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N,N'-Bis(4-bromobenzylidene)ethane-1,2-diamine

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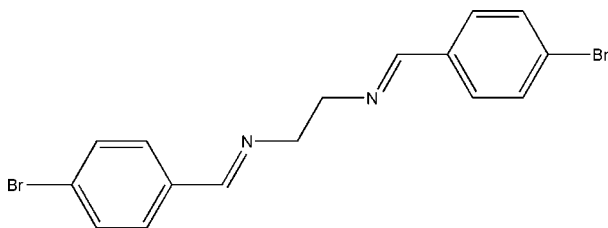
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 21.7.

The molecule of the title Schiff base compound, $\text{C}_{16}\text{H}_{14}\text{Br}_2\text{N}_2$, lies across a crystallographic inversion centre and adopts an *E* configuration with respect to the azomethine $\text{C}=\text{N}$ bond. The imino group is coplanar with the aromatic ring. Within the molecule, the planar units are parallel, but extend in opposite directions from the dimethylene bridge. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\pi$ interactions and $\text{Br}\cdots\text{Br}$ [3.6307 (4) Å] short contacts.

Related literature

For the values of bond lengths, see Allen *et al.* (1987). For related structures see, for example: Fun, Kargar & Kia (2008); Fun, Kia & Kargar (2008); Habibi *et al.* (2007); Calligaris & Randaccio, (1987). For information on Schiff base complexes and their applications, see, for example: Kia, Mirkhani, Harkema & van Hummel (2007); Kia, Mirkhani, Kalman & Deak (2007); Amirnasr *et al.* (2002); Pal *et al.* (2005); Hou *et al.* (2001); Ren *et al.* (2002).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{14}\text{Br}_2\text{N}_2$ $a = 13.8417$ (5) Å
 $M_r = 394.11$ $b = 7.4796$ (3) Å
 Monoclinic, $P2_1/c$ $c = 7.1531$ (3) Å

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$\beta = 95.692$ (1)°
 $V = 736.91$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 5.49$ mm⁻¹
 $T = 100.0$ (1) K
 $0.45 \times 0.24 \times 0.03$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker 2005)
 $T_{\min} = 0.189$, $T_{\max} = 0.853$

10096 measured reflections
 2148 independent reflections
 1773 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.069$
 $S = 1.06$
 2148 reflections
 99 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.73$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C7}-\text{H7A}\cdots\text{Cg1}$	0.93	2.99	3.7143 (19)	136

Cg1 is the centroid of the C1–C6 benzene ring.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2584).

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supporting information

Acta Cryst. (2008). E64, o1374–o1375 [doi:10.1107/S1600536808019594]

N,N'*-Bis(4-bromobenzylidene)ethane-1,2-diamine*Hoong-Kun Fun, Valiollah Mirkhani, Reza Kia and Akbar Rostami Vartooni****S1. Comment**

Schiff bases are one of most prevalent mixed-donor ligands in the field of coordination chemistry. There has been growing interest in Schiff base ligands, mainly because of their wide application in the field of biochemistry, synthesis, and catalysis (Kia *et al.*, 2007a,b; Habibi *et al.*, 2007; Amirnasr *et al.*, 2002; Pal *et al.*, 2005; Hou *et al.*, 2001; Ren *et al.*, 2002). Many Schiff base complexes have been structurally characterized, but only a relatively small number of free Schiff bases have been characterized. As an extension of our work (Fun *et al.*, 2008a,b) on the structural characterization of Schiff base compounds, the title compound (I), (Fig. 1), is reported here.

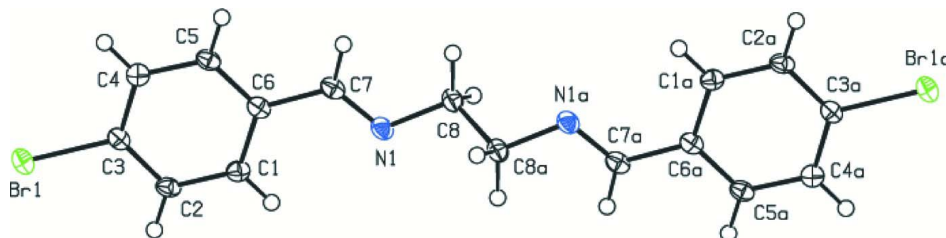
The molecule of the title compound, (I), (Fig. 1), lies across a crystallographic inversion centre and adopts an *E* configuration with respect to the azomethine C=N bond. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The asymmetric unit of the compound is composed of one-half of the molecule. The two planar units are parallel but extend in opposite directions from the methylene bridge. The interesting feature of the structure is Br \cdots Brⁱ [symmetry code: (i) 2 - x, 1 - y, 1 - z] interactions with distance 3.6307 (4) Å. In the crystal structure, molecules (Fig. 2) are arranged into columns along the *c* axis by C—H \cdots π interactions (Table 1).

S2. Experimental

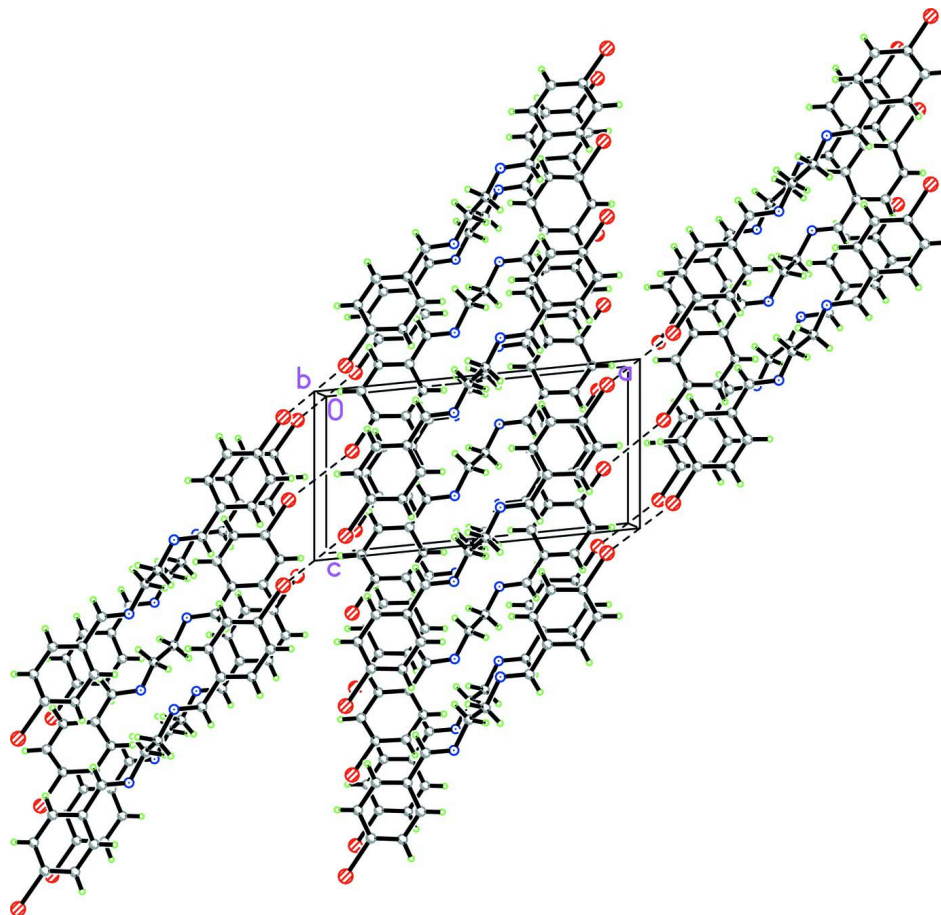
The synthetic method has been described earlier (Fun *et al.*, 2008a,b). Single crystals suitable for X-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

S3. Refinement

H atoms bound to C8 were located from the difference Fourier map and freely refined. The rest of the hydrogen atoms were positioned geometrically with C—H = 0.93 Å and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

**Figure 1**

The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms [symmetry code for a: -x, 0.5 + y, 0.5 - z].

**Figure 2**

The crystal packing, showing column arrangement of the molecules along the *c*-axis. The Br...Br contacts are shown as dashed lines.

N,N'-Bis(4-bromobenzylidene)ethane-1,2-diamine

Crystal data

$C_{16}H_{14}Br_2N_2$

$M_r = 394.11$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 13.8417\ (5)\ \text{\AA}$

$b = 7.4796\ (3)\ \text{\AA}$

$c = 7.1531\ (3)\ \text{\AA}$

$\beta = 95.692\ (1)^\circ$

$V = 736.91\ (5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 388$

$D_x = 1.776\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3320 reflections

$\theta = 3.1\text{--}31.6^\circ$

$\mu = 5.49\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, colourless

$0.45 \times 0.24 \times 0.03\ \text{mm}$

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker 2005)

$T_{\min} = 0.189$, $T_{\max} = 0.853$

10096 measured reflections

2148 independent reflections

1773 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$
 $\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 3.0^\circ$

$h = -19 \rightarrow 19$
 $k = -10 \rightarrow 9$
 $l = -10 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.069$
 $S = 1.06$
 2148 reflections
 99 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 0.1298P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.73 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.45 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.901280 (16)	0.57354 (3)	-0.36941 (3)	0.02279 (8)
N1	0.57142 (14)	0.4729 (2)	0.2936 (2)	0.0199 (4)
C1	0.67242 (16)	0.5432 (3)	-0.0377 (3)	0.0185 (4)
H1A	0.6068	0.5727	-0.0490	0.022*
C2	0.72773 (16)	0.5762 (2)	-0.1849 (3)	0.0187 (4)
H2A	0.7001	0.6316	-0.2937	0.022*
C3	0.82508 (15)	0.5259 (3)	-0.1685 (3)	0.0172 (4)
C4	0.86807 (16)	0.4432 (2)	-0.0085 (3)	0.0183 (4)
H4A	0.9327	0.4073	-0.0005	0.022*
C5	0.81247 (16)	0.4149 (2)	0.1402 (3)	0.0179 (4)
H5A	0.8408	0.3615	0.2496	0.021*
C6	0.71515 (16)	0.4652 (2)	0.1284 (3)	0.0169 (4)
C7	0.65967 (17)	0.4292 (2)	0.2901 (3)	0.0185 (4)
H7A	0.6909	0.3717	0.3944	0.022*
C8	0.52516 (17)	0.4197 (3)	0.4604 (3)	0.0202 (4)
H8A	0.4726 (17)	0.323 (3)	0.418 (3)	0.025 (6)*
H8B	0.5700 (17)	0.359 (3)	0.553 (3)	0.014 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02663 (14)	0.02485 (12)	0.01759 (12)	-0.00239 (9)	0.00569 (9)	0.00236 (8)
N1	0.0245 (9)	0.0218 (8)	0.0134 (8)	0.0011 (7)	0.0025 (7)	0.0012 (6)
C1	0.0196 (10)	0.0176 (10)	0.0178 (10)	0.0016 (7)	-0.0005 (8)	-0.0006 (7)
C2	0.0250 (11)	0.0172 (9)	0.0131 (9)	0.0030 (8)	-0.0015 (8)	0.0005 (7)
C3	0.0231 (11)	0.0143 (8)	0.0143 (9)	-0.0018 (8)	0.0024 (8)	-0.0009 (7)
C4	0.0193 (10)	0.0164 (9)	0.0188 (9)	-0.0014 (7)	0.0006 (8)	-0.0018 (7)
C5	0.0239 (11)	0.0148 (9)	0.0144 (9)	-0.0008 (8)	-0.0008 (8)	0.0002 (7)
C6	0.0249 (11)	0.0122 (8)	0.0135 (9)	-0.0011 (7)	0.0013 (8)	-0.0026 (6)
C7	0.0265 (11)	0.0155 (9)	0.0132 (9)	-0.0012 (8)	0.0002 (8)	-0.0010 (7)
C8	0.0231 (11)	0.0215 (10)	0.0167 (10)	0.0002 (8)	0.0050 (8)	0.0021 (8)

Geometric parameters (\AA , $^\circ$)

Br1—C3	1.8987 (19)	C4—C5	1.389 (3)
N1—C7	1.267 (3)	C4—H4A	0.9300
N1—C8	1.464 (3)	C5—C6	1.393 (3)
C1—C2	1.384 (3)	C5—H5A	0.9300
C1—C6	1.400 (3)	C6—C7	1.475 (3)
C1—H1A	0.9300	C7—H7A	0.9300
C2—C3	1.393 (3)	C8—C8 ⁱ	1.526 (4)
C2—H2A	0.9300	C8—H8A	1.05 (2)
C3—C4	1.383 (3)	C8—H8B	0.97 (2)
C7—N1—C8	116.51 (18)	C4—C5—H5A	119.4
C2—C1—C6	120.0 (2)	C6—C5—H5A	119.4
C2—C1—H1A	120.0	C5—C6—C1	119.23 (18)
C6—C1—H1A	120.0	C5—C6—C7	118.59 (18)
C1—C2—C3	119.43 (19)	C1—C6—C7	122.15 (19)
C1—C2—H2A	120.3	N1—C7—C6	123.10 (19)
C3—C2—H2A	120.3	N1—C7—H7A	118.5
C4—C3—C2	121.58 (18)	C6—C7—H7A	118.5
C4—C3—Br1	119.00 (15)	N1—C8—C8 ⁱ	109.9 (2)
C2—C3—Br1	119.42 (15)	N1—C8—H8A	107.5 (13)
C3—C4—C5	118.43 (19)	C8 ⁱ —C8—H8A	108.8 (13)
C3—C4—H4A	120.8	N1—C8—H8B	112.2 (12)
C5—C4—H4A	120.8	C8 ⁱ —C8—H8B	113.6 (13)
C4—C5—C6	121.22 (19)	H8A—C8—H8B	104.4 (18)
C6—C1—C2—C3	2.1 (3)	C4—C5—C6—C7	179.13 (17)
C1—C2—C3—C4	0.1 (3)	C2—C1—C6—C5	-2.6 (3)
C1—C2—C3—Br1	-179.35 (14)	C2—C1—C6—C7	179.26 (17)
C2—C3—C4—C5	-1.7 (3)	C8—N1—C7—C6	176.96 (18)
Br1—C3—C4—C5	177.70 (14)	C5—C6—C7—N1	178.68 (18)

C3—C4—C5—C6	1.2 (3)	C1—C6—C7—N1	-3.2 (3)
C4—C5—C6—C1	1.0 (3)	C7—N1—C8—C8 ⁱ	129.5 (3)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C7—H7A...Cg1	0.93	2.99	3.7143 (19)	136