Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Saeed Dehghanpour,[a]* Farzaneh Afshariazar,[a] Shan Gao[b] and Seik Weng Ng[c]

[a]Department of Chemistry, Alzahra University, Vanak, Tehran, Iran, [b]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: dehganpour_farasha@yahoo.com

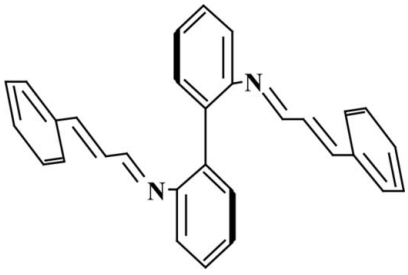
Received 7 January 2009; accepted 7 January 2009

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.

supporting information

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

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

Saeed Dehghanpour, Farzaneh Afshariazar, Shan Gao and Seik Weng Ng

S1. 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%.

S2. 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

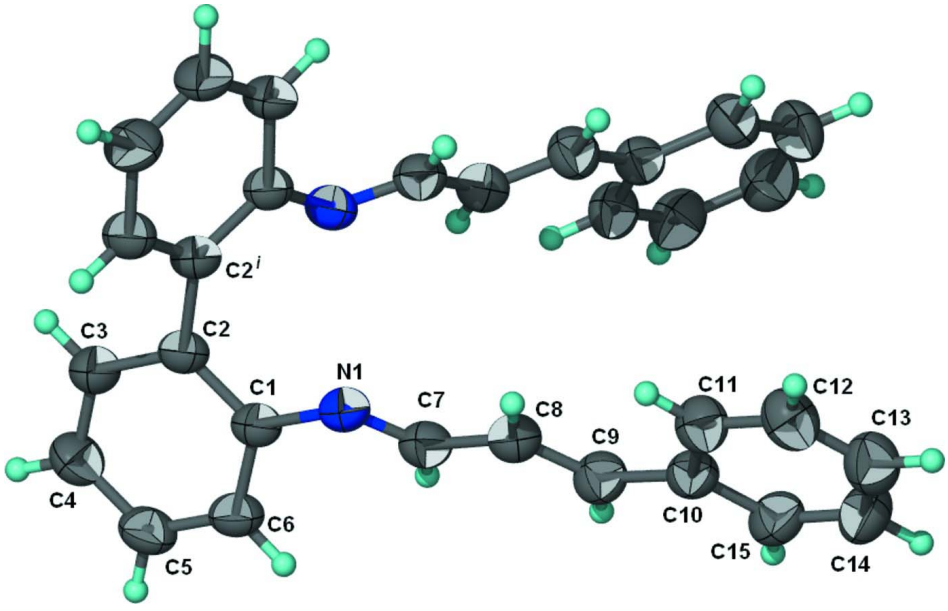


Figure 1

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

$C_{30}H_{24}N_2$
M_r = 412.51
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
a = 15.4354 (12) Å
b = 31.783 (2) Å
c = 9.6188 (8) Å
V = 4718.8 (6) Å^3
Z = 8
F(000) = 1744

D_x = 1.161 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7049 reflections
θ = 3.2–27.5°
μ = 0.07 mm^{-1}
T = 295 K
Cuboid, light yellow
0.27 × 0.21 × 0.16 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} = 0.982, T_{max} = 0.989
11331 measured reflections
1427 independent reflections
1021 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −20→19
k = −41→41
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.110
S = 1.07
1427 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 0.8672P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −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 (Å²)

	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, º)

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