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

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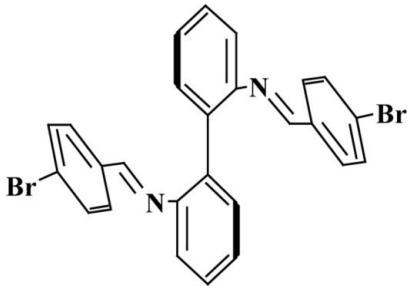
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.034; wR factor = 0.116; data-to-parameter ratio = 18.7.

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).

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

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supplementary materials

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

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

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Comment

(type here to add)

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.

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.

Figures

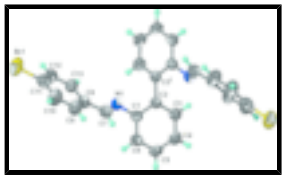

Fig. 1. Thermal ellipsoid plot (Barbour, 2001); displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. (Symmetry code: *i* = 2 - *x*, 3 - *y*, *z*).

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

Crystal data

$C_{26}H_{18}Br_2N_2$	F_{000} = 1032
M_r = 518.24	D_x = 1.539 Mg m^{-3}
Orthorhombic, *Aba*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: A 2 -2ac	Cell parameters from 5898 reflections
a = 15.9691 (10) Å	θ = 3.0–27.4°
b = 8.3482 (5) Å	μ = 3.64 mm^{-1}
c = 16.7767 (11) Å	*T* = 295 (2) K
V = 2236.6 (2) Å^3	Cuboid, light yellow
Z = 4	0.28 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2542 independent reflections
Radiation source: fine-focus sealed tube	1333 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.4°$
$T = 295(2)$ K	$\theta_{min} = 3.0°$
ω scans	$h = -18 \rightarrow 20$
Absorption correction: Multi-scan (ABSCOR; Higashi, 1995)	$k = -10 \rightarrow 10$
$T_{min} = 0.429$, $T_{max} = 0.545$	$l = -21 \rightarrow 21$
10424 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.116$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.98$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
2542 reflections	$\Delta\rho_{min} = -0.36$ e Å^{-3}
136 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1209 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.013 (15)
Secondary atom site location: difference Fourier map	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	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 (Å^2)

	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, °)

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 codes: (i) −*x*+2, −*y*+3, *z*.

Fig. 1