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(*E*)-*N*′-[1-(4-Bromophenyl)ethylidene]-2-hydroxybenzohydrazide

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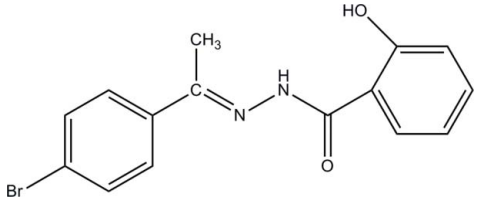
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.111; data-to-parameter ratio = 13.2.

In the title compound, $C_{15}H_{13}BrN_2O_2$, the two aromatic rings form a dihedral angle of 7.9 (1)° and an intramolecular N—H···O hydrogen bond influences the molecular conformation. In the crystal, intermolecular O—H···O hydrogen bonds link the molecules into chains propagated in [001]. The crystal packing exhibits also π–π interactions, which pair molecules into centrosymmetric dimers with short intermolecular distances of 3.671 (4) Å between the centroids of aromatic rings.

Related literature

For the biological properties of Schiff base ligands, see: Jeewoth *et al.* (1999). For related structures, see: Fun *et al.* (2008); Cui *et al.* (2009); Nie (2008).



Experimental

Crystal data

$C_{15}H_{13}BrN_2O_2$
M_r = 333.18
Monoclinic, $C2/c$
a = 27.805 (3) Å
b = 7.9061 (9) Å
c = 13.5002 (15) Å
β = 113.344 (2)°
V = 2724.8 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.02 mm^{-1}
T = 298 K
0.39 × 0.14 × 0.12 mm

Data collection

Siemens SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.386, T_{max} = 0.713
6480 measured reflections
2397 independent reflections
1602 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.111
S = 0.95
2397 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.95	2.637 (3)	136
O2—H2···O1^{i}	0.82	1.86	2.677 (3)	178

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: CV2623).

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supporting information

Acta Cryst. (2009). E**65**, o2792 [https://doi.org/10.1107/S1600536809042081]

(*E*)-*N*′-[1-(4-Bromophenyl)ethylidene]-2-hydroxybenzohydrazide

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S1. Comment

Schiff base compounds have received considerable attention during the last decades due to their structures and biological properties (Jeewoth *et al.*, 1999). We report here the crystal structure of the title Schiff base compound (I).

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to the values observed in similar compounds (Nie, 2008; Fun *et al.*, 2008; Cui *et al.*, 2009). The C9=N2 bond length in the molecule is 1.282 (4) °, showing the double-bond character. The dihedral angle between the benzene ring C2-C7 and the benzene ring C10-C15 is 7.9 (1)°, indicating that two these rings are approximately coplanar.

In the crystal, intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into chains propagated in direction [001]. The crystal packing exhibits also $\pi\cdots\pi$ interactions, which pair molecules into centrosymmetric dimers with short intermolecular distance of 3.671 (4) Å between the centroids of aromatic rings.

S2. Experimental

Salicyloyl hydrazide (5.0 mmol), 20 ml e thanol and 4-bromoacetophenone (5.0 mmol) were mixed in 50 ml flash. After refluxing 3 h, the resulting mixture was cooled to room temperature, and recrystallized from ethanol. Elemental analysis: calculated for $C_{15}H_{13}BrN_2O_2$: C 54.07, H 3.93, N 8.41%; found: C 54.21, H 3.85, N 8.52%.

S3. Refinement

All H atoms were placed in geometrically idealized positions (O—H 0.82, N—H 0.86 and C—H = 0.93–0.96 Å) and treated as riding, with U_{iso}(H) = 1.2U-1.5U_{eq} of the parent atom.

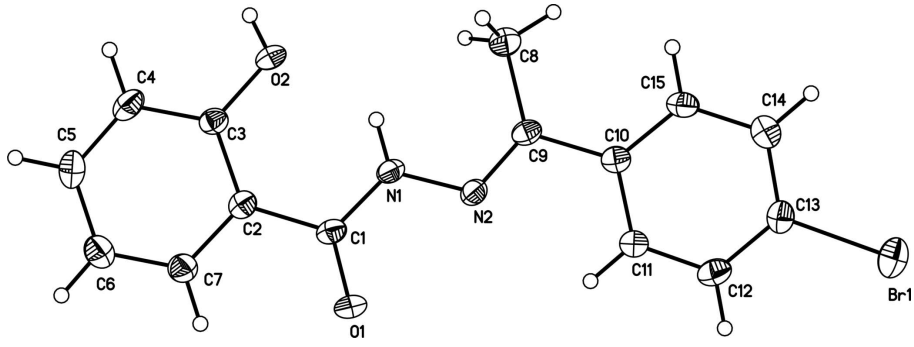

Figure 1

The molecular structure of (I) showing the atomic numbering scheme and 30% probability displacement ellipsoids.

(*E*)-*N*′-[1-(4-Bromophenyl)ethylidene]-2-hydroxybenzohydrazide

Crystal data

$C_{15}H_{13}BrN_2O_2$
$M_r = 333.18$
Monoclinic, $C2/c$
$a = 27.805$ (3) Å
$b = 7.9061$ (9) Å
$c = 13.5002$ (15) Å
$\beta = 113.344$ (2)°
$V = 2724.8$ (5) Å^3
$Z = 8$
$F(000) = 1344$
$D_x = 1.624$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1955 reflections
$\theta = 2.7$–$26.0°$
$\mu = 3.02$ mm^{-1}
$T = 298$ K
Block, colourless
0.39 × 0.14 × 0.12 mm

Data collection

Siemens SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.386$, $T_{max} = 0.713$
6480 measured reflections
2397 independent reflections
1602 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -32 \rightarrow 32$
$k = -5 \rightarrow 9$
$l = -16 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.111$
$S = 0.95$
2397 reflections
181 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ 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}
Br1	1.171700 (16)	1.05278 (6)	1.41157 (3)	0.0585 (2)
N1	0.92749 (11)	0.6137 (4)	0.9225 (2)	0.0342 (8)
H1	0.9291	0.6170	0.8602	0.041*
N2	0.96688 (11)	0.6843 (4)	1.0103 (2)	0.0325 (7)
O1	0.88354 (11)	0.5298 (4)	1.02232 (19)	0.0555 (9)

O2	0.88245 (10)	0.5567 (4)	0.71317 (18)	0.0434 (7)
H2	0.8821	0.5286	0.6545	0.065*
C1	0.88626 (13)	0.5393 (5)	0.9337 (3)	0.0329 (9)
C2	0.84455 (14)	0.4681 (5)	0.8353 (3)	0.0317 (9)
C3	0.84277 (13)	0.4765 (5)	0.7298 (3)	0.0325 (9)
C4	0.80124 (15)	0.4043 (6)	0.6450 (3)	0.0450 (11)
H4	0.7998	0.4127	0.5752	0.054*
C5	0.76224 (15)	0.3206 (6)	0.6629 (3)	0.0467 (11)
H5	0.7347	0.2722	0.6053	0.056*
C6	0.76374 (15)	0.3079 (5)	0.7662 (3)	0.0461 (11)
H6	0.7376	0.2496	0.7787	0.055*
C7	0.80399 (14)	0.3818 (5)	0.8496 (3)	0.0394 (10)
H7	0.8044	0.3744	0.9187	0.047*
C8	1.01117 (15)	0.7562 (6)	0.8889 (3)	0.0453 (11)
H8A	1.0056	0.6454	0.8573	0.068*
H8B	1.0457	0.7943	0.9003	0.068*
H8C	0.9858	0.8331	0.8413	0.068*
C9	1.00561 (13)	0.7498 (5)	0.9952 (2)	0.0314 (9)
C10	1.04721 (13)	0.8237 (5)	1.0939 (3)	0.0312 (9)
C11	1.04697 (14)	0.7866 (5)	1.1949 (3)	0.0387 (10)
H11	1.0216	0.7137	1.1993	0.046*
C12	1.08322 (15)	0.8551 (6)	1.2876 (3)	0.0441 (10)
H12	1.0822	0.8297	1.3540	0.053*
C13	1.12116 (14)	0.9617 (5)	1.2819 (3)	0.0376 (9)
C14	1.12300 (16)	0.9996 (6)	1.1834 (3)	0.0446 (10)
H14	1.1487	1.0713	1.1795	0.054*
C15	1.08594 (14)	0.9290 (5)	1.0911 (3)	0.0393 (10)
H15	1.0873	0.9537	1.0248	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0516 (3)	0.0628 (4)	0.0480 (3)	−0.0060 (3)	0.0059 (2)	−0.0110 (2)
N1	0.0355 (17)	0.045 (2)	0.0228 (15)	0.0001 (16)	0.0125 (13)	−0.0005 (14)
N2	0.0320 (17)	0.039 (2)	0.0259 (16)	0.0008 (15)	0.0105 (14)	−0.0028 (14)
O1	0.0562 (18)	0.088 (3)	0.0281 (14)	−0.0174 (17)	0.0231 (13)	−0.0038 (15)
O2	0.0502 (16)	0.060 (2)	0.0236 (12)	−0.0083 (15)	0.0181 (12)	−0.0062 (12)
C1	0.036 (2)	0.038 (2)	0.0268 (19)	0.0080 (19)	0.0146 (16)	0.0022 (17)
C2	0.0311 (19)	0.032 (2)	0.0301 (19)	0.0081 (18)	0.0104 (16)	0.0016 (17)
C3	0.034 (2)	0.035 (2)	0.0305 (19)	0.0059 (18)	0.0151 (17)	0.0000 (17)
C4	0.050 (3)	0.054 (3)	0.027 (2)	0.003 (2)	0.0108 (19)	−0.0065 (19)
C5	0.034 (2)	0.048 (3)	0.048 (2)	−0.001 (2)	0.0052 (19)	−0.009 (2)
C6	0.038 (2)	0.049 (3)	0.053 (3)	−0.002 (2)	0.020 (2)	−0.002 (2)
C7	0.037 (2)	0.044 (3)	0.036 (2)	0.001 (2)	0.0145 (18)	0.0041 (19)
C8	0.048 (2)	0.054 (3)	0.039 (2)	−0.003 (2)	0.0221 (19)	−0.005 (2)
C9	0.037 (2)	0.032 (2)	0.0277 (19)	0.0079 (18)	0.0145 (17)	0.0014 (16)
C10	0.031 (2)	0.031 (2)	0.0338 (19)	0.0078 (18)	0.0158 (16)	0.0012 (17)
C11	0.040 (2)	0.044 (3)	0.035 (2)	−0.005 (2)	0.0175 (18)	−0.0008 (19)

C12	0.051 (2)	0.052 (3)	0.030 (2)	0.004 (2)	0.0164 (19)	0.0058 (19)
C13	0.032 (2)	0.036 (2)	0.041 (2)	0.0022 (19)	0.0106 (17)	−0.0046 (18)
C14	0.042 (2)	0.043 (3)	0.049 (2)	−0.005 (2)	0.018 (2)	−0.001 (2)
C15	0.043 (2)	0.044 (3)	0.036 (2)	0.000 (2)	0.0210 (18)	0.0068 (19)

Geometric parameters (Å, º)

Br1—C13	1.899 (4)	C6—H6	0.9300
N1—C1	1.349 (5)	C7—H7	0.9300
N1—N2	1.374 (4)	C8—C9	1.504 (4)
N1—H1	0.8600	C8—H8A	0.9600
N2—C9	1.282 (4)	C8—H8B	0.9600
O1—C1	1.231 (4)	C8—H8C	0.9600
O2—C3	1.366 (4)	C9—C10	1.494 (5)
O2—H2	0.8200	C10—C15	1.374 (5)
C1—C2	1.485 (5)	C10—C11	1.398 (5)
C2—C7	1.395 (5)	C11—C12	1.369 (5)
C2—C3	1.407 (5)	C11—H11	0.9300
C3—C4	1.386 (5)	C12—C13	1.376 (5)
C4—C5	1.371 (5)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.384 (5)
C5—C6	1.383 (5)	C14—C15	1.382 (5)
C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.365 (5)	C15—H15	0.9300
C1—N1—N2	120.2 (3)	C9—C8—H8B	109.5
C1—N1—H1	119.9	H8A—C8—H8B	109.5
N2—N1—H1	119.9	C9—C8—H8C	109.5
C9—N2—N1	117.3 (3)	H8A—C8—H8C	109.5
C3—O2—H2	109.5	H8B—C8—H8C	109.5
O1—C1—N1	121.2 (3)	N2—C9—C10	114.8 (3)
O1—C1—C2	121.3 (3)	N2—C9—C8	125.2 (3)
N1—C1—C2	117.6 (3)	C10—C9—C8	120.1 (3)
C7—C2—C3	117.2 (3)	C15—C10—C11	117.5 (3)
C7—C2—C1	116.7 (3)	C15—C10—C9	123.4 (3)
C3—C2—C1	126.1 (3)	C11—C10—C9	119.1 (3)
O2—C3—C4	121.2 (3)	C12—C11—C10	121.5 (4)
O2—C3—C2	118.8 (3)	C12—C11—H11	119.3
C4—C3—C2	120.0 (3)	C10—C11—H11	119.3
C5—C4—C3	120.8 (3)	C11—C12—C13	119.7 (3)
C5—C4—H4	119.6	C11—C12—H12	120.2
C3—C4—H4	119.6	C13—C12—H12	120.2
C4—C5—C6	120.2 (4)	C12—C13—C14	120.5 (3)
C4—C5—H5	119.9	C12—C13—Br1	119.0 (3)
C6—C5—H5	119.9	C14—C13—Br1	120.5 (3)
C7—C6—C5	119.2 (4)	C15—C14—C13	118.8 (4)
C7—C6—H6	120.4	C15—C14—H14	120.6
C5—C6—H6	120.4	C13—C14—H14	120.6

C6—C7—C2	122.6 (3)	C10—C15—C14	122.2 (3)
C6—C7—H7	118.7	C10—C15—H15	118.9
C2—C7—H7	118.7	C14—C15—H15	118.9
C9—C8—H8A	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.95	2.637 (3)	136
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