Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(3-phenylallylidene)biphenyl-2,2′-diamine

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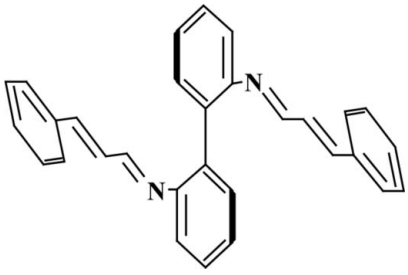
Received 7 January 2009; accepted 7 January 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.110; data-to-parameter ratio = 9.8.

In the title Schiff base, $C_{30}H_{24}N_2$, the complete molecule is generated by a crystallographic twofold axis; the aromatic rings of the biphenyl unit are twisted by 60.78 (1)°. The imine double bond has a *trans* configuration.

Related literature

For a list of the crystal structures of Schiff bases formed by condensing biphenyl-2,2′-diamine with aldehydes or ketones, see: Dehghanpour *et al.* (2009).



Experimental

Crystal data

$C_{30}H_{24}N_2$
M_r = 412.51
Orthorhombic, *Fdd*2
a = 15.4354 (12) Å
b = 31.783 (2) Å
c = 9.6188 (8) Å
V = 4718.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 (2) K
0.27 × 0.21 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.982, T_{max} = 0.989
11331 measured reflections
1427 independent reflections
1021 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.110
S = 1.07
1427 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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: BT2848).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Dehghanpour, S., Asadizadeh, S., Gao, S. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o306.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
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.

supplementary materials

Acta Cryst. (2009). E**65**, o307 [**doi:10.1107/S1600536809000804**]

N,*N*'-Bis(3-phenylallylidene)biphenyl-2,2'-diamine

S. Dehghanpour, F. Afshariazar, S. Gao and S. W. Ng

Experimental

Biphenyl-2,2'-diamine (5 mmol) and cinnamaldehyde (10 mmol) were dissolved in diethyl ether (50 ml). The mixture was stirred for 30 min. Evaporation of the solvent gave a solid that was recrystallized from ethanol twice. Yield: 80%. CH&N elemental analysis. Calculated for $C_{30}H_{24}N_2$: C 87.35, H 5.86, N 6.79%; found: C 87.30, H 5.81, N 9.82%.

Refinement

H atoms were placed in calculated positions [C—H 0.93 Å and U_{iso}(H) 1.2U_{eq}(C)], and were included in the refinement in the riding-model approximation. Friedel pairs were merged

Figures

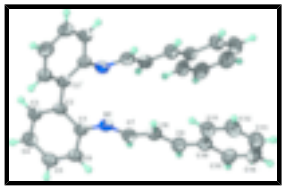


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001); displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. (Symmetry code *i*: -*x*, -*y*, *z*).

N,*N*'-Bis(3-phenylallylidene)biphenyl-2,2'-diamine

Crystal data

$C_{30}H_{24}N_2$	F_{000} = 1744
M_r = 412.51	D_x = 1.161 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 7049 reflections
a = 15.4354 (12) Å	θ = 3.2–27.5º
b = 31.783 (2) Å	μ = 0.07 mm^{-1}
c = 9.6188 (8) Å	*T* = 295 (2) K
V = 4718.8 (6) Å^3	Cuboid, light yellow
Z = 8	0.27 × 0.21 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	1427 independent reflections
Radiation source: fine-focus sealed tube	1021 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.029
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.2º
ω scans	h = −20→19
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −41→41
T_{min} = 0.982, T_{max} = 0.989	l = −12→12
11331 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.034	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.110	H-atom parameters constrained
S = 1.07	$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 0.8672P]$ where $P = (F_o^2 + 2F_c^2)/3$
1427 reflections	$(\Delta/\sigma)_{max}$ = 0.001
145 parameters	$\Delta\rho_{max}$ = 0.11 e Å^{-3}
1 restraint	$\Delta\rho_{min}$ = −0.15 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	−0.01193 (13)	0.05064 (6)	0.5676 (2)	0.0523 (5)
C2	−0.02328 (13)	0.02045 (6)	0.4634 (2)	0.0541 (5)
C3	−0.07746 (15)	0.02974 (7)	0.3523 (3)	0.0641 (6)
H3A	−0.0859	0.0097	0.2831	0.077*
C4	−0.11943 (16)	0.06833 (8)	0.3424 (3)	0.0724 (7)
H4A	−0.1561	0.0739	0.2679	0.087*
C5	−0.10622 (16)	0.09796 (7)	0.4433 (3)	0.0695 (7)
H5A	−0.1333	0.1240	0.4363	0.083*
C6	−0.05334 (14)	0.08962 (6)	0.5546 (3)	0.0609 (6)
H6A	−0.0449	0.1101	0.6223	0.073*
C7	0.03355 (16)	0.05664 (7)	0.7976 (3)	0.0598 (6)
H7A	−0.0185	0.0702	0.8165	0.072*
C8	0.09664 (17)	0.05217 (7)	0.9066 (3)	0.0629 (6)
H8A	0.1467	0.0370	0.8870	0.075*
C9	0.08822 (15)	0.06818 (7)	1.0333 (3)	0.0637 (6)

H9A	0.0374	0.0829	1.0516	0.076*
C10	0.15066 (15)	0.06500 (7)	1.1471 (3)	0.0588 (6)
C11	0.22801 (16)	0.04272 (7)	1.1346 (3)	0.0669 (6)
H11A	0.2417	0.0301	1.0502	0.080*
C12	0.28461 (18)	0.03901 (9)	1.2443 (3)	0.0771 (8)
H12A	0.3361	0.0241	1.2337	0.093*
C13	0.2651 (2)	0.05718 (9)	1.3688 (3)	0.0822 (8)
H13A	0.3033	0.0547	1.4431	0.099*
C14	0.18916 (19)	0.07916 (10)	1.3845 (3)	0.0829 (8)
H14A	0.1758	0.0913	1.4697	0.099*
C15	0.13291 (17)	0.08318 (8)	1.2745 (3)	0.0703 (7)
H15A	0.0820	0.0984	1.2860	0.084*
N1	0.04738 (12)	0.04246 (5)	0.6758 (2)	0.0584 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0562 (11)	0.0430 (9)	0.0576 (14)	0.0011 (8)	0.0025 (11)	0.0017 (9)
C2	0.0626 (11)	0.0412 (10)	0.0584 (14)	0.0000 (9)	0.0012 (11)	0.0017 (9)
C3	0.0792 (15)	0.0510 (11)	0.0622 (15)	0.0019 (11)	−0.0095 (13)	−0.0006 (11)
C4	0.0809 (15)	0.0638 (13)	0.0725 (16)	0.0109 (12)	−0.0124 (14)	0.0089 (12)
C5	0.0807 (15)	0.0509 (11)	0.0770 (18)	0.0140 (11)	0.0009 (15)	0.0072 (12)
C6	0.0714 (13)	0.0432 (9)	0.0681 (15)	0.0043 (9)	0.0024 (13)	−0.0018 (10)
C7	0.0649 (13)	0.0496 (11)	0.0648 (16)	−0.0036 (10)	−0.0008 (13)	0.0007 (11)
C8	0.0707 (14)	0.0538 (11)	0.0641 (16)	0.0005 (10)	−0.0006 (12)	−0.0019 (12)
C9	0.0645 (13)	0.0638 (13)	0.0627 (16)	0.0013 (11)	0.0043 (13)	−0.0040 (12)
C10	0.0632 (13)	0.0539 (11)	0.0593 (14)	−0.0054 (10)	0.0053 (12)	−0.0010 (10)
C11	0.0663 (14)	0.0743 (14)	0.0600 (16)	0.0005 (11)	0.0086 (12)	0.0008 (12)
C12	0.0688 (15)	0.0864 (18)	0.076 (2)	0.0019 (13)	0.0035 (14)	0.0137 (15)
C13	0.0814 (17)	0.0908 (19)	0.074 (2)	−0.0112 (15)	−0.0109 (17)	0.0062 (16)
C14	0.100 (2)	0.0861 (17)	0.0621 (18)	−0.0064 (16)	−0.0005 (17)	−0.0145 (15)
C15	0.0763 (15)	0.0673 (13)	0.0673 (17)	0.0006 (12)	0.0044 (14)	−0.0112 (13)
N1	0.0707 (11)	0.0445 (8)	0.0599 (13)	0.0019 (8)	−0.0044 (10)	−0.0029 (9)

Geometric parameters (Å, °)

C1—C2	1.399 (3)	C8—C9	1.327 (4)
C1—C6	1.400 (3)	C8—H8A	0.9300
C1—N1	1.410 (3)	C9—C10	1.461 (3)
C2—C3	1.389 (3)	C9—H9A	0.9300
C2—C2^{i}	1.485 (4)	C10—C15	1.383 (4)
C3—C4	1.390 (3)	C10—C11	1.393 (3)
C3—H3A	0.9300	C11—C12	1.375 (4)
C4—C5	1.368 (4)	C11—H11A	0.9300
C4—H4A	0.9300	C12—C13	1.362 (4)
C5—C6	1.373 (4)	C12—H12A	0.9300
C5—H5A	0.9300	C13—C14	1.373 (4)
C6—H6A	0.9300	C13—H13A	0.9300

C7—N1	1.273 (3)	C14—C15	1.375 (4)
C7—C8	1.438 (4)	C14—H14A	0.9300
C7—H7A	0.9300	C15—H15A	0.9300
C2—C1—C6	119.1 (2)	C7—C8—H8A	117.8
C2—C1—N1	118.93 (17)	C8—C9—C10	126.6 (2)
C6—C1—N1	121.7 (2)	C8—C9—H9A	116.7
C3—C2—C1	118.76 (18)	C10—C9—H9A	116.7
C3—C2—C2^{i}	118.52 (15)	C15—C10—C11	117.3 (2)
C1—C2—C2^{i}	122.67 (16)	C15—C10—C9	120.3 (2)
C2—C3—C4	121.4 (2)	C11—C10—C9	122.4 (2)
C2—C3—H3A	119.3	C12—C11—C10	121.5 (3)
C4—C3—H3A	119.3	C12—C11—H11A	119.3
C5—C4—C3	119.3 (3)	C10—C11—H11A	119.3
C5—C4—H4A	120.4	C13—C12—C11	119.8 (3)
C3—C4—H4A	120.4	C13—C12—H12A	120.1
C4—C5—C6	120.6 (2)	C11—C12—H12A	120.1
C4—C5—H5A	119.7	C12—C13—C14	120.1 (3)
C6—C5—H5A	119.7	C12—C13—H13A	120.0
C5—C6—C1	120.8 (2)	C14—C13—H13A	120.0
C5—C6—H6A	119.6	C13—C14—C15	120.1 (3)
C1—C6—H6A	119.6	C13—C14—H14A	119.9
N1—C7—C8	121.5 (2)	C15—C14—H14A	119.9
N1—C7—H7A	119.3	C14—C15—C10	121.2 (2)
C8—C7—H7A	119.3	C14—C15—H15A	119.4
C9—C8—C7	124.4 (2)	C10—C15—H15A	119.4
C9—C8—H8A	117.8	C7—N1—C1	120.32 (19)
C6—C1—C2—C3	−1.9 (3)	C8—C9—C10—C15	−179.7 (2)
N1—C1—C2—C3	−175.9 (2)	C8—C9—C10—C11	−2.0 (4)
C6—C1—C2—C2^{i}	175.3 (2)	C15—C10—C11—C12	−0.2 (4)
N1—C1—C2—C2^{i}	1.4 (3)	C9—C10—C11—C12	−177.9 (2)
C1—C2—C3—C4	0.7 (3)	C10—C11—C12—C13	0.4 (4)
C2^{i}—C2—C3—C4	−176.6 (2)	C11—C12—C13—C14	0.0 (5)
C2—C3—C4—C5	0.8 (4)	C12—C13—C14—C15	−0.5 (5)
C3—C4—C5—C6	−1.1 (4)	C13—C14—C15—C10	0.7 (5)
C4—C5—C6—C1	−0.1 (4)	C11—C10—C15—C14	−0.4 (4)
C2—C1—C6—C5	1.7 (3)	C9—C10—C15—C14	177.4 (2)
N1—C1—C6—C5	175.4 (2)	C8—C7—N1—C1	−174.1 (2)
N1—C7—C8—C9	176.2 (2)	C2—C1—N1—C7	−147.5 (2)
C7—C8—C9—C10	−179.2 (2)	C6—C1—N1—C7	38.7 (3)

Symmetry codes: (i) −*x*, −*y*, *z*.

Fig. 1