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Biphenyl-4-carbaldehyde azine

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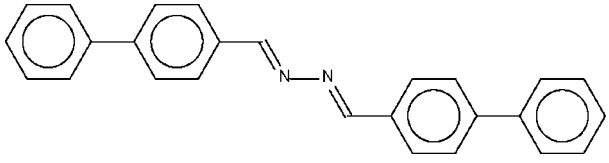
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.127; data-to-parameter ratio = 16.6.

The complete molecule of the title compound, $C_{26}H_{20}N_2$, is generated by crystallographic inversion symmetry. The terminal phenyl ring is twisted by 19.2 (1)° with respect to the adjacent phenylene ring.

Related literature

For the synthesis, see: Malkes & Timchenko (1961). For biological evaluation, see: Cremlyn *et al.* (1991). The compound is a formylating agent for aromatic compounds; see: Kantlehner *et al.* (2004). When treated with cerium ammonium nitrate, the aldehyde is regenerated; see Giurg & Mlochowski (1999).



Experimental

Crystal data

$C_{26}H_{20}N_2$ M_r = 360.44
Monoclinic, $P2_1/c$
a = 20.5417 (6) Å
b = 7.1358 (2) Å
c = 6.3402 (2) Å
β = 93.632 (2)°
V = 927.49 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
0.40 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: none
6044 measured reflections
2104 independent reflections
1607 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.127
S = 1.05
2104 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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, 2008).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2856).

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supporting information

Acta Cryst. (2008). E**64**, o2444 [doi:10.1107/S1600536808038622]

Biphenyl-4-carbaldehyde azine

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S1. Comment

The complete molecule of the title compound, (I) is generated by crystallographic inversion symmetry (Fig. 1). The terminal phenyl ring is twisted by 19.2 (1) ° with respect to the phenylene ring.

S2. Experimental

4-Phenyl benzaldehyde (0.72 g, 4 mmol) and 80% hydrazine hydrate (0.10 g, 2 mmol) were heated in ethanol (25 ml) for 1 h. The resulting product was filtered and washed with ethanol and then recrystallized from hexane to yield yellow prisms of (I).

S3. Refinement

The H atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with U(H) = 1.2U(C).

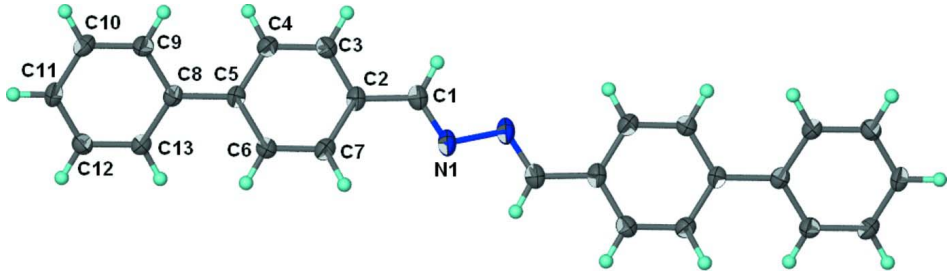

Figure 1

The molecular structure of (I) with atoms shown at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radiius. The unlabelled atoms are generated by the symmetry operation (1–x, 1–y, 1–z).

Biphenyl-4-carbaldehyde azine

Crystal data

$C_{26}H_{20}N_2$
M_r = 360.44
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 20.5417 (6) Å
b = 7.1358 (2) Å
c = 6.3402 (2) Å
β = 93.632 (2)°
V = 927.49 (5) Å^3
Z = 2
F(000) = 380
D_x = 1.291 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1869 reflections
θ = 2.9–26.2°
μ = 0.08 mm^{-1}
T = 100 K
Prism, yellow
0.40 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6044 measured reflections
2104 independent reflections
1607 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.0°$
$h = -25 \rightarrow 26$
$k = -8 \rightarrow 9$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.127$
$S = 1.06$
2104 reflections
127 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.2493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.46654 (6)	0.48506 (18)	0.47390 (19)	0.0260 (3)
C1	0.45139 (7)	0.5211 (2)	0.2795 (2)	0.0229 (3)
H1	0.4847	0.5598	0.1916	0.027*
C2	0.38464 (7)	0.50463 (19)	0.1880 (2)	0.0202 (3)
C3	0.37032 (7)	0.5594 (2)	−0.0206 (2)	0.0218 (3)
H3	0.4045	0.6006	−0.1034	0.026*
C4	0.30685 (7)	0.5548 (2)	−0.1095 (2)	0.0205 (3)
H4	0.2983	0.5927	−0.2522	0.025*
C5	0.25534 (6)	0.49541 (19)	0.0078 (2)	0.0169 (3)
C6	0.27039 (7)	0.43846 (19)	0.2177 (2)	0.0198 (3)
H6	0.2363	0.3972	0.3008	0.024*
C7	0.33352 (7)	0.4412 (2)	0.3054 (2)	0.0212 (3)
H7	0.3424	0.3998	0.4467	0.025*
C8	0.18693 (6)	0.49529 (18)	−0.08434 (19)	0.0170 (3)
C9	0.16848 (7)	0.60293 (19)	−0.2631 (2)	0.0202 (3)
H9	0.2005	0.6745	−0.3287	0.024*
C10	0.10445 (7)	0.6072 (2)	−0.3461 (2)	0.0215 (3)
H10	0.0932	0.6811	−0.4676	0.026*
C11	0.05681 (7)	0.5041 (2)	−0.2529 (2)	0.0200 (3)
H11	0.0128	0.5083	−0.3084	0.024*
C12	0.07425 (6)	0.39455 (19)	−0.0772 (2)	0.0197 (3)

H12	0.0420	0.3224	−0.0132	0.024*
C13	0.13839 (6)	0.38970 (19)	0.0054 (2)	0.0186 (3)
H13	0.1496	0.3133	0.1249	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0154 (6)	0.0334 (7)	0.0285 (7)	−0.0007 (5)	−0.0034 (5)	−0.0004 (5)
C1	0.0174 (7)	0.0249 (8)	0.0261 (7)	0.0009 (5)	−0.0003 (5)	−0.0009 (6)
C2	0.0171 (7)	0.0195 (7)	0.0235 (7)	0.0013 (5)	−0.0018 (5)	−0.0020 (5)
C3	0.0181 (7)	0.0244 (7)	0.0231 (7)	−0.0002 (5)	0.0028 (5)	0.0015 (5)
C4	0.0205 (7)	0.0229 (7)	0.0178 (6)	0.0009 (5)	0.0002 (5)	0.0015 (5)
C5	0.0168 (7)	0.0149 (6)	0.0187 (6)	0.0012 (5)	−0.0017 (5)	−0.0015 (5)
C6	0.0188 (7)	0.0209 (7)	0.0196 (6)	−0.0007 (5)	0.0013 (5)	0.0015 (5)
C7	0.0221 (7)	0.0225 (7)	0.0186 (6)	0.0005 (5)	−0.0020 (5)	0.0007 (5)
C8	0.0185 (7)	0.0164 (6)	0.0160 (6)	0.0012 (5)	−0.0010 (5)	−0.0028 (5)
C9	0.0203 (7)	0.0201 (7)	0.0200 (6)	−0.0024 (5)	0.0000 (5)	0.0025 (5)
C10	0.0245 (7)	0.0213 (7)	0.0182 (6)	0.0011 (5)	−0.0036 (5)	0.0020 (5)
C11	0.0170 (7)	0.0227 (7)	0.0197 (6)	0.0018 (5)	−0.0037 (5)	−0.0036 (5)
C12	0.0185 (7)	0.0210 (7)	0.0196 (6)	−0.0016 (5)	0.0022 (5)	−0.0010 (5)
C13	0.0195 (7)	0.0191 (7)	0.0169 (6)	0.0008 (5)	−0.0004 (5)	0.0010 (5)

Geometric parameters (Å, º)

N1—C1	1.2784 (19)	C6—H6	0.9500
N1—N1^{i}	1.410 (2)	C7—H7	0.9500
C1—C2	1.4592 (18)	C8—C13	1.3989 (18)
C1—H1	0.9500	C8—C9	1.4012 (18)
C2—C3	1.3927 (18)	C9—C10	1.3858 (19)
C2—C7	1.4006 (19)	C9—H9	0.9500
C3—C4	1.3874 (18)	C10—C11	1.3863 (19)
C3—H3	0.9500	C10—H10	0.9500
C4—C5	1.3969 (19)	C11—C12	1.3888 (19)
C4—H4	0.9500	C11—H11	0.9500
C5—C6	1.4073 (18)	C12—C13	1.3870 (18)
C5—C8	1.4873 (17)	C12—H12	0.9500
C6—C7	1.3784 (18)	C13—H13	0.9500
C1—N1—N1^{i}	111.73 (15)	C6—C7—H7	119.7
N1—C1—C2	122.17 (13)	C2—C7—H7	119.7
N1—C1—H1	118.9	C13—C8—C9	117.44 (12)
C2—C1—H1	118.9	C13—C8—C5	121.38 (11)
C3—C2—C7	118.38 (12)	C9—C8—C5	121.17 (12)
C3—C2—C1	119.45 (13)	C10—C9—C8	121.38 (12)
C7—C2—C1	122.14 (12)	C10—C9—H9	119.3
C4—C3—C2	121.03 (12)	C8—C9—H9	119.3
C4—C3—H3	119.5	C9—C10—C11	120.34 (12)
C2—C3—H3	119.5	C9—C10—H10	119.8

C3—C4—C5	121.01 (12)	C11—C10—H10	119.8
C3—C4—H4	119.5	C10—C11—C12	119.17 (12)
C5—C4—H4	119.5	C10—C11—H11	120.4
C4—C5—C6	117.55 (12)	C12—C11—H11	120.4
C4—C5—C8	121.34 (11)	C13—C12—C11	120.49 (13)
C6—C5—C8	121.11 (12)	C13—C12—H12	119.8
C7—C6—C5	121.48 (12)	C11—C12—H12	119.8
C7—C6—H6	119.3	C12—C13—C8	121.16 (12)
C5—C6—H6	119.3	C12—C13—H13	119.4
C6—C7—C2	120.53 (12)	C8—C13—H13	119.4
N1^{i}—N1—C1—C2	−178.70 (14)	C4—C5—C8—C13	161.70 (13)
N1—C1—C2—C3	175.14 (14)	C6—C5—C8—C13	−19.36 (19)
N1—C1—C2—C7	−2.6 (2)	C4—C5—C8—C9	−19.07 (19)
C7—C2—C3—C4	1.2 (2)	C6—C5—C8—C9	159.86 (13)
C1—C2—C3—C4	−176.66 (13)	C13—C8—C9—C10	0.99 (19)
C2—C3—C4—C5	0.1 (2)	C5—C8—C9—C10	−178.27 (12)
C3—C4—C5—C6	−0.8 (2)	C8—C9—C10—C11	0.1 (2)
C3—C4—C5—C8	178.21 (13)	C9—C10—C11—C12	−0.9 (2)
C4—C5—C6—C7	0.1 (2)	C10—C11—C12—C13	0.7 (2)
C8—C5—C6—C7	−178.86 (12)	C11—C12—C13—C8	0.5 (2)
C5—C6—C7—C2	1.2 (2)	C9—C8—C13—C12	−1.26 (19)
C3—C2—C7—C6	−1.8 (2)	C5—C8—C13—C12	177.99 (12)
C1—C2—C7—C6	175.96 (13)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.