}
Br1	0.84586 (4)	0.69664 (2)	0.07515 (6)	0.07832 (19)
O1	0.5849 (2)	0.09555 (15)	−0.3004 (2)	0.0534 (5)
H1	0.6305	0.1342	−0.2516	0.080*
O2	0.7840 (2)	0.33361 (14)	−0.1658 (2)	0.0481 (5)
N1	0.7189 (2)	0.16000 (16)	−0.0568 (2)	0.0389 (5)
N2	0.7749 (2)	0.23255 (16)	0.0345 (3)	0.0405 (5)
C1	0.6433 (2)	−0.00290 (19)	−0.0791 (3)	0.0368 (6)
C2	0.5861 (3)	0.0088 (2)	−0.2268 (3)	0.0409 (6)
C3	0.5269 (3)	−0.0700 (2)	−0.3001 (4)	0.0538 (8)
H3	0.4882	−0.0620	−0.3974	0.065*
C4	0.5246 (3)	−0.1593 (2)	−0.2315 (4)	0.0587 (9)
H4	0.4853	−0.2116	−0.2831	0.070*
C5	0.5801 (3)	−0.1726 (2)	−0.0866 (4)	0.0567 (9)
H5	0.5784	−0.2336	−0.0405	0.068*
C6	0.6378 (3)	−0.0954 (2)	−0.0110 (4)	0.0491 (7)
H6	0.6740	−0.1043	0.0873	0.059*
C7	0.7039 (3)	0.07677 (19)	0.0056 (3)	0.0398 (6)
H7	0.7325	0.0676	0.1067	0.048*
C8	0.8024 (3)	0.31817 (18)	−0.0293 (3)	0.0365 (6)
C9	0.8582 (2)	0.39488 (19)	0.0755 (3)	0.0359 (6)
C10	0.8331 (3)	0.4917 (2)	0.0361 (3)	0.0416 (7)
H10	0.7829	0.5067	−0.0518	0.050*
C11	0.8834 (3)	0.5656 (2)	0.1290 (4)	0.0474 (7)
C12	0.9601 (3)	0.5450 (2)	0.2575 (4)	0.0552 (8)
H12	0.9943	0.5954	0.3184	0.066*
C13	0.9855 (3)	0.4493 (2)	0.2948 (3)	0.0572 (9)
H13	1.0377	0.4349	0.3811	0.069*
C14	0.9343 (3)	0.3738 (2)	0.2055 (3)	0.0468 (7)
H14	0.9509	0.3091	0.2329	0.056*
H2	0.778 (4)	0.223 (3)	0.1343 (14)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0724 (3)	0.03681 (19)	0.1239 (4)	0.00291 (16)	0.0012 (2)	−0.01230 (19)
O1	0.0719 (16)	0.0428 (11)	0.0428 (12)	−0.0081 (10)	−0.0072 (10)	0.0057 (9)
O2	0.0717 (14)	0.0422 (10)	0.0285 (11)	−0.0023 (10)	−0.0047 (9)	−0.0005 (8)
N1	0.0472 (14)	0.0350 (11)	0.0338 (12)	−0.0024 (10)	0.0004 (10)	−0.0045 (10)
N2	0.0559 (15)	0.0350 (11)	0.0292 (12)	−0.0041 (11)	−0.0022 (11)	−0.0036 (10)
C1	0.0382 (15)	0.0318 (13)	0.0409 (15)	0.0024 (11)	0.0057 (12)	−0.0011 (11)
C2	0.0441 (16)	0.0392 (14)	0.0397 (16)	−0.0023 (12)	0.0052 (12)	−0.0023 (12)
C3	0.060 (2)	0.0524 (18)	0.0481 (18)	−0.0130 (15)	−0.0005 (15)	−0.0042 (14)
C4	0.060 (2)	0.0435 (16)	0.073 (2)	−0.0143 (15)	0.0066 (18)	−0.0148 (16)
C5	0.060 (2)	0.0345 (15)	0.076 (2)	−0.0035 (14)	0.0107 (18)	0.0042 (15)
C6	0.0550 (18)	0.0398 (15)	0.0517 (18)	0.0034 (13)	0.0019 (14)	0.0053 (13)
C7	0.0452 (16)	0.0388 (14)	0.0342 (15)	0.0032 (12)	−0.0013 (12)	−0.0013 (11)
C8	0.0428 (16)	0.0359 (14)	0.0301 (15)	0.0035 (11)	0.0008 (11)	−0.0004 (11)
C9	0.0397 (15)	0.0373 (14)	0.0304 (14)	−0.0036 (11)	0.0028 (11)	−0.0023 (11)
C10	0.0437 (16)	0.0390 (15)	0.0410 (16)	−0.0004 (12)	−0.0012 (12)	−0.0042 (12)
C11	0.0468 (17)	0.0357 (14)	0.061 (2)	−0.0029 (12)	0.0098 (15)	−0.0069 (13)
C12	0.063 (2)	0.0560 (19)	0.0470 (19)	−0.0200 (16)	0.0056 (16)	−0.0149 (15)
C13	0.066 (2)	0.067 (2)	0.0364 (17)	−0.0203 (17)	−0.0083 (15)	0.0003 (15)
C14	0.0564 (19)	0.0464 (16)	0.0358 (16)	−0.0079 (14)	−0.0036 (14)	0.0043 (12)

Geometric parameters (Å, °)

Br1—C11	1.889 (3)	C5—C6	1.371 (4)
O1—C2	1.354 (3)	C5—H5	0.93
O1—H1	0.82	C6—H6	0.93
O2—C8	1.228 (3)	C7—H7	0.93
N1—C7	1.284 (3)	C8—C9	1.491 (4)
N1—N2	1.384 (3)	C9—C14	1.384 (4)
N2—C8	1.348 (3)	C9—C10	1.390 (4)
N2—H2	0.89 (1)	C10—C11	1.383 (4)
C1—C2	1.404 (4)	C10—H10	0.93
C1—C6	1.406 (4)	C11—C12	1.376 (5)
C1—C7	1.446 (4)	C12—C13	1.372 (5)
C2—C3	1.385 (4)	C12—H12	0.93
C3—C4	1.367 (5)	C13—C14	1.385 (4)
C3—H3	0.93	C13—H13	0.93
C4—C5	1.379 (5)	C14—H14	0.93
C4—H4	0.93		
C2—O1—H1	109.5	N1—C7—H7	119.5
C7—N1—N2	116.7 (2)	C1—C7—H7	119.5
C8—N2—N1	118.6 (2)	O2—C8—N2	123.0 (2)
C8—N2—H2	124 (3)	O2—C8—C9	120.8 (2)
N1—N2—H2	117 (3)	N2—C8—C9	116.3 (2)
C2—C1—C6	118.1 (3)	C14—C9—C10	119.7 (3)

C2—C1—C7	122.5 (2)	C14—C9—C8	123.2 (2)
C6—C1—C7	119.4 (3)	C10—C9—C8	117.0 (2)
O1—C2—C3	118.2 (3)	C11—C10—C9	119.2 (3)
O1—C2—C1	122.2 (2)	C11—C10—H10	120.4
C3—C2—C1	119.5 (3)	C9—C10—H10	120.4
C4—C3—C2	121.0 (3)	C12—C11—C10	121.3 (3)
C4—C3—H3	119.5	C12—C11—Br1	120.1 (2)
C2—C3—H3	119.5	C10—C11—Br1	118.6 (2)
C3—C4—C5	120.5 (3)	C13—C12—C11	119.1 (3)
C3—C4—H4	119.7	C13—C12—H12	120.5
C5—C4—H4	119.7	C11—C12—H12	120.5
C6—C5—C4	119.5 (3)	C12—C13—C14	120.9 (3)
C6—C5—H5	120.2	C12—C13—H13	119.6
C4—C5—H5	120.2	C14—C13—H13	119.6
C5—C6—C1	121.3 (3)	C9—C14—C13	119.8 (3)
C5—C6—H6	119.3	C9—C14—H14	120.1
C1—C6—H6	119.3	C13—C14—H14	120.1
N1—C7—C1	121.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.93	2.639 (3)	145
N2—H2···O2^{i}	0.89 (1)	1.934 (15)	2.806 (3)	165 (4)
C7—H7···O2^{i}	0.93	2.45	3.206 (3)	139

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

Fig. 1

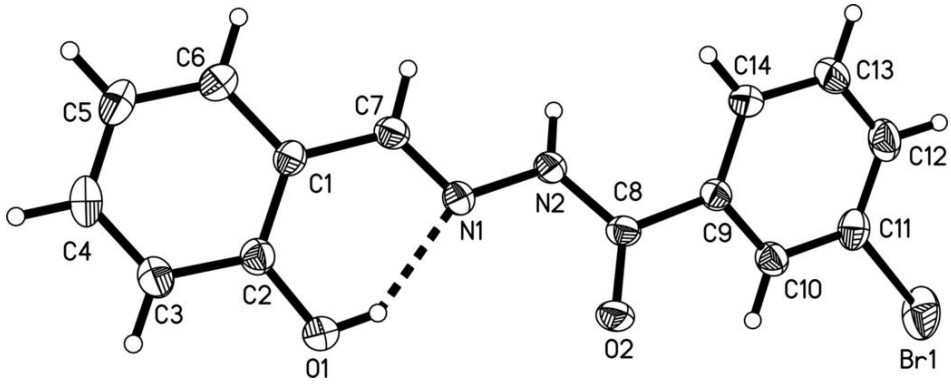

Fig. 2