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(*E*)-4-Bromo-*N*-(2-chlorobenzylidene)-aniline

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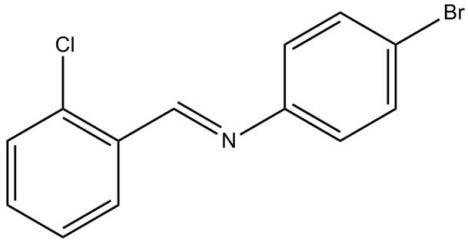
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.048; wR factor = 0.138; data-to-parameter ratio = 15.3.

In the title Schiff base molecule, $C_{13}H_9BrClN$, the dihedral angle between the benzene rings is 49.8 (2)° and the molecule has an E configuration about the C=N bond. In the crystal, there are no directional interactions but only van der Waals intermolecular interaction forces between neighbouring molecules.

Related literature

For the antibacterial activities of Schiff base compounds, see: El Masry *et al.* (2000). For the anticancer properties of Schiff base compounds, see: Dao *et al.* (2000). For related crystal structures, see: Sun *et al.* (2011*a*,*b*); Guo *et al.* (2011). For standard bond-length values, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_9BrClN$
M_r = 294.57
Monoclinic, $P2_1/n$
a = 15.243 (13) Å
b = 4.020 (4) Å
c = 20.142 (18) Å
β = 103.248 (8)°
V = 1201.4 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.61 mm^{-1}
T = 296 K
0.25 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.465, T_{max} = 0.518
7879 measured reflections
2219 independent reflections
1413 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.138
S = 1.04
2219 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

The author wishes to thank Professor Shao, Lanzhou University, for collecting the X-ray diffraction data.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2298).

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supporting information

Acta Cryst. (2011). E**67**, o2204 [doi:10.1107/S1600536811029977]

(*E*)-4-Bromo-*N*-(2-chlorobenzylidene)aniline

Chuang Wang

S1. Comment

Schiff bases compounds have attracted a lot of attention for a long time, because of their applications as antibacterial (El Masry *et al.*, 2000), and anticancer (Dao *et al.*, 2000) agents. We report herein, on the crystal structure of the title new Schiff base compound.

The molecular structure of the title molecule is illustrated in Fig. 1. The geometric parameters agree well with those reported for similar structures (Sun *et al.*, 2011*a*,*b*; Guo *et al.*, 2011), and all the bond lengths are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the two aromatic rings in the Schiff base molecule is 49.8 (2)°.

In the crystal, there are only van der Waals intermolecular forces between neighbouring molecules.

S2. Experimental

A mixture of 2-chlorobenzaldehyde (10 mmol), 4-bromoaniline (10 mmol) and methanol (50 ml) was refluxed for 6 h. It was then allowed to cool and was filtered. Recrystallization of the crude product from methanol yielded colourless crystals, suitable for X-ray diffraction analysis.

S3. Refinement

The H atoms were positioned geometrically and refined using the riding-model approximation: C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C).

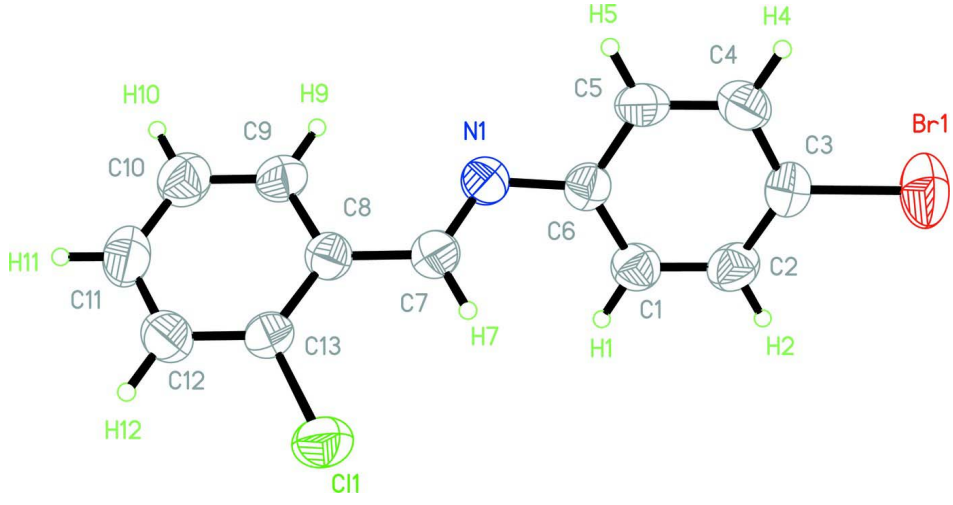

Figure 1

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

(*E*)-4-Bromo-*N*-(2-chlorobenzylidene)aniline

Crystal data

$C_{13}H_9BrClN$
$M_r = 294.57$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.243$ (13) Å
$b = 4.020$ (4) Å
$c = 20.142$ (18) Å
$\beta = 103.248$ (8)°
$V = 1201.4$ (18) Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.629$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1725 reflections
$\theta = 2.8$–21.7°
$\mu = 3.61$ mm^{-1}
$T = 296$ K
Block, colourless
0.25 × 0.23 × 0.21 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)
$T_{min} = 0.465$, $T_{max} = 0.518$
7879 measured reflections
2219 independent reflections
1413 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.8°$
$h = -18\rightarrow17$
$k = -4\rightarrow4$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.138$
$S = 1.04$
2219 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 0.0187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ 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	0.28006 (4)	0.71850 (15)	1.03703 (3)	0.0824 (3)
C1	0.4330 (3)	0.6328 (11)	0.8929 (2)	0.0499 (11)
H1	0.4917	0.6854	0.8906	0.060*
C2	0.4042 (3)	0.6997 (11)	0.9513 (2)	0.0544 (12)

H2	0.4431	0.8014	0.9880	0.065*
C3	0.3186 (3)	0.6179 (11)	0.9560 (2)	0.0501 (11)
C4	0.2584 (3)	0.4713 (12)	0.9009 (2)	0.0544 (12)
H4	0.2003	0.4154	0.9041	0.065*
C5	0.2870 (3)	0.4110 (12)	0.8416 (2)	0.0527 (12)
H5	0.2469	0.3189	0.8042	0.063*
C6	0.3744 (3)	0.4854 (11)	0.8366 (2)	0.0440 (10)
C7	0.4763 (3)	0.2977 (10)	0.7752 (2)	0.0479 (11)
H7	0.5136	0.2425	0.8171	0.057*
C8	0.5086 (3)	0.2397 (10)	0.7133 (2)	0.0438 (10)
C9	0.4571 (3)	0.3496 (11)	0.6495 (2)	0.0506 (11)
H9	0.4020	0.4532	0.6473	0.061*
C10	0.4871 (4)	0.3061 (12)	0.5909 (3)	0.0603 (13)
H10	0.4520	0.3800	0.5495	0.072*
C11	0.5684 (4)	0.1546 (13)	0.5928 (3)	0.0633 (14)
H11	0.5886	0.1297	0.5528	0.076*
C12	0.6206 (3)	0.0384 (12)	0.6542 (2)	0.0575 (13)
H12	0.6753	−0.0670	0.6557	0.069*
C13	0.5897 (3)	0.0821 (11)	0.7133 (2)	0.0452 (10)
Cl1	0.65673 (8)	−0.0722 (3)	0.78942 (6)	0.0647 (4)
N1	0.3988 (2)	0.4211 (9)	0.77412 (18)	0.0491 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1072 (6)	0.0843 (5)	0.0678 (4)	−0.0119 (3)	0.0453 (4)	−0.0171 (3)
C1	0.046 (2)	0.052 (3)	0.052 (3)	−0.006 (2)	0.011 (2)	0.002 (2)
C2	0.054 (3)	0.057 (3)	0.049 (3)	−0.011 (2)	0.004 (2)	−0.005 (2)
C3	0.061 (3)	0.046 (3)	0.045 (3)	0.002 (2)	0.016 (2)	0.000 (2)
C4	0.043 (2)	0.057 (3)	0.065 (3)	−0.004 (2)	0.015 (2)	−0.010 (2)
C5	0.038 (3)	0.062 (3)	0.053 (3)	0.000 (2)	0.001 (2)	−0.004 (2)
C6	0.048 (3)	0.042 (3)	0.042 (2)	0.006 (2)	0.009 (2)	0.002 (2)
C7	0.047 (3)	0.051 (3)	0.045 (3)	0.000 (2)	0.008 (2)	0.000 (2)
C8	0.044 (2)	0.042 (3)	0.045 (3)	0.000 (2)	0.010 (2)	−0.002 (2)
C9	0.049 (3)	0.054 (3)	0.045 (3)	0.003 (2)	0.003 (2)	0.005 (2)
C10	0.064 (3)	0.065 (3)	0.050 (3)	−0.001 (3)	0.010 (2)	0.004 (2)
C11	0.073 (3)	0.068 (3)	0.053 (3)	−0.006 (3)	0.022 (3)	−0.012 (3)
C12	0.046 (3)	0.062 (3)	0.066 (3)	−0.001 (2)	0.015 (2)	−0.014 (3)
C13	0.043 (2)	0.047 (3)	0.043 (2)	−0.005 (2)	0.005 (2)	−0.005 (2)
Cl1	0.0567 (7)	0.0718 (9)	0.0585 (8)	0.0150 (6)	−0.0019 (6)	−0.0042 (6)
N1	0.046 (2)	0.052 (2)	0.048 (2)	0.0069 (19)	0.0096 (17)	−0.0027 (18)

Geometric parameters (Å, º)

Br1—C3	1.900 (5)	C7—C8	1.461 (6)
C1—C2	1.374 (6)	C7—H7	0.9300
C1—C6	1.404 (6)	C8—C13	1.390 (6)
C1—H1	0.9300	C8—C9	1.414 (6)

C2—C3	1.369 (7)	C9—C10	1.371 (7)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.399 (6)	C10—C11	1.374 (8)
C4—C5	1.384 (6)	C10—H10	0.9300
C4—H4	0.9300	C11—C12	1.390 (7)
C5—C6	1.391 (6)	C11—H11	0.9300
C5—H5	0.9300	C12—C13	1.387 (6)
C6—N1	1.416 (5)	C12—H12	0.9300
C7—N1	1.276 (5)	C13—Cl1	1.750 (4)
C2—C1—C6	120.3 (4)	C8—C7—H7	118.7
C2—C1—H1	119.9	C13—C8—C9	116.8 (4)
C6—C1—H1	119.9	C13—C8—C7	123.2 (4)
C3—C2—C1	120.6 (4)	C9—C8—C7	120.0 (4)
C3—C2—H2	119.7	C10—C9—C8	121.2 (4)
C1—C2—H2	119.7	C10—C9—H9	119.4
C2—C3—C4	120.6 (4)	C8—C9—H9	119.4
C2—C3—Br1	119.7 (4)	C9—C10—C11	120.7 (5)
C4—C3—Br1	119.7 (3)	C9—C10—H10	119.7
C5—C4—C3	118.7 (4)	C11—C10—H10	119.7
C5—C4—H4	120.7	C10—C11—C12	120.1 (5)
C3—C4—H4	120.7	C10—C11—H11	119.9
C4—C5—C6	121.4 (4)	C12—C11—H11	119.9
C4—C5—H5	119.3	C13—C12—C11	118.9 (4)
C6—C5—H5	119.3	C13—C12—H12	120.5
C5—C6—C1	118.4 (4)	C11—C12—H12	120.5
C5—C6—N1	118.4 (4)	C12—C13—C8	122.4 (4)
C1—C6—N1	123.1 (4)	C12—C13—Cl1	117.5 (3)
N1—C7—C8	122.6 (4)	C8—C13—Cl1	120.1 (3)
N1—C7—H7	118.7	C7—N1—C6	119.1 (4)
C6—C1—C2—C3	1.3 (7)	C7—C8—C9—C10	178.2 (4)
C1—C2—C3—C4	−1.4 (7)	C8—C9—C10—C11	−0.2 (7)
C1—C2—C3—Br1	−179.2 (3)	C9—C10—C11—C12	1.1 (8)
C2—C3—C4—C5	−0.1 (7)	C10—C11—C12—C13	−0.8 (7)
Br1—C3—C4—C5	177.7 (4)	C11—C12—C13—C8	−0.3 (7)
C3—C4—C5—C6	1.6 (7)	C11—C12—C13—Cl1	179.2 (4)
C4—C5—C6—C1	−1.7 (7)	C9—C8—C13—C12	1.2 (6)
C4—C5—C6—N1	−179.3 (4)	C7—C8—C13—C12	−178.0 (4)
C2—C1—C6—C5	0.2 (6)	C9—C8—C13—Cl1	−178.4 (3)
C2—C1—C6—N1	177.7 (4)	C7—C8—C13—Cl1	2.5 (6)
N1—C7—C8—C13	−174.9 (4)	C8—C7—N1—C6	−176.8 (4)
N1—C7—C8—C9	6.0 (6)	C5—C6—N1—C7	−139.1 (4)
C13—C8—C9—C10	−1.0 (7)	C1—C6—N1—C7	43.5 (6)