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N-[(*E*)-4-Bromobenzylidene]-2,3-dimethylaniline

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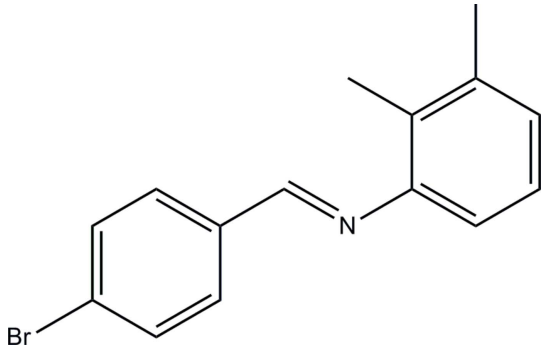
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 16.0.

The title compound, $C_{15}H_{14}BrN$, has an *E* conformation about the C=N bond and the dihedral angle between the benzene rings is 50.7 (2)°. In the crystal, molecules are linked *via* C—H$\cdots\pi$ interactions, forming columns propagating along [010].

Related literature

Schiff base derivatives have many pharmaceutical activities. For their antifungal effects, see: Aziz *et al.* (2010), for their radical scavenging activity, see: Lu *et al.* (2012), for their inhibition of enzyme activity, see: Schmidt *et al.* (2009) and for their antibacterial activity, see: Shi *et al.* (2010). For related structures, see: Sun *et al.* (2011*a*,*b*); Guo *et al.* (2011). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{14}BrN$
M_r = 288.18
Monoclinic, $P2_1/n$
a = 12.945 (9) Å
b = 7.857 (5) Å
c = 14.497 (10) Å
β = 113.384 (8)°
V = 1353.3 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.02 mm^{-1}
T = 296 K
0.25 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.519, T_{max} = 0.598
5865 measured reflections
2525 independent reflections
1154 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 0.94
2525 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C8–C13 and C1–C6 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots Cg2^{i}$	0.93	2.99	3.830 (6)	151
C15—H15*B*$\cdots Cg1^{ii}$	0.96	2.99	3.781 (6)	140

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $-x, -y+1, -z+1$.

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: *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: SU2578).

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supplementary materials

Acta Cryst. (2013). E**69**, o630 [doi:10.1107/S1600536813008088]

N-[(*E*)-4-Bromobenzylidene]-2,3-dimethylaniline

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Comment

Schiff base ligands have received much more attention during the past years. They have many pharmaceutical activities, such as antifungal effects (Aziz *et al.*, 2010), radical scavenging activity (Lu *et al.*, 2012), inhibition of enzyme activity (Schmidt *et al.*, 2009), and antibacterial activities (Shi *et al.*, 2010). We report herein on the crystal structure of a new Schiff base compound.

In the title molecule, Fig. 1, the bond lengths (Allen *et al.*, 1987) and angles are normal and comparable to the values observed in similar compounds (Sun *et al.*, 2011*a*,*b*; Guo *et al.*, 2011). The molecule has an E conformation about the C7═N1 bond and is twisted with the dihedral angle between the two aromatic rings being 50.7 (2) °.

In the crystal, molecules are linked via C-H···π interactions (Table 1).

Experimental

A mixture of 4-bromobenzaldehyde (5 mmol), 2,3-dimethylaniline (5 mmol) and methanol (50 ml) was refluxed for 6 h. The mixture was then allowed to cool and filtered. Recrystallization of the crude product from methanol yielded yellow block-like crystals.

Refinement

H atoms were positioned geometrically and refined using the riding-model approximation: C—H = 0.93 and 0.96 Å for CH and CH_3 H atoms, respectively, with U_{iso}(H) = 1.5U_{eq}(C-methyl) and = 1.2U_{eq}(C) for other H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); 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* (Sheldrick, 2008).

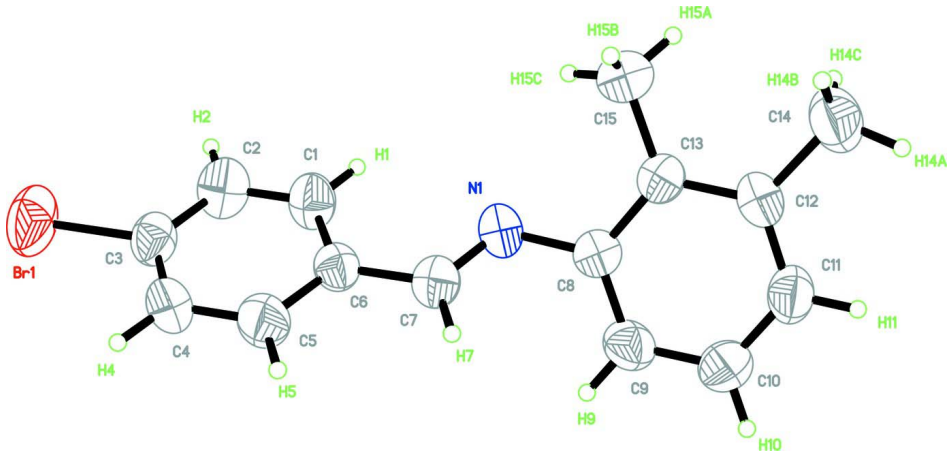

Figure 1

The molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 50% probability level.

N-[(*E*)-4-Bromobenzylidene]-2,3-dimethylaniline

Crystal data

$C_{15}H_{14}BrN$
$M_r = 288.18$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.945$ (9) Å
$b = 7.857$ (5) Å
$c = 14.497$ (10) Å
$\beta = 113.384$ (8)°
$V = 1353.3$ (16) Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.414$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2505 reflections
$\theta = 2.7$–25.5°
$\mu = 3.02$ mm^{-1}
$T = 296$ K
Block, yellow
0.25 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.519$, $T_{max} = 0.598$
5865 measured reflections
2525 independent reflections
1154 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.7°$
$h = -15\rightarrow10$
$k = -9\rightarrow7$
$l = -15\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.112$
$S = 0.94$
2525 reflections
157 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
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0298 (19)

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	0.07853 (5)	0.88838 (7)	0.11686 (4)	0.0919 (4)
C1	0.0611 (4)	0.8732 (5)	0.3942 (3)	0.0581 (13)
H1	0.0091	0.9056	0.4205	0.070*
C2	0.0362 (4)	0.8999 (5)	0.2939 (3)	0.0643 (13)
H2	−0.0315	0.9504	0.2529	0.077*
C3	0.1122 (5)	0.8513 (5)	0.2554 (3)	0.0547 (12)
C4	0.2111 (4)	0.7767 (7)	0.3137 (4)	0.0736 (15)
H4	0.2616	0.7431	0.2860	0.088*
C5	0.2363 (4)	0.7508 (6)	0.4154 (3)	0.0682 (15)
H5	0.3042	0.7002	0.4557	0.082*
C6	0.1617 (4)	0.7992 (5)	0.4572 (3)	0.0477 (11)
C7	0.1882 (4)	0.7675 (5)	0.5637 (3)	0.0513 (12)
H7	0.2592	0.7258	0.6036	0.062*
C8	0.1554 (4)	0.7691 (5)	0.7095 (3)	0.0434 (11)
C9	0.2578 (4)	0.8290 (6)	0.7761 (3)	0.0582 (13)
H9	0.3060	0.8842	0.7525	0.070*
C10	0.2887 (4)	0.8071 (7)	0.8781 (3)	0.0713 (14)
H10	0.3586	0.8452	0.9231	0.086*
C11	0.2169 (4)	0.7295 (6)	0.9130 (3)	0.0602 (13)
H11	0.2382	0.7163	0.9818	0.072*
C12	0.1130 (4)	0.6702 (5)	0.8474 (3)	0.0500 (12)
C13	0.0802 (3)	0.6918 (5)	0.7437 (3)	0.0449 (11)
C14	0.0371 (4)	0.5812 (6)	0.8890 (4)	0.0776 (16)
H14A	0.0750	0.5718	0.9607	0.116*
H14B	0.0191	0.4695	0.8602	0.116*
H14C	−0.0309	0.6457	0.8726	0.116*
C15	−0.0326 (4)	0.6292 (6)	0.6700 (3)	0.0758 (15)
H15A	−0.0869	0.6384	0.6995	0.114*
H15B	−0.0262	0.5124	0.6535	0.114*
H15C	−0.0564	0.6970	0.6100	0.114*
N1	0.1199 (3)	0.7938 (4)	0.6039 (2)	0.0501 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1350 (6)	0.0914 (5)	0.0529 (3)	−0.0264 (4)	0.0410 (3)	0.0038 (3)
C1	0.064 (3)	0.061 (3)	0.052 (3)	0.015 (3)	0.025 (3)	0.005 (2)
C2	0.075 (4)	0.054 (3)	0.061 (3)	0.021 (3)	0.024 (3)	0.008 (3)
C3	0.069 (3)	0.050 (3)	0.044 (2)	−0.006 (3)	0.023 (3)	0.005 (2)
C4	0.069 (4)	0.104 (4)	0.061 (3)	−0.012 (3)	0.039 (3)	−0.015 (3)
C5	0.051 (3)	0.095 (4)	0.060 (3)	0.013 (3)	0.024 (3)	0.000 (3)
C6	0.051 (3)	0.047 (3)	0.048 (3)	−0.001 (2)	0.023 (2)	−0.001 (2)
C7	0.058 (3)	0.047 (3)	0.050 (3)	0.002 (2)	0.022 (3)	0.000 (2)
C8	0.047 (3)	0.034 (3)	0.049 (3)	0.004 (2)	0.018 (2)	0.001 (2)
C9	0.062 (3)	0.055 (3)	0.063 (3)	−0.015 (3)	0.030 (3)	−0.005 (2)
C10	0.065 (3)	0.089 (4)	0.057 (3)	−0.024 (3)	0.021 (3)	−0.020 (3)
C11	0.072 (4)	0.066 (4)	0.044 (3)	−0.004 (3)	0.024 (3)	−0.002 (2)
C12	0.062 (3)	0.043 (3)	0.053 (3)	0.002 (2)	0.032 (3)	0.003 (2)
C13	0.051 (3)	0.037 (3)	0.046 (2)	0.002 (2)	0.018 (2)	−0.005 (2)
C14	0.093 (4)	0.080 (4)	0.070 (3)	−0.008 (3)	0.042 (3)	0.009 (3)
C15	0.059 (3)	0.100 (4)	0.062 (3)	−0.015 (3)	0.018 (3)	−0.005 (3)
N1	0.061 (2)	0.048 (2)	0.048 (2)	0.004 (2)	0.028 (2)	0.0032 (17)

Geometric parameters (Å, º)

Br1—C3	1.901 (4)	C8—N1	1.426 (5)
C1—C2	1.375 (6)	C9—C10	1.380 (6)
C1—C6	1.387 (5)	C9—H9	0.9300
C1—H1	0.9300	C10—C11	1.366 (6)
C2—C3	1.365 (6)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.383 (6)
C3—C4	1.355 (6)	C11—H11	0.9300
C4—C5	1.393 (6)	C12—C13	1.401 (5)
C4—H4	0.9300	C12—C14	1.513 (6)
C5—C6	1.382 (5)	C13—C15	1.509 (6)
C5—H5	0.9300	C14—H14A	0.9600
C6—C7	1.464 (5)	C14—H14B	0.9600
C7—N1	1.253 (5)	C14—H14C	0.9600
C7—H7	0.9300	C15—H15A	0.9600
C8—C9	1.377 (5)	C15—H15B	0.9600
C8—C13	1.395 (5)	C15—H15C	0.9600
C2—C1—C6	121.6 (4)	C10—C9—H9	120.1
C2—C1—H1	119.2	C11—C10—C9	120.1 (4)
C6—C1—H1	119.2	C11—C10—H10	120.0
C3—C2—C1	119.1 (4)	C9—C10—H10	120.0
C3—C2—H2	120.5	C10—C11—C12	121.0 (4)
C1—C2—H2	120.5	C10—C11—H11	119.5
C4—C3—C2	121.5 (4)	C12—C11—H11	119.5
C4—C3—Br1	119.2 (4)	C11—C12—C13	119.6 (4)
C2—C3—Br1	119.3 (4)	C11—C12—C14	119.3 (4)
C3—C4—C5	119.3 (4)	C13—C12—C14	121.0 (4)

C3—C4—H4	120.4	C8—C13—C12	118.5 (4)
C5—C4—H4	120.4	C8—C13—C15	120.3 (4)
C6—C5—C4	120.9 (4)	C12—C13—C15	121.1 (4)
C6—C5—H5	119.6	C12—C14—H14A	109.5
C4—C5—H5	119.6	C12—C14—H14B	109.5
C5—C6—C1	117.7 (4)	H14A—C14—H14B	109.5
C5—C6—C7	120.2 (4)	C12—C14—H14C	109.5
C1—C6—C7	122.1 (4)	H14A—C14—H14C	109.5
N1—C7—C6	123.3 (4)	H14B—C14—H14C	109.5
N1—C7—H7	118.4	C13—C15—H15A	109.5
C6—C7—H7	118.4	C13—C15—H15B	109.5
C9—C8—C13	120.8 (4)	H15A—C15—H15B	109.5
C9—C8—N1	121.1 (4)	C13—C15—H15C	109.5
C13—C8—N1	117.9 (4)	H15A—C15—H15C	109.5
C8—C9—C10	119.9 (4)	H15B—C15—H15C	109.5
C8—C9—H9	120.1	C7—N1—C8	119.4 (4)

C6—C1—C2—C3	0.4 (7)	C9—C10—C11—C12	0.6 (8)
C1—C2—C3—C4	0.4 (7)	C10—C11—C12—C13	−0.8 (7)
C1—C2—C3—Br1	−179.8 (3)	C10—C11—C12—C14	178.5 (4)
C2—C3—C4—C5	−0.7 (7)	C9—C8—C13—C12	−2.6 (6)
Br1—C3—C4—C5	179.5 (4)	N1—C8—C13—C12	−178.6 (4)
C3—C4—C5—C6	0.3 (7)	C9—C8—C13—C15	179.0 (4)
C4—C5—C6—C1	0.4 (7)	N1—C8—C13—C15	3.0 (6)
C4—C5—C6—C7	178.6 (4)	C11—C12—C13—C8	1.7 (6)
C2—C1—C6—C5	−0.8 (7)	C14—C12—C13—C8	−177.6 (4)
C2—C1—C6—C7	−178.9 (4)	C11—C12—C13—C15	−179.9 (4)
C5—C6—C7—N1	−173.1 (4)	C14—C12—C13—C15	0.9 (6)
C1—C6—C7—N1	4.9 (7)	C6—C7—N1—C8	−176.2 (4)
C13—C8—C9—C10	2.5 (6)	C9—C8—N1—C7	44.6 (6)
N1—C8—C9—C10	178.4 (4)	C13—C8—N1—C7	−139.3 (4)
C8—C9—C10—C11	−1.5 (7)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C8–C13 and C1–C6 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*2^{i}	0.93	2.99	3.830 (6)	151
C15—H15*B*···*Cg*1^{ii}	0.96	2.99	3.781 (6)	140

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