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2-[(3-Bromophenyl)iminomethyl]phenol

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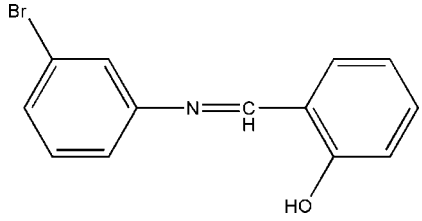
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.019 Å; R factor = 0.083; wR factor = 0.229; data-to-parameter ratio = 12.6.

The title compound, $C_{13}H_{10}BrNO$, was prepared by reaction of 3-bromoaniline with 2-hydroxybenzaldehyde at 377 K. The molecular structure and packing are stabilized by an intramolecular O—H···N hydrogen-bond interaction.

Related literature

For related literature, see: Jian *et al.* (2006); Rozwadowski *et al.* (1999).



Experimental

Crystal data

$C_{13}H_{10}BrNO$
M_r = 276.13
Monoclinic, $P2_1$
a = 3.9700 (8) Å
b = 10.540 (2) Å
c = 13.200 (3) Å
β = 98.00 (3)°
V = 546.96 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.73 mm^{-1}
T = 293 (2) K
0.12 × 0.10 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
2736 measured reflections
1822 independent reflections
1666 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.229
S = 1.13
1822 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.43 e Å^{-3}
$\Delta\rho_{min}$ = −1.17 e Å^{-3}
Absolute structure: Flack (1983), 787 Freidel pairs
Flack parameter: 0.1 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.86	2.599 (17)	149

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2611).

References

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Jian, F.-F., Zhuang, R.-R., Wang, K.-F., Zhao, P.-S. & Xiao, H.-L. (2006). *Acta Cryst.* E**62**, o3198–o3199.
Rozwadowski, Z., Majewski, E., Dziembowska, T. & Hansen, P. E. (1999). *J. Chem. Soc. Perkin Trans. 2*, pp. 2809–2817.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1863 [https://doi.org/10.1107/S1600536808027360]

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S1. Comment

The recent growing interest in Schiff bases is also due to their ability to form intramolecular hydrogen bonds by electron coupling between acid–base centers (Rozwadowski *et al.*, 1999). The part of our research is to find Schiff base with higher biological activity, we synthesized the title compound (I) and report its crystal structure here.

In the crystal structure of compound (I) (Fig. 1), the dihedral angle between the benzene rings (C1–C6) and (C7–C12) was 4.6 (2)°. The C═N bond length [1.273 (1) Å] is in agreement with that observed before (Jian *et al.*, 2006). There are intramolecular O—H···N hydrogen-bond interactions to stabilize the crystal structure (Table 1, Fig. 2).

S2. Experimental

A mixture of 2-nitrobenzaldehyde (0.02 mol) and 4-methoxyaniline (0.02 mol) was stirred with ethanol (50 mL) at 377 K for 5 h, affording the title compound (4.33 g, yield 84.5%). Single crystals suitable for X-ray measurements were obtained by recrystallization from acetone at room temperature.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with O—H and C—H distances of 0.82 and 0.93 Å, respectively, and with U_{iso}(H) = 1.2 or 1.5U_{eq} of the parent atoms.

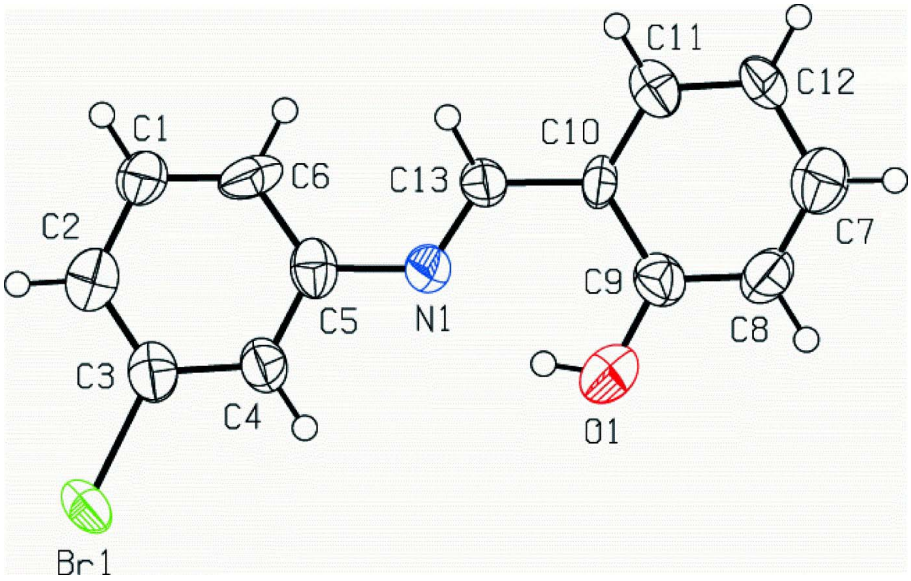

Figure 1

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

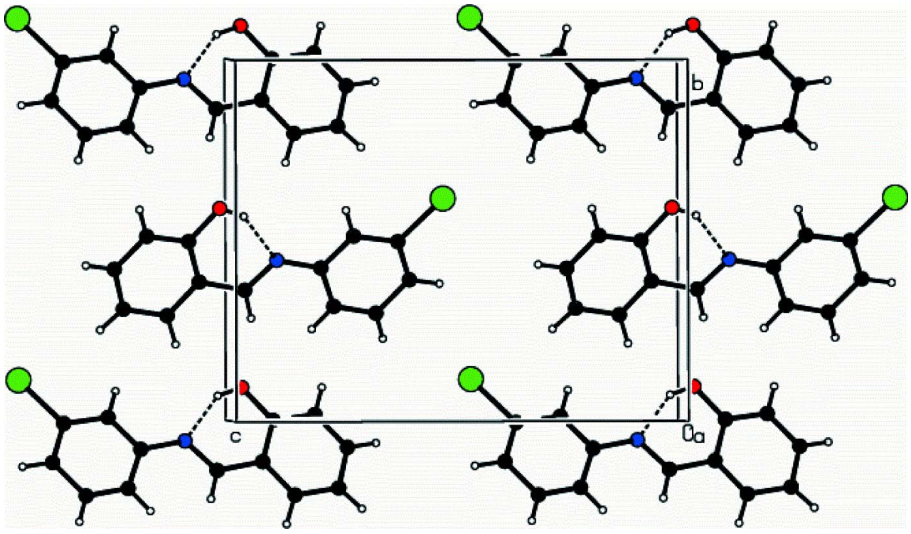

Figure 2

A view of the packing and the intramolecular hydrogen bonding (dashed lines) of (I) in the unitcell.

2-[(3-Bromophenyl)iminomethyl]phenol

Crystal data

$C_{13}H_{10}BrNO$
$M_r = 276.13$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 3.9700\ (8)$ Å
$b = 10.540\ (2)$ Å
$c = 13.200\ (3)$ Å
$\beta = 98.00\ (3)°$
$V = 546.96\ (19)$ Å^3
$Z = 2$
$F(000) = 276.0$
$D_x = 1.676$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1666 reflections
$\theta = 1.6–25.0°$
$\mu = 3.73$ mm^{-1}
$T = 293$ K
Bar, yellow
0.12 × 0.10 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
2736 measured reflections
1822 independent reflections
1666 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -4\rightarrow4$
$k = -12\rightarrow12$
$l = -12\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.082$
$wR(F^2) = 0.229$
$S = 1.13$
1822 reflections
145 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1154P)^2 + 2.8393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.43$ e Å^{-3}
$\Delta\rho_{min} = -1.17$ e Å^{-3}

Absolute structure: Flack (1983), 787 Freidel pairs

Absolute structure parameter: 0.1 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.4943 (3)	0.6144 (2)	0.53030 (8)	0.0544 (5)
N1	0.643 (3)	0.4449 (9)	0.9014 (8)	0.041 (2)
C4	0.538 (4)	0.5109 (12)	0.7289 (10)	0.046 (3)
H4A	0.6652	0.5830	0.7485	0.055*
C10	0.793 (3)	0.3864 (10)	1.0766 (9)	0.036 (3)
C3	0.402 (4)	0.4950 (13)	0.6277 (11)	0.049 (3)
C11	0.800 (4)	0.2937 (12)	1.1480 (10)	0.043 (3)
H11A	0.7186	0.2137	1.1274	0.052*
C5	0.487 (3)	0.4229 (12)	0.8000 (10)	0.043 (3)
C8	1.128 (4)	0.5145 (14)	1.2004 (12)	0.057 (4)
H8A	1.2470	0.5889	1.2187	0.068*
C12	0.918 (4)	0.3124 (13)	1.2476 (10)	0.052 (4)
H12A	0.8763	0.2550	1.2978	0.062*
C13	0.644 (4)	0.3630 (11)	0.9723 (11)	0.041 (3)
H13A	0.5431	0.2846	0.9561	0.050*
C9	0.978 (4)	0.4994 (12)	1.1041 (10)	0.045 (3)
C7	1.110 (4)	0.4238 (15)	1.2716 (13)	0.060 (4)
H7A	1.2254	0.4348	1.3373	0.072*
O1	0.995 (3)	0.5906 (16)	1.0355 (8)	0.081 (6)
H1	0.8925	0.5681	0.9801	0.121*
C6	0.304 (3)	0.3157 (12)	0.7675 (13)	0.050 (4)
H6A	0.2798	0.2530	0.8157	0.060*
C2	0.216 (4)	0.3883 (13)	0.5982 (12)	0.049 (3)
H2A	0.1275	0.3769	0.5298	0.059*
C1	0.157 (5)	0.2960 (13)	0.6708 (11)	0.054 (4)
H1B	0.0231	0.2250	0.6527	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0649 (8)	0.0635 (8)	0.0338 (6)	−0.0095 (9)	0.0028 (5)	0.0168 (7)
N1	0.053 (6)	0.034 (5)	0.034 (5)	−0.002 (4)	0.001 (5)	−0.001 (4)
C4	0.060 (8)	0.041 (7)	0.035 (7)	0.005 (6)	−0.002 (6)	0.001 (5)

C10	0.042 (7)	0.035 (6)	0.026 (6)	0.004 (5)	−0.009 (5)	−0.007 (5)
C3	0.053 (8)	0.053 (8)	0.040 (7)	0.006 (6)	0.000 (6)	−0.002 (6)
C11	0.052 (8)	0.045 (7)	0.035 (7)	0.015 (6)	0.009 (6)	0.002 (6)
C5	0.039 (7)	0.049 (7)	0.038 (7)	0.013 (6)	−0.002 (5)	−0.002 (5)
C8	0.061 (9)	0.043 (7)	0.060 (9)	−0.009 (6)	−0.015 (7)	−0.003 (6)
C12	0.073 (10)	0.045 (7)	0.034 (7)	0.001 (7)	−0.007 (6)	0.013 (6)
C13	0.060 (8)	0.028 (6)	0.034 (7)	0.004 (5)	0.000 (6)	0.000 (4)
C9	0.056 (8)	0.039 (6)	0.041 (7)	0.007 (6)	0.003 (6)	0.003 (6)
C7	0.052 (9)	0.066 (9)	0.060 (9)	0.002 (7)	−0.001 (7)	−0.005 (7)
O1	0.096 (8)	0.077 (16)	0.065 (7)	−0.043 (8)	−0.005 (6)	−0.004 (7)
C6	0.035 (7)	0.032 (6)	0.079 (10)	−0.009 (5)	−0.002 (7)	0.004 (6)
C2	0.039 (7)	0.059 (9)	0.049 (8)	0.003 (6)	0.006 (6)	−0.010 (7)
C1	0.084 (11)	0.043 (8)	0.037 (7)	−0.011 (7)	0.014 (7)	−0.013 (6)

Geometric parameters (Å, º)

Br1—C3	1.872 (15)	C8—C7	1.35 (2)
N1—C13	1.273 (17)	C8—H8A	0.9300
N1—C5	1.414 (16)	C12—C7	1.41 (2)
C4—C5	1.354 (19)	C12—H12A	0.9300
C4—C3	1.379 (19)	C13—H13A	0.9300
C4—H4A	0.9300	C9—O1	1.328 (19)
C10—C11	1.355 (18)	C7—H7A	0.9300
C10—C9	1.420 (18)	O1—H1	0.8200
C10—C13	1.443 (18)	C6—C1	1.34 (2)
C3—C2	1.37 (2)	C6—H6A	0.9300
C11—C12	1.348 (19)	C2—C1	1.41 (2)
C11—H11A	0.9300	C2—H2A	0.9300
C5—C6	1.381 (18)	C1—H1B	0.9300
C8—C9	1.34 (2)		
C13—N1—C5	122.7 (11)	C7—C12—H12A	121.8
C5—C4—C3	120.8 (13)	N1—C13—C10	123.0 (11)
C5—C4—H4A	119.6	N1—C13—H13A	118.5
C3—C4—H4A	119.6	C10—C13—H13A	118.5
C11—C10—C9	117.9 (11)	O1—C9—C8	120.3 (13)
C11—C10—C13	120.4 (11)	O1—C9—C10	120.4 (11)
C9—C10—C13	121.1 (11)	C8—C9—C10	119.3 (12)
C2—C3—C4	119.8 (14)	C8—C7—C12	120.8 (14)
C2—C3—Br1	120.4 (11)	C8—C7—H7A	119.6
C4—C3—Br1	119.7 (11)	C12—C7—H7A	119.6
C12—C11—C10	122.9 (13)	C9—O1—H1	109.5
C12—C11—H11A	118.6	C1—C6—C5	124.1 (13)
C10—C11—H11A	118.6	C1—C6—H6A	117.9
C4—C5—C6	117.9 (13)	C5—C6—H6A	117.9
C4—C5—N1	117.2 (12)	C3—C2—C1	120.5 (14)
C6—C5—N1	124.8 (13)	C3—C2—H2A	119.8
C9—C8—C7	121.2 (14)	C1—C2—H2A	119.8

C9—C8—H8A	119.4	C6—C1—C2	116.7 (13)
C7—C8—H8A	119.4	C6—C1—H1B	121.6
C11—C12—C7	116.5 (14)	C2—C1—H1B	121.6
C11—C12—H12A	121.8		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.86	2.599 (17)	149