Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(4-bromobenzylidene)biphenyl-2,2′-diamine

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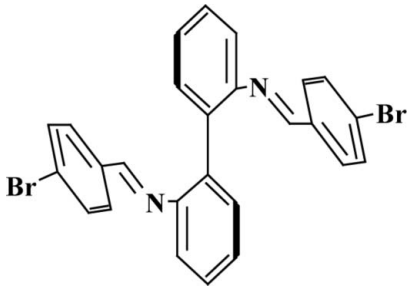
Received 7 January 2009; accepted 8 January 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.116; data-to-parameter ratio = 18.7.

The complete molecule of the title Schiff base, $C_{26}H_{18}Br_2N_2$, is generated by crystallographic twofold symmetry. The aromatic rings of the biphenylene portion of the molecule are twisted, as shown by the dihedral of 61.8 (1)° formed between them.

Related literature

There are relatively few crystallographic reports of Schiff bases formed by condensing biphenyl-2,2′-diamine with aldehydes or ketones. See: Alajarín *et al.* (2007); Coxall *et al.* (2003); Cunningham *et al.* (2004); Finder *et al.* (1973); Pruszynski *et al.* (1992).



Experimental

Crystal data

$C_{26}H_{18}Br_2N_2$ M_r = 518.24
Orthorhombic, *Aba*2
a = 15.9691 (10) Å
b = 8.3482 (5) Å
c = 16.7767 (11) Å
V = 2236.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.64 mm^{-1}
T = 295 (2) K
0.28 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.429, T_{max} = 0.545
(expected range = 0.394–0.501)
10424 measured reflections
2542 independent reflections
1333 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.116
S = 0.98
2542 reflections
136 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 1209 Friedel pairs
Flack parameter: −0.013 (15)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the Alzahra University Research Council and Natural Resources, and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2356).

References

Alajarín, M., Bonillo, B., Sánchez-Andrada, P., Vidal, Á. & Bautista, D. (2007). *J. Org. Chem.* **72**, 5863–5866.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Coxall, R. A., Lindoy, L. F., Miller, H. A., Parkin, A., Parsons, S., Tasker, P. A. & White, D. J. (2003). *Dalton Trans.* pp. 55–64.
Cunningham, D., Gilligan, K., Hannon, M., Kelly, K., McArdle, P. & O'Malley, A. (2004). *Organometallics*, **23**, 984–994.
Finder, C. J., Newton, M. G. & Allinger, N. L. (1973). *J. Chem. Soc. Perkin Trans. 2*, pp. 1929–1932.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Pruszynski, P., Leffek, K. T., Borecka, B. & Cameron, T. S. (1992). *Acta Cryst.* C**48**, 1638–1641.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, o306 [doi:10.1107/S1600536809000993]

N,*N*′-Bis(4-bromobenzylidene)biphenyl-2,2′-diamine

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S1. Experimental

Biphenyl-2,2′-diamine (5 mmol) and 4-bromobenzaldehyde (10 mmol) were dissolved in ethanol (50 ml). The solution was heated for 5 h; the solid that separated from the cooled solution was collected and recrystallized from chloroform; a second recrystallization was effected with ethanol. The yield as 90%. Analysis found: C 60.20, H 3.54, N 5.43; $C_{26}H_{18}Br_2N_2$ requires: C 60.26, H 3.50, N 5.41.

S2. Refinement

Carbon-bound H atoms were placed in calculated positions [C—H 0.93 Å and U_{iso}(H) 1.2–1.5U_{eq}(C)] and were included in the refinement in the riding-model approximation.

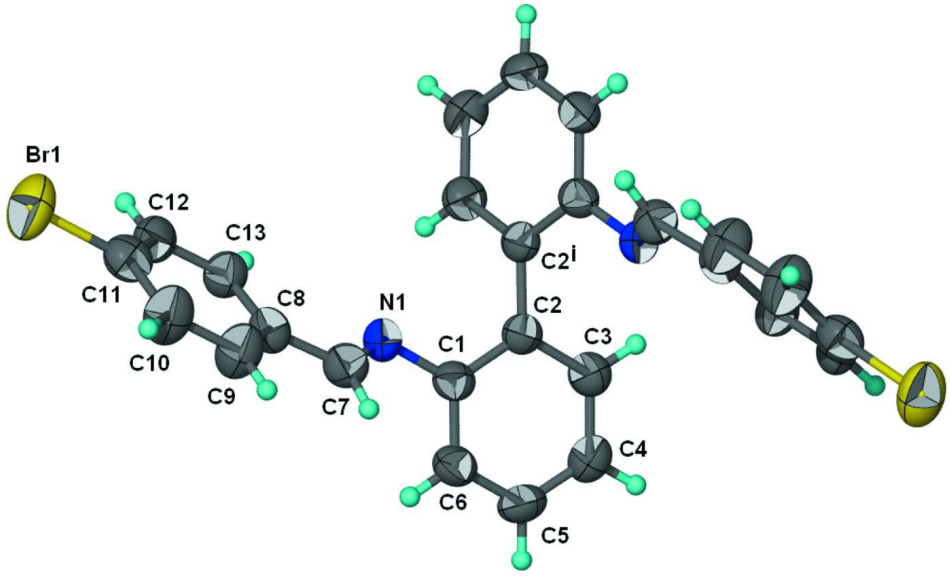

Figure 1

Thermal ellipsoid plot (Barbour, 2001); displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. (Symmetry code: *i* = 2 - *x*, 3 - *y*, *z*).

N,*N*′-Bis(4-bromobenzylidene)biphenyl-2,2′-diamine

Crystal data

$C_{26}H_{18}Br_2N_2$
M_r = 518.24
Orthorhombic, *Aba*2
Hall symbol: A 2 -2ac
a = 15.9691 (10) Å
b = 8.3482 (5) Å
c = 16.7767 (11) Å
V = 2236.6 (2) Å^3

$Z = 4$
$F(000) = 1032$
$D_x = 1.539$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5898 reflections
$\theta = 3.0$–$27.4°$
$\mu = 3.64$ mm^{-1}
$T = 295$ K
Cuboid, light yellow
0.28 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.429$, $T_{max} = 0.545$
10424 measured reflections
2542 independent reflections
1333 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -18 \rightarrow 20$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.116$
$S = 0.98$
2542 reflections
136 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Absolute structure: Flack (1983), 1209 Friedel pairs
Absolute structure parameter: −0.013 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.89090 (4)	0.63217 (6)	0.50003 (6)	0.1058 (3)
N1	0.8979 (2)	1.3119 (4)	0.7320 (3)	0.0604 (9)
C1	0.8877 (2)	1.4642 (5)	0.7689 (3)	0.0555 (10)
C2	0.9576 (2)	1.5394 (4)	0.8036 (2)	0.0537 (9)
C3	0.9461 (3)	1.6846 (5)	0.8415 (3)	0.0650 (11)
H3	0.9920	1.7371	0.8636	0.078*
C4	0.8672 (3)	1.7534 (6)	0.8471 (4)	0.0676 (13)
H4	0.8605	1.8514	0.8727	0.081*
C5	0.7989 (3)	1.6768 (5)	0.8150 (3)	0.0685 (12)
H5	0.7459	1.7214	0.8205	0.082*
C6	0.8087 (2)	1.5347 (5)	0.7748 (3)	0.0656 (12)
H6	0.7626	1.4854	0.7514	0.079*
C7	0.8654 (3)	1.2832 (7)	0.6649 (3)	0.0633 (12)
H7	0.8381	1.3663	0.6387	0.076*
C8	0.8685 (3)	1.1275 (5)	0.6264 (3)	0.0597 (11)
C9	0.8443 (3)	1.1094 (5)	0.5480 (3)	0.0818 (14)
H9	0.8236	1.1973	0.5202	0.098*
C10	0.8505 (3)	0.9629 (6)	0.5101 (4)	0.0891 (14)

H10	0.8346	0.9518	0.4570	0.107*
C11	0.8805 (3)	0.8339 (6)	0.5523 (3)	0.0714 (13)
C12	0.9015 (3)	0.8464 (5)	0.6305 (3)	0.0703 (13)
H12	0.9195	0.7566	0.6585	0.084*
C13	0.8961 (2)	0.9926 (5)	0.6683 (3)	0.0646 (11)
H13	0.9108	1.0016	0.7217	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1445 (6)	0.0704 (3)	0.1026 (5)	−0.0098 (2)	0.0284 (5)	−0.0131 (4)
N1	0.058 (2)	0.0512 (18)	0.072 (3)	−0.0048 (15)	0.0000 (19)	−0.0029 (19)
C1	0.050 (3)	0.058 (2)	0.058 (3)	0.0000 (18)	0.0025 (18)	0.009 (2)
C2	0.054 (2)	0.052 (2)	0.056 (2)	−0.0007 (16)	0.0007 (19)	0.0069 (19)
C3	0.063 (3)	0.064 (2)	0.067 (3)	−0.001 (2)	−0.005 (2)	−0.004 (2)
C4	0.081 (4)	0.057 (3)	0.065 (3)	0.004 (2)	−0.002 (3)	−0.002 (2)
C5	0.059 (3)	0.064 (2)	0.082 (3)	0.017 (2)	0.008 (2)	0.008 (2)
C6	0.052 (3)	0.065 (3)	0.080 (3)	−0.0025 (19)	0.000 (2)	0.014 (2)
C7	0.066 (3)	0.066 (3)	0.058 (3)	0.000 (2)	−0.007 (2)	0.010 (2)
C8	0.062 (2)	0.065 (3)	0.052 (3)	−0.0084 (18)	−0.002 (2)	0.001 (2)
C9	0.111 (4)	0.068 (3)	0.066 (3)	0.004 (3)	−0.020 (3)	0.002 (2)
C10	0.127 (4)	0.075 (3)	0.066 (3)	−0.001 (3)	−0.024 (4)	0.010 (3)
C11	0.065 (3)	0.084 (3)	0.065 (3)	−0.006 (2)	0.008 (2)	0.004 (3)
C12	0.070 (3)	0.058 (2)	0.083 (4)	−0.0047 (19)	−0.004 (3)	0.015 (2)
C13	0.074 (3)	0.060 (3)	0.059 (3)	0.001 (2)	−0.008 (2)	0.006 (2)

Geometric parameters (Å, º)

Br1—C11	1.906 (5)	C6—H6	0.9300
N1—C7	1.262 (6)	C7—C8	1.452 (7)
N1—C1	1.424 (6)	C7—H7	0.9300
C1—C6	1.395 (5)	C8—C9	1.378 (7)
C1—C2	1.407 (6)	C8—C13	1.399 (6)
C2—C3	1.381 (6)	C9—C10	1.383 (6)
C2—C2^{i}	1.506 (7)	C9—H9	0.9300
C3—C4	1.389 (6)	C10—C11	1.376 (7)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.373 (7)	C11—C12	1.358 (8)
C4—H4	0.9300	C12—C13	1.378 (6)
C5—C6	1.374 (6)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C7—N1—C1	120.7 (4)	N1—C7—H7	118.2
C6—C1—C2	120.0 (4)	C8—C7—H7	118.2
C6—C1—N1	120.8 (4)	C9—C8—C13	118.6 (4)
C2—C1—N1	119.2 (3)	C9—C8—C7	120.9 (4)
C3—C2—C1	118.5 (4)	C13—C8—C7	120.5 (5)
C3—C2—C2^{i}	120.2 (4)	C8—C9—C10	121.1 (4)

C1—C2—C2^{i}	121.2 (4)	C8—C9—H9	119.5
C2—C3—C4	121.0 (4)	C10—C9—H9	119.5
C2—C3—H3	119.5	C9—C10—C11	118.7 (5)
C4—C3—H3	119.5	C9—C10—H10	120.7
C5—C4—C3	120.1 (4)	C11—C10—H10	120.7
C5—C4—H4	120.0	C12—C11—C10	121.6 (5)
C3—C4—H4	120.0	C12—C11—Br1	119.4 (4)
C6—C5—C4	120.3 (4)	C10—C11—Br1	119.0 (4)
C6—C5—H5	119.8	C11—C12—C13	119.8 (5)
C4—C5—H5	119.8	C11—C12—H12	120.1
C5—C6—C1	120.1 (4)	C13—C12—H12	120.1
C5—C6—H6	119.9	C12—C13—C8	120.1 (5)
C1—C6—H6	119.9	C12—C13—H13	119.9
N1—C7—C8	123.6 (5)	C8—C13—H13	119.9

C7—N1—C1—C6	48.5 (6)	C1—N1—C7—C8	−175.6 (4)
C7—N1—C1—C2	−135.0 (5)	N1—C7—C8—C9	−169.2 (5)
C6—C1—C2—C3	−1.4 (6)	N1—C7—C8—C13	10.8 (7)
N1—C1—C2—C3	−177.9 (4)	C13—C8—C9—C10	−2.8 (8)
C6—C1—C2—C2^{i}	175.4 (3)	C7—C8—C9—C10	177.2 (5)
N1—C1—C2—C2^{i}	−1.1 (5)	C8—C9—C10—C11	0.6 (8)
C1—C2—C3—C4	1.6 (6)	C9—C10—C11—C12	2.1 (7)
C2^{i}—C2—C3—C4	−175.3 (4)	C9—C10—C11—Br1	−179.0 (4)
C2—C3—C4—C5	0.2 (8)	C10—C11—C12—C13	−2.7 (7)
C3—C4—C5—C6	−2.2 (8)	Br1—C11—C12—C13	178.5 (3)
C4—C5—C6—C1	2.4 (7)	C11—C12—C13—C8	0.4 (7)
C2—C1—C6—C5	−0.6 (7)	C9—C8—C13—C12	2.2 (7)
N1—C1—C6—C5	175.9 (4)	C7—C8—C13—C12	−177.8 (4)

Symmetry code: (i) −*x*+2, −*y*+3, *z*.