Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-[(4-Bromobenzylidene)amino]-phenol

Jasmine P. Vennila,[a] D. John Thiruvadigal,[b] Helen P. Kavitha,[c] B. Gunasekaran[d] and V. Manivannan[e]*

[a]Department of Physics, Panimalar Institute of Technology, Chennai 602 103, India, [b]Department of Physics, SRM University, Kattankulathur Campus, Chennai, India, [c]Department of Chemistry, SRM University, Ramapuram Campus, Chennai 600 089, India, [d]Department of Physics, AMET University, Kanathur, Chennai 603 112, India, and [e]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: manivan_1999@yahoo.com

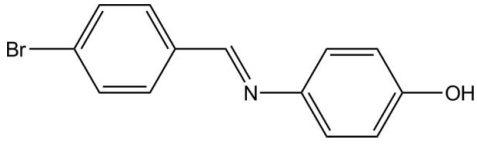
Received 22 December 2009; accepted 24 December 2009

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.086; data-to-parameter ratio = 18.3.

In the title compound, $C_{13}H_{10}BrNO$, the dihedral angle between the benzene rings is 35.20 (8)°. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming a zigzag chain along the *a* axis. A weak C—H···π interaction is observed between the chains.

Related literature

For the biological activity of benzylidene derivatives, see: El Masry *et al.* (2000); Fegade *et al.* (2009); Foroumadi *et al.* (2007); Hodnett & Dunn (1970); Hu & Zhou (2004); Jada *et al.* (2008); Samadhiya & Halve (2001); Singh & Dash (1988). For related structures, see: Cui *et al.* (2009); Sun *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{10}BrNO$
M_r = 276.13
Orthorhombic, *Pbca*
a = 12.7035 (4) Å
b = 10.3897 (3) Å
c = 17.0899 (6) Å
V = 2255.62 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.62 mm^{-1}
T = 295 K
0.20 × 0.16 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.503, T_{max} = 0.581
13273 measured reflections
2670 independent reflections
1710 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.00
2670 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

*Cg*1 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.05	2.848 (3)	164
C5—H5···*Cg*1^{ii}	0.93	2.89	3.374 (3)	114

Symmetry codes: (i) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (ii) $-x, -y, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors wish to acknowledge the SAIF, IIT, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2508).

References

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 (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cui, C., Meng, Q. & Wang, Y. (2009). *Acta Cryst.* E**65**, o2472.
El Masry, A. H., Fahmy, H. H. & Abdelwahed, S. H. A. (2000). *Molecules*, **5**, 1429–1438.
Fegade, J. D., Rane, S. S., Chaudhari, R. Y. & Patil, V. R. (2009). *Digest J. Nanomater. Biostruct.* **4**, 145–154.
Foroumadi, A., Samzadeh Kermani, A., Emami, S., Dehghan, G., Sorkhi, M., Arabsorkhi, F., Heidari, M. R., Abdollahi, M. & Shafiee, A. (2007). *Bioorg. Med. Chem. Lett.* **17**, 6764–6769.
Hodnett, E. M. & Dunn, W. J. (1970). *J. Med. Chem.* **13**, 768–770.
Hu, W. & Zhou, W. (2004). *Bioorg. Med. Chem. Lett.* **14**, 621–622.
Jada, S. R., Matthews, C., Saad, M. S., Hamzah, A. S., Lajis, N. H., Stevens, M. F. G. & Stanslas, J. (2008). *Br. J. Pharmacol.* **155**, 641–654.
Samadhiya, S. & Halve, A. (2001). *Orient J. Chem.* **17**, 119–122.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, W. M. & Dash, B. C. (1988). *Pesticides*, **22**, 33–37.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Sun, Y., Fu, S., Zhang, J., Wang, X. & Wang, D. (2009). *Acta Cryst.* E**65**, o237.

supporting information

Acta Cryst. (2010). E**66**, o316 [https://doi.org/10.1107/S160053680905538X]

(*E*)-4-[(4-Bromobenzylidene)amino]phenol

Jasmine P. Vennila, D. John Thiruvadigal, Helen P. Kavitha, B. Gunasekaran and V. Manivannan

S1. Comment

Benzylidene derivatives exhibit antitumor (Hu & Zhou 2004) and antioxidant (Foroumadi *et al.*, 2007) activities. Some *N*-benzylidene aniline derivatives show biological activities sucs as antibacterial (El Masry *et al.*, 2000), antifungal (Singh & Dash, 1988), anticancer (Hodnett & Dunn, 1970) and herbicidal (Samadhiya & Halve, 2001). In addition, benzylidene derivatives of andrographolide are potential anticancer agents (Jada *et al.*, 2008) and some of the benzylidene derivatives are acting as selective cyclooxygenase-2-inhibitors (Fegade *et al.*, 2009).

The geometric parameters of the title compound (Fig. 1) agree well with reported similar structures (Cui *et al.*, 2009; Sun *et al.*, 2009). The dihedral angle between the benzene rings is 35.20 (8)°. The C—Br bond distance is 1.894 (2) Å, which is comparable to the literature value of 1.883 (15) Å (Allen *et al.*, 1987). The crystal packing is stabilized by an O—H···N hydrogen bond and a weak C—H···π interaction (Table 1).

S2. Experimental

A mixture of 4-bromobenzaldehyde (5 mmol), 4-aminophenol (5 mmol) and ethanol (40 ml) was refluxed for 2 h. It was then allowed to cool and filtered. Recrystallization of the crude product from ethanol yielded brown colored crystals.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(O), and C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

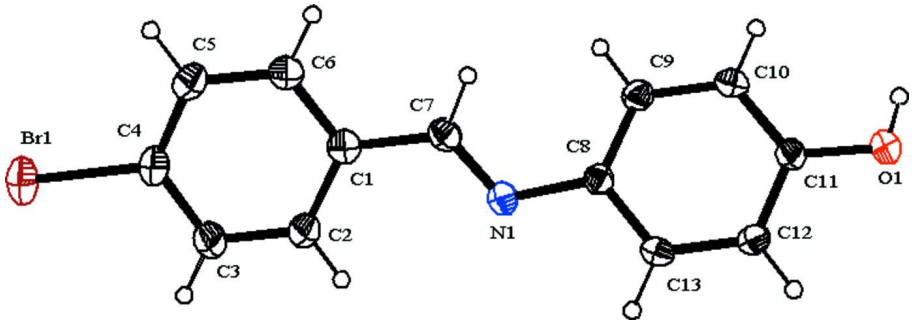


Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

(*E*)-4-[(4-Bromobenzylidene)amino]phenol

Crystal data

$C_{13}H_{10}BrNO$
$M_r = 276.13$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.7035$ (4) Å
$b = 10.3897$ (3) Å
$c = 17.0899$ (6) Å
$V = 2255.62$ (12) Å^3
$Z = 8$
$F(000) = 1104$
$D_x = 1.626$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2371 reflections
$\theta = 2.4$–$23.7°$
$\mu = 3.62$ mm^{-1}
$T = 295$ K
Block, brown
0.20 × 0.16 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.503$, $T_{max} = 0.581$
13273 measured reflections
2670 independent reflections
1710 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.8°$, $\theta_{min} = 2.4°$
$h = -12 \rightarrow 16$
$k = -12 \rightarrow 13$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.086$
$S = 1.00$
2670 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.8359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.16600 (18)	0.0270 (2)	0.54592 (14)	0.0371 (6)
C2	0.2620 (2)	−0.0367 (3)	0.54384 (16)	0.0463 (7)
H2	0.2727	−0.1086	0.5753	0.056*
C3	0.34124 (19)	0.0056 (3)	0.49578 (18)	0.0520 (7)
H3	0.4054	−0.0374	0.4944	0.062*
C4	0.32501 (19)	0.1120 (3)	0.44968 (15)	0.0422 (6)
C5	0.2319 (2)	0.1769 (3)	0.45068 (16)	0.0463 (7)
H5	0.2220	0.2490	0.4192	0.056*

C6	0.1528 (2)	0.1340 (3)	0.49907 (16)	0.0449 (7)
H6	0.0891	0.1780	0.5002	0.054*
C7	0.07751 (18)	−0.0183 (3)	0.59347 (15)	0.0383 (6)
H7	0.0158	0.0298	0.5927	0.046*
C8	−0.01245 (17)	−0.1551 (2)	0.67752 (14)	0.0325 (5)
C9	−0.08369 (16)	−0.0690 (2)	0.70991 (15)	0.0365 (6)
H9	−0.0736	0.0189	0.7031	0.044*
C10	−0.16897 (17)	−0.1120 (2)	0.75198 (14)	0.0368 (6)
H10	−0.2155	−0.0532	0.7740	0.044*
C11	−0.18585 (16)	−0.2426 (2)	0.76165 (15)	0.0360 (6)
C12	−0.11568 (19)	−0.3294 (2)	0.72949 (16)	0.0412 (6)
H12	−0.1267	−0.4174	0.7355	0.049*
C13	−0.02907 (18)	−0.2855 (2)	0.68836 (15)	0.0388 (6)
H13	0.0186	−0.3443	0.6677	0.047*
N1	0.07946 (14)	−0.1183 (2)	0.63553 (12)	0.0367 (5)
O1	−0.26777 (13)	−0.29148 (18)	0.80295 (12)	0.0497 (5)
H1	−0.3015	−0.2324	0.8226	0.075*
Br1	0.43298 (2)	0.16639 (3)	0.38080 (2)	0.06483 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0383 (13)	0.0383 (15)	0.0348 (14)	−0.0034 (11)	−0.0019 (11)	−0.0038 (12)
C2	0.0458 (14)	0.0461 (16)	0.0471 (16)	0.0036 (12)	0.0056 (13)	0.0117 (14)
C3	0.0386 (14)	0.0573 (19)	0.0599 (19)	0.0045 (13)	0.0086 (14)	0.0115 (15)
C4	0.0427 (14)	0.0468 (16)	0.0371 (15)	−0.0113 (12)	0.0046 (12)	0.0009 (13)
C5	0.0549 (16)	0.0432 (16)	0.0407 (16)	−0.0024 (13)	0.0003 (13)	0.0081 (13)
C6	0.0406 (14)	0.0464 (17)	0.0476 (17)	0.0047 (11)	0.0009 (13)	0.0066 (13)
C7	0.0322 (13)	0.0420 (16)	0.0406 (14)	0.0007 (10)	−0.0006 (11)	−0.0023 (13)
C8	0.0268 (11)	0.0357 (14)	0.0349 (13)	−0.0010 (10)	−0.0028 (10)	0.0021 (11)
C9	0.0337 (12)	0.0305 (13)	0.0452 (16)	−0.0010 (10)	−0.0018 (11)	0.0006 (12)
C10	0.0332 (13)	0.0360 (15)	0.0411 (15)	0.0066 (10)	−0.0012 (11)	−0.0013 (12)
C11	0.0291 (12)	0.0387 (16)	0.0403 (15)	0.0004 (10)	0.0010 (11)	0.0041 (11)
C12	0.0361 (12)	0.0308 (14)	0.0566 (18)	0.0013 (11)	0.0019 (12)	0.0056 (13)
C13	0.0319 (12)	0.0364 (15)	0.0480 (16)	0.0076 (11)	0.0022 (11)	0.0021 (13)
N1	0.0314 (10)	0.0404 (12)	0.0384 (13)	−0.0021 (8)	0.0016 (9)	0.0000 (10)
O1	0.0371 (10)	0.0431 (11)	0.0688 (14)	0.0020 (8)	0.0169 (9)	0.0058 (10)
Br1	0.0582 (2)	0.0736 (3)	0.0627 (2)	−0.01461 (15)	0.01935 (16)	0.01033 (18)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C8—C13	1.383 (3)
C1—C2	1.388 (3)	C8—C9	1.388 (3)
C1—C7	1.465 (3)	C8—N1	1.423 (3)
C2—C3	1.371 (4)	C9—C10	1.375 (3)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.373 (4)	C10—C11	1.383 (4)
C3—H3	0.9300	C10—H10	0.9300

C4—C5	1.362 (4)	C11—O1	1.356 (3)
C4—Br1	1.894 (2)	C11—C12	1.382 (3)
C5—C6	1.376 (4)	C12—C13	1.383 (3)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—N1	1.264 (3)	O1—H1	0.8200
C7—H7	0.9300		

C6—C1—C2	118.4 (2)	C13—C8—C9	118.6 (2)
C6—C1—C7	119.2 (2)	C13—C8—N1	117.1 (2)
C2—C1—C7	122.4 (2)	C9—C8—N1	124.3 (2)
C3—C2—C1	120.5 (3)	C10—C9—C8	120.9 (2)
C3—C2—H2	119.8	C10—C9—H9	119.6
C1—C2—H2	119.8	C8—C9—H9	119.6
C2—C3—C4	119.4 (2)	C9—C10—C11	120.2 (2)
C2—C3—H3	120.3	C9—C10—H10	119.9
C4—C3—H3	120.3	C11—C10—H10	119.9
C5—C4—C3	121.5 (2)	O1—C11—C12	117.2 (2)
C5—C4—Br1	119.3 (2)	O1—C11—C10	123.3 (2)
C3—C4—Br1	119.2 (2)	C12—C11—C10	119.5 (2)
C4—C5—C6	118.7 (3)	C11—C12—C13	120.0 (2)
C4—C5—H5	120.6	C11—C12—H12	120.0
C6—C5—H5	120.6	C13—C12—H12	120.0
C5—C6—C1	121.4 (2)	C12—C13—C8	120.8 (2)
C5—C6—H6	119.3	C12—C13—H13	119.6
C1—C6—H6	119.3	C8—C13—H13	119.6
N1—C7—C1	124.4 (2)	C7—N1—C8	119.4 (2)
N1—C7—H7	117.8	C11—O1—H1	109.5
C1—C7—H7	117.8		

C6—C1—C2—C3	−0.5 (4)	N1—C8—C9—C10	−177.8 (2)
C7—C1—C2—C3	177.0 (3)	C8—C9—C10—C11	−1.0 (4)
C1—C2—C3—C4	0.1 (5)	C9—C10—C11—O1	179.4 (2)
C2—C3—C4—C5	0.2 (5)	C9—C10—C11—C12	0.8 (4)
C2—C3—C4—Br1	−177.9 (2)	O1—C11—C12—C13	−178.4 (2)
C3—C4—C5—C6	−0.1 (4)	C10—C11—C12—C13	0.3 (4)
Br1—C4—C5—C6	177.9 (2)	C11—C12—C13—C8	−1.2 (4)
C4—C5—C6—C1	−0.2 (4)	C9—C8—C13—C12	1.0 (4)
C2—C1—C6—C5	0.5 (4)	N1—C8—C13—C12	179.1 (2)
C7—C1—C6—C5	−177.0 (3)	C1—C7—N1—C8	−178.2 (2)
C6—C1—C7—N1	176.6 (3)	C13—C8—N1—C7	147.6 (3)
C2—C1—C7—N1	−0.9 (4)	C9—C8—N1—C7	−34.5 (4)
C13—C8—C9—C10	0.1 (4)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.05	2.848 (3)	164
C5—H5···*Cg*1^{ii}	0.93	2.89	3.374 (3)	114

Symmetry codes: (i) *x*−1/2, *y*, −*z*+3/2; (ii) −*x*, −*y*, −*z*+1.