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N-(4-Bromobenzylidene)-2-hydroxyaniline

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.110
Data-to-parameter ratio = 17.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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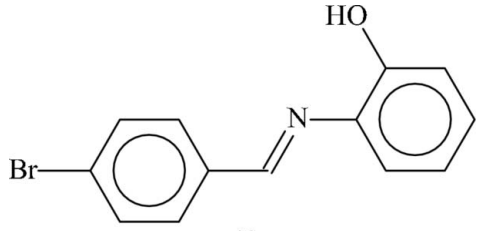
N-(4-Bromobenzylidene)-2-hydroxyaniline, $C_{13}H_{10}BrNO$, exists as a planar molecule in which the hydroxy group is intramolecularly hydrogen bonded to the imino N atom.

Comment

The preceding study reports the Schiff base that is derived by condensing *p*-bromobenzaldehyde and a substituted aniline; the compound adopts a non-planar conformation (Sun *et al.*, 2006). The present study reports the product, (I), obtained by condensing the aldehyde with *o*-hydroxyaniline. The product exists as a planar molecule (Fig. 1), in which the hydroxy group forms an intramolecular hydrogen bond to the imino N atom (Table 1). The hydrogen bond appears to be crucial for a planar conformation; hydrogen bonds are important for the manifestation of this feature in other similar Schiff bases (Huo *et al.*, 2004).



(I)

Experimental

p-Bromobenzaldehyde (3.24 g, 17.5 mmol) and *o*-hydroxyaniline (1.92 g, 17.6 mmol) were dissolved in ethanol (30 ml) along with 1 ml formic acid. The solution was refluxed for 6 h. The removal of the

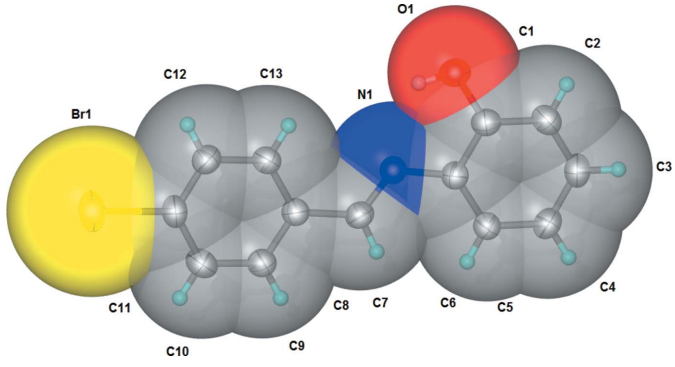


Figure 1
The molecular structure of (I), with the van der Waals surfaces. Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii.

solvent and recrystallization from a 1:1 ethanol/dichloromethane mixture (30 ml) gave the compound in about 75% yield. Crystals were grown from ethanol. Elemental analysis calculated for $C_{13}H_{10}BrNO$: C 56.55, H 3.65, N 5.07%; found: C 56.70, H 3.71, N 5.10%.

Crystal data

$C_{13}H_{10}BrNO$
M_r = 276.13
Monoclinic, $P2_1/n$
a = 13.389 (1) Å
b = 5.8745 (5) Å
c = 14.902 (1) Å
β = 102.457 (1)°
V = 1144.50 (15) Å^3
Z = 4
D_x = 1.603 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.57 mm^{-1}
T = 292 (2) K
Block, yellow
0.20 × 0.10 × 0.08 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.442, T_{max} = 0.752
10362 measured reflections
2608 independent reflections
1677 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
S = 1.02
2608 reflections
149 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.1771P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.85 (1)	2.08 (3)	2.624 (3)	122 (3)
O1—H1···O1^{i}	0.85 (1)	2.41 (3)	2.913 (4)	119 (3)

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

Carbon-bound H atoms were placed in calculated positions (C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and were included in the refinement in the riding-model approximation. The hydroxy H atom was located in a difference Fourier map, and was refined with a distance restraint of O–H 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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