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2-Benzyloxybenzaldehyde azine

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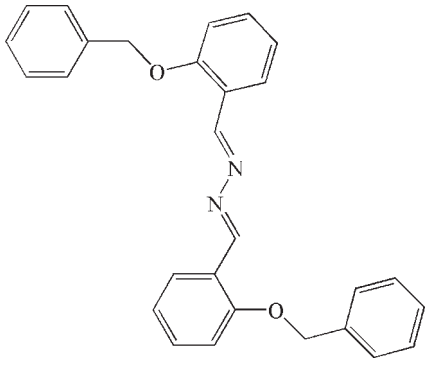
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.119; data-to-parameter ratio = 14.6.

The complete molecule of the title compound, $C_{28}H_{24}N_2O_2$, is generated by a centre of inversion (at the mid-point of the N—N bond). The substituents at the ends of the C=N bonds adopt an *E*,*E* configuration. The central –CH=N—N=CH– fragment is planar, but as a whole the molecule is not: the benzyloxy group is rotated about the O—C bond by 69.3 (2)° with respect to the plane of the benzylidene hydrazine unit.

Related literature

For general background to the coordination capability and biological activity of Schiff bases, see: Amadei *et al.* (1998); Xu *et al.* (2007). For related structures, see: Glidewell *et al.* (2006); Chattopadhyay *et al.* (2008). For the synthesis, see: Fu (2007).



Experimental

Crystal data

$C_{28}H_{24}N_2O_2$
M_r = 420.49
Monoclinic, $P2_1/n$
a = 11.222 (2) Å
b = 8.1157 (15) Å
c = 12.799 (2) Å
β = 102.297 (3)°
V = 1138.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 K
0.30 × 0.22 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
8428 measured reflections
2125 independent reflections
1143 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.119
S = 1.02
2125 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2064).

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Xu, C., Mao, H. Y., Shen, X. Q., Zhang, H. Y., Liu, H. L., Wu, Q. A., Hou, H. W. & Zhu, Y. (2007). *J. Coord. Chem.* **60**, 193–200.

supporting information

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2-Benzyloxybenzaldehyde azine

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S1. Comment

Schiff bases have received much attention during the past decades because of their strong coordination capability and diverse biological activities (Amadei *et al.*, 1998; Xu *et al.*, 2007). Among them, azines are obtained from the condensation of an aldehyde or ketone with hydrazine.

The title compound possesses a crystallographically imposed center of symmetry at the midpoint of the N—N bond (Fig.1). It adopts an *E*, *E* configuration, which is similar to those of the related compounds (Glidewell, *et al.*, 2007; Chattopadhyay *et al.*, 2008). The C7—N1 [1.266 (2) Å] and N1—N1A [1.414 (3) Å] distances indicate these correspond to double and single bonds, respectively. The central –CH=N—N=CH– fragment is planar, but as a whole the molecule is not planar. The benzyloxy group is rotated about the O—C bond by 69.3 (2)° with respect to the plane of the benzylidene hydrazine moiety.

S2. Experimental

The title compound was prepared as described in literature (Fu, 2007) and recrystallized from ethanol at room temperature to give the desired crystals suitable for single-crystal X-ray diffraction.

S3. Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with U_{iso}(H)=1.2–1.5U_{eq}(C).

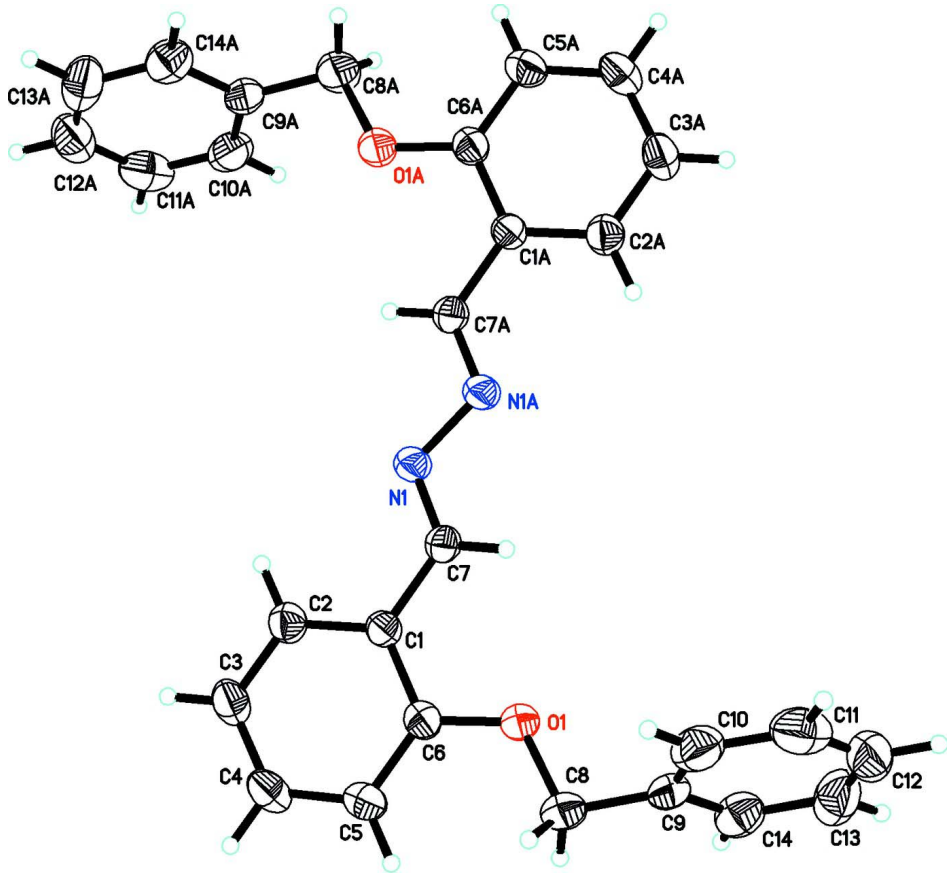

Figure 1

The molecular structure of the title compound with displacement ellipsoids at the 30% probability level (suffix A denotes the symmetry code: -*x* + 2, -*y*, -*z*).

2-Benzyloxybenzaldehyde azine

Crystal data

$C_{28}H_{24}N_2O_2$
$M_r = 420.49$
Monoclinic, $P2_1/n$
$a = 11.222\ (2)$ Å
$b = 8.1157\ (15)$ Å
$c = 12.799\ (2)$ Å
$\beta = 102.297\ (3)°$
$V = 1138.9\ (4)$ Å^3
$Z = 2$
$F(000) = 444$
$D_x = 1.226$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 930 reflections
$\theta = 2.7–20.6°$
$\mu = 0.08$ mm^{-1}
$T = 294$ K
BLOCK, yellow
0.30 × 0.22 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
8428 measured reflections
2125 independent reflections
1143 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.7°$
$h = -13\rightarrow13$
$k = -9\rightarrow9$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 1.02$
2125 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.1257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.015 (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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.76645 (18)	0.1813 (2)	−0.07028 (15)	0.0456 (5)
C2	0.7692 (2)	0.2275 (3)	−0.17414 (17)	0.0558 (6)
H2	0.8364	0.1990	−0.2022	0.067*
C3	0.6754 (2)	0.3140 (3)	−0.23634 (18)	0.0665 (7)
H3	0.6790	0.3436	−0.3058	0.080*
C4	0.5764 (2)	0.3566 (3)	−0.1955 (2)	0.0692 (7)
H4	0.5130	0.4163	−0.2374	0.083*
C5	0.5694 (2)	0.3123 (3)	−0.09323 (19)	0.0651 (7)
H5	0.5013	0.3405	−0.0665	0.078*
C6	0.66432 (19)	0.2253 (3)	−0.03029 (17)	0.0529 (6)
C7	0.86788 (18)	0.0949 (2)	−0.00285 (16)	0.0475 (5)
H7	0.8684	0.0807	0.0693	0.057*
C8	0.5779 (2)	0.2404 (4)	0.1251 (2)	0.0907 (9)
H8A	0.4976	0.1985	0.0925	0.109*
H8B	0.5762	0.3596	0.1194	0.109*
C9	0.6111 (2)	0.1903 (3)	0.2398 (2)	0.0626 (7)
C10	0.7017 (2)	0.2695 (3)	0.3102 (3)	0.0799 (8)
H10	0.7445	0.3551	0.2866	0.096*
C11	0.7299 (3)	0.2228 (5)	0.4164 (3)	0.0935 (9)

H11	0.7907	0.2782	0.4643	0.112*
C12	0.6691 (4)	0.0959 (5)	0.4514 (2)	0.0952 (10)
H12	0.6888	0.0640	0.5228	0.114*
C13	0.5805 (3)	0.0169 (4)	0.3821 (3)	0.0938 (9)
H13	0.5391	−0.0699	0.4059	0.113*
C14	0.5506 (2)	0.0633 (3)	0.2766 (2)	0.0742 (8)
H14	0.4888	0.0081	0.2297	0.089*
N1	0.95554 (14)	0.0385 (2)	−0.04001 (12)	0.0503 (5)
O1	0.66609 (13)	0.17497 (19)	0.07219 (12)	0.0690 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0451 (12)	0.0464 (13)	0.0445 (12)	0.0027 (10)	0.0074 (10)	0.0012 (10)
C2	0.0595 (14)	0.0573 (14)	0.0508 (14)	0.0035 (12)	0.0126 (12)	0.0019 (11)
C3	0.0826 (18)	0.0636 (16)	0.0512 (14)	0.0121 (14)	0.0092 (14)	0.0112 (12)
C4	0.0698 (17)	0.0688 (17)	0.0615 (16)	0.0169 (13)	−0.0027 (14)	0.0088 (13)
C5	0.0565 (15)	0.0718 (17)	0.0654 (16)	0.0181 (13)	0.0095 (13)	0.0077 (13)
C6	0.0550 (14)	0.0542 (14)	0.0496 (13)	0.0073 (11)	0.0113 (11)	0.0055 (11)
C7	0.0486 (12)	0.0534 (13)	0.0411 (12)	0.0016 (10)	0.0104 (10)	−0.0024 (10)
C8	0.0831 (18)	0.124 (2)	0.0752 (19)	0.0530 (17)	0.0391 (16)	0.0188 (17)
C9	0.0586 (15)	0.0706 (17)	0.0656 (17)	0.0217 (13)	0.0291 (13)	0.0060 (14)
C10	0.0663 (18)	0.080 (2)	0.100 (2)	0.0011 (15)	0.0325 (17)	0.0067 (17)
C11	0.0693 (19)	0.113 (3)	0.092 (2)	0.0163 (18)	0.0034 (18)	−0.022 (2)
C12	0.115 (3)	0.107 (3)	0.069 (2)	0.046 (2)	0.030 (2)	0.0131 (19)
C13	0.123 (3)	0.076 (2)	0.096 (2)	0.0074 (19)	0.053 (2)	0.0160 (18)
C14	0.0758 (18)	0.0684 (18)	0.083 (2)	0.0021 (14)	0.0279 (16)	−0.0083 (15)
N1	0.0446 (10)	0.0636 (12)	0.0415 (10)	0.0078 (9)	0.0067 (8)	−0.0011 (8)
O1	0.0666 (10)	0.0865 (12)	0.0603 (10)	0.0333 (9)	0.0278 (8)	0.0168 (9)

Geometric parameters (Å, º)

C1—C2	1.388 (3)	C8—C9	1.492 (3)
C1—C6	1.398 (3)	C8—H8A	0.9700
C1—C7	1.454 (3)	C8—H8B	0.9700
C2—C3	1.370 (3)	C9—C10	1.368 (3)
C2—H2	0.9300	C9—C14	1.372 (3)
C3—C4	1.370 (3)	C10—C11	1.382 (4)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.376 (3)	C11—C12	1.362 (4)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.384 (3)	C12—C13	1.346 (4)
C5—H5	0.9300	C12—H12	0.9300
C6—O1	1.370 (2)	C13—C14	1.373 (4)
C7—N1	1.266 (2)	C13—H13	0.9300
C7—H7	0.9300	C14—H14	0.9300
C8—O1	1.417 (2)	N1—N1^{i}	1.414 (3)

C2—C1—C6	117.99 (19)	O1—C8—H8B	110.0
C2—C1—C7	121.61 (19)	C9—C8—H8B	110.0
C6—C1—C7	120.36 (18)	H8A—C8—H8B	108.4
C3—C2—C1	121.6 (2)	C10—C9—C14	118.7 (2)
C3—C2—H2	119.2	C10—C9—C8	121.0 (3)
C1—C2—H2	119.2	C14—C9—C8	120.3 (3)
C4—C3—C2	119.5 (2)	C9—C10—C11	120.1 (3)
C4—C3—H3	120.2	C9—C10—H10	119.9
C2—C3—H3	120.2	C11—C10—H10	119.9
C3—C4—C5	120.8 (2)	C12—C11—C10	120.3 (3)
C3—C4—H4	119.6	C12—C11—H11	119.8
C5—C4—H4	119.6	C10—C11—H11	119.8
C4—C5—C6	119.7 (2)	C13—C12—C11	119.7 (3)
C4—C5—H5	120.2	C13—C12—H12	120.1
C6—C5—H5	120.2	C11—C12—H12	120.1
O1—C6—C5	124.2 (2)	C12—C13—C14	120.6 (3)
O1—C6—C1	115.37 (18)	C12—C13—H13	119.7
C5—C6—C1	120.4 (2)	C14—C13—H13	119.7
N1—C7—C1	121.61 (18)	C9—C14—C13	120.6 (3)
N1—C7—H7	119.2	C9—C14—H14	119.7
C1—C7—H7	119.2	C13—C14—H14	119.7
O1—C8—C9	108.35 (19)	C7—N1—N1^{i}	111.88 (19)
O1—C8—H8A	110.0	C6—O1—C8	118.49 (17)
C9—C8—H8A	110.0		

C6—C1—C2—C3	0.2 (3)	O1—C8—C9—C14	−102.1 (3)
C7—C1—C2—C3	−177.7 (2)	C14—C9—C10—C11	−0.8 (4)
C1—C2—C3—C4	0.1 (3)	C8—C9—C10—C11	179.1 (2)
C2—C3—C4—C5	−0.6 (4)	C9—C10—C11—C12	1.1 (4)
C3—C4—C5—C6	0.8 (4)	C10—C11—C12—C13	−0.6 (4)
C4—C5—C6—O1	−179.8 (2)	C11—C12—C13—C14	−0.1 (4)
C4—C5—C6—C1	−0.5 (3)	C10—C9—C14—C13	0.1 (3)
C2—C1—C6—O1	179.35 (18)	C8—C9—C14—C13	−179.8 (2)
C7—C1—C6—O1	−2.8 (3)	C12—C13—C14—C9	0.4 (4)
C2—C1—C6—C5	0.0 (3)	C1—C7—N1—N1^{i}	179.20 (19)
C7—C1—C6—C5	177.9 (2)	C5—C6—O1—C8	−12.4 (3)
C2—C1—C7—N1	−9.7 (3)	C1—C6—O1—C8	168.4 (2)
C6—C1—C7—N1	172.5 (2)	C9—C8—O1—C6	−170.5 (2)
O1—C8—C9—C10	78.1 (3)		

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