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The Schiff base *N*,*N*′-bis(3-nitrobenzylidene)propane-1,3-diamine

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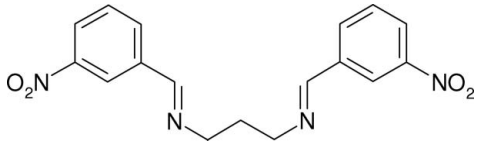
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.104; data-to-parameter ratio = 8.8.

The molecule of the title Schiff base compound, $C_{17}H_{16}N_4O_4$, has crystallographic twofold rotation symmetry. The nitro and CH=N—C substituents are coplanar with the benzene ring in each half of the molecule. These two planar units are parallel, but extend in opposite directions from the central methylene bridge, so there is no intramolecular π-stacking. Instead, molecules pack with approximately parallel interleaved benzene rings providing intermolecular π-stacking, the centroid-to-centroid separation being 3.7196 (18) Å.

Related literature

For related structures, see: Li *et al.* (2005), Bomfim *et al.* (2005), Glidewell *et al.* (2005, 2006) and Sun *et al.* (2004).



Experimental

Crystal data

$C_{17}H_{16}N_4O_4$
M_r = 340.34
Orthorhombic, *Fdd*2
a = 12.994 (3) Å
b = 35.859 (12) Å
c = 6.983 (2) Å
V = 3253.7 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 150 (2) K
0.45 × 0.40 × 0.40 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
7631 measured reflections
1004 independent reflections
858 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
S = 1.15
1004 reflections
114 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2251).

References

Bomfim, J. A. S., Wardell, J. L., Low, J. N., Skakle, J. M. S. & Glidewell, C. (2005). *Acta Cryst.* C**61**, o53–o56.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2005). *Acta Cryst.* E**61**, o3551–o3553.
Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2006). *Acta Cryst.* C**62**, o1–o4.
Li, Y.-G., Zhu, H.-L., Chen, X.-Z. & Song, Y. (2005). *Acta Cryst.* E**61**, o4156–o4157.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (2005). *SHELXTL*. Version 6. Bruker AXS Inc., Madison, Wisconsin, USA.
Sun, Y.-X., You, Z.-L. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, o1707–o1708.

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supplementary materials

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The Schiff base *N*,*N*'-bis(3-nitrobenzylidene)propane-1,3-diamine

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Comment

Schiff base compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and molecular architectures. Structures of Schiff bases derived from nitrobenzaldehydes and closely related to the title compound have been reported by Li *et al.* (2005), Bomfin *et al.* (2005), Glidewell *et al.* (2005, 2006), and Sun *et al.* (2004).

The title compound, (I), was prepared by the condensation of 3-nitrobenzaldehyde and 1,3-diaminopropane in a 2:1 molar ratio. A view of the molecular structure is shown in Fig. 1. The molecule has crystallographic twofold rotation symmetry. Bond lengths and angles are unexceptional. The nitro and CH═N—C substituents are coplanar with the benzene ring in each half of the molecule. These two planar units are parallel by symmetry, but extend in opposite directions from the central methylene bridge, so there is no intramolecular π-stacking. Instead, molecules pack with approximately parallel interleaved benzene rings providing intermolecular π-stacking, the centroid-to-centroid separation being 3.7196 (18) Å (Fig. 2).

Experimental

A solution of 1,3-propanediamine (0.1 mmol, 0.074 g) in chloroform (5 ml) was slowly added to a solution of 3-nitrobenzaldehyde (0.2 mmol, 0.30 g) in the same solvent (5 ml). Recrystallization of the resulting solid from ethanol afforded colourless crystals, 81% yield.

Refinement

Hydrogen atoms were positioned geometrically with C—H = 0.95 (aromatic) or 0.98 Å (CH_2), and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Figures

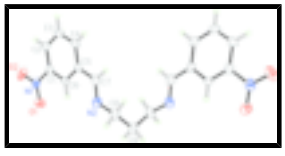

Fig. 1. The molecular structure with atom labels and 50% probability ellipsoids for non-H atoms [symmetry code for unlabelled atoms: -x, -y, z].

Fig. 2. The packing, viewed down the c axis, showing stacking of the benzene rings.

N,*N*'-bis(3-nitrobenzylidene)propane-1,3-diamine

Crystal data

$C_{17}H_{16}N_4O_4$	$D_x = 1.390$ Mg m^{-3}
$M_r = 340.34$	Melting point: 390 K
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 106 reflections
$a = 12.994$ (3) Å	θ = 2.5–27.5º
$b = 35.859$ (12) Å	μ = 0.10 mm^{-1}
$c = 6.983$ (2) Å	$T = 150$ (2) K
$V = 3253.7$ (16) Å^3	Block, colourless
$Z = 8$	0.45 × 0.40 × 0.40 mm
$F_{000} = 1424$	

Data collection

Nonius KappaCCD diffractometer	858 reflections with $I > 2\sigma(I)$
Radiation source: sealed tube	$R_{int} = 0.038$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 150(2)$ K	$\theta_{min} = 4.3$º
φ and ω scans	$h = -16 \rightarrow 11$
Absorption correction: none	$k = -46 \rightarrow 46$
7631 measured reflections	$l = -7 \rightarrow 9$
1004 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 1.1167P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.15$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
1004 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
114 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
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}
O1	0.06407 (16)	0.18127 (4)	0.6914 (3)	0.0409 (5)
O2	0.09163 (14)	0.21456 (5)	0.4384 (3)	0.0446 (5)
N1	0.08005 (15)	0.18443 (5)	0.5184 (3)	0.0304 (5)
N2	0.09255 (14)	0.04422 (5)	0.6668 (3)	0.0310 (5)
C1	0.08638 (15)	0.15000 (6)	0.4017 (3)	0.0249 (5)
C2	0.09912 (17)	0.15330 (7)	0.2039 (4)	0.0298 (5)
H2	0.1014	0.1770	0.1435	0.036*
C3	0.10824 (18)	0.12071 (7)	0.0994 (4)	0.0349 (6)
H3	0.1162	0.1219	−0.0357	0.042*
C4	0.10585 (17)	0.08602 (7)	0.1900 (3)	0.0308 (6)
H4	0.1130	0.0639	0.1161	0.037*
C5	0.09300 (15)	0.08339 (6)	0.3882 (3)	0.0259 (6)
C6	0.08196 (16)	0.11602 (6)	0.4955 (3)	0.0226 (5)
H6	0.0716	0.1149	0.6300	0.027*
C7	0.09518 (17)	0.04671 (6)	0.4865 (4)	0.0296 (6)
H7	0.0986	0.0246	0.4120	0.036*
C8	0.09691 (18)	0.00688 (6)	0.7532 (4)	0.0324 (6)
H8A	0.1585	0.0049	0.8361	0.039*
H8B	0.1024	−0.0122	0.6512	0.039*
C9	0.0000	0.0000	0.8718 (5)	0.0292 (7)
H9A	0.0118	−0.0219	0.9555	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0569 (11)	0.0346 (9)	0.0313 (11)	−0.0037 (8)	0.0078 (9)	−0.0082 (8)
O2	0.0501 (11)	0.0270 (9)	0.0566 (14)	−0.0030 (7)	0.0149 (10)	0.0076 (9)
N1	0.0243 (10)	0.0299 (11)	0.0369 (13)	−0.0018 (7)	0.0044 (9)	−0.0007 (9)
N2	0.0316 (11)	0.0238 (9)	0.0377 (12)	0.0004 (7)	0.0007 (9)	0.0014 (8)
C1	0.0178 (10)	0.0302 (12)	0.0267 (14)	−0.0016 (8)	−0.0022 (9)	−0.0004 (9)
C2	0.0232 (11)	0.0400 (12)	0.0263 (14)	−0.0040 (9)	−0.0006 (10)	0.0074 (11)
C3	0.0256 (13)	0.0613 (18)	0.0180 (12)	−0.0071 (10)	−0.0023 (10)	0.0008 (12)
C4	0.0236 (11)	0.0436 (13)	0.0253 (14)	−0.0042 (9)	−0.0002 (10)	−0.0100 (11)
C5	0.0192 (11)	0.0313 (12)	0.0272 (15)	−0.0031 (8)	−0.0023 (9)	−0.0041 (9)
C6	0.0190 (11)	0.0298 (11)	0.0191 (12)	−0.0019 (8)	−0.0002 (9)	−0.0006 (9)
C7	0.0257 (12)	0.0268 (11)	0.0364 (15)	−0.0028 (8)	0.0032 (10)	−0.0082 (10)
C8	0.0335 (12)	0.0225 (11)	0.0412 (15)	0.0024 (9)	0.0012 (11)	0.0017 (10)
C9	0.0288 (16)	0.0238 (14)	0.0350 (18)	0.0029 (12)	0.000	0.000

Geometric parameters (Å, °)

O1—N1	1.231 (3)	C4—C5	1.397 (3)
O2—N1	1.226 (3)	C5—C6	1.397 (3)
N1—C1	1.482 (3)	C5—C7	1.484 (3)
N2—C7	1.263 (4)	C6—H6	0.950

N2—C8	1.470 (3)	C7—H7	0.950
C1—C2	1.396 (4)	C8—H8A	0.990
C1—C6	1.384 (3)	C8—H8B	0.990
C2—H2	0.950	C8—C9	1.527 (3)
C2—C3	1.383 (3)	C9—C8^{i}	1.527 (3)
C3—H3	0.950	C9—H9A	0.990
C3—C4	1.396 (4)	C9—H9A^{i}	0.990
C4—H4	0.950		
O1—N1—O2	123.3 (2)	C1—C6—C5	118.6 (2)
O1—N1—C1	118.20 (19)	C1—C6—H6	120.7
O2—N1—C1	118.5 (2)	C5—C6—H6	120.7
C7—N2—C8	118.2 (2)	N2—C7—C5	121.6 (2)
N1—C1—C2	118.7 (2)	N2—C7—H7	119.2
N1—C1—C6	118.1 (2)	C5—C7—H7	119.2
C2—C1—C6	123.2 (2)	N2—C8—H8A	109.7
C1—C2—H2	121.3	N2—C8—H8B	109.7
C1—C2—C3	117.4 (2)	N2—C8—C9	109.75 (16)
H2—C2—C3	121.3	H8A—C8—H8B	108.2
C2—C3—H3	119.6	H8A—C8—C9	109.7
C2—C3—C4	120.8 (2)	H8B—C8—C9	109.7
H3—C3—C4	119.6	C8—C9—C8^{i}	114.3 (3)
C3—C4—H4	119.6	C8—C9—H9A	108.7
C3—C4—C5	120.8 (2)	C8^{i}—C9—H9A	108.7
H4—C4—C5	119.6	C8—C9—H9A^{i}	108.7
C4—C5—C6	119.1 (2)	C8^{i}—C9—H9A^{i}	108.7
C4—C5—C7	121.0 (2)	H9A—C9—H9A^{i}	107.6
C6—C5—C7	119.8 (2)		
O1—N1—C1—C2	176.7 (2)	N1—C1—C6—C5	−176.85 (18)
O1—N1—C1—C6	−4.9 (3)	C2—C1—C6—C5	1.4 (3)
O2—N1—C1—C2	−3.8 (3)	C4—C5—C6—C1	−1.4 (3)
O2—N1—C1—C6	174.61 (18)	C7—C5—C6—C1	176.16 (18)
N1—C1—C2—C3	177.89 (19)	C8—N2—C7—C5	−178.89 (18)
C6—C1—C2—C3	−0.4 (3)	C4—C5—C7—N2	173.8 (2)
C1—C2—C3—C4	−0.7 (3)	C6—C5—C7—N2	−3.7 (3)
C2—C3—C4—C5	0.7 (3)	C7—N2—C8—C9	−120.0 (2)
C3—C4—C5—C6	0.3 (3)	N2—C8—C9—C8^{i}	73.30 (18)
C3—C4—C5—C7	−177.17 (19)		

Symmetry codes: (i) −*x*, −*y*, *z*.

Fig. 1

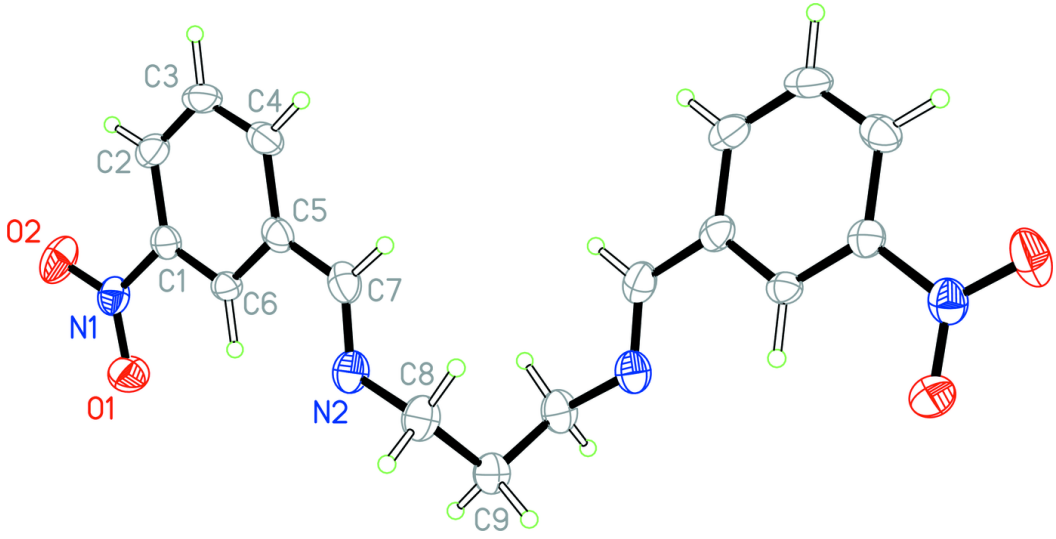

Fig. 2