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N,*N*′-Bis(4-nitrobenzylidene)ethane-1,2-diamine

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.133
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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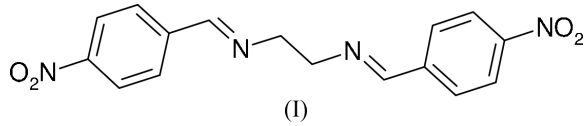
The title compound, $C_{16}H_{14}N_4O_4$, acts as an important precursor for the synthesis of Schiff base complexes. The molecule lies across a crystallographic inversion centre. The crystal packing is stabilized by C—H···O hydrogen bonds and π–π interactions.

Comment

Recently, we reported a few Schiff base compounds (You *et al.*, 2003, 2004). As an extension of our work on the structural characterization of Schiff base compounds, the title compound, (I), is reported here.



(I)

The asymmetric unit contains one-half of the molecule of (I), the other half being inversion-related by (2 − *x*, −*y*, 2 − *z*) (Fig. 1). All the bond lengths are within normal ranges (Allen *et al.*, 1987). The C7═N1 bond length of 1.261 (2) Å conforms to the value for a double bond, while the C8—N1 bond length of 1.457 (2) Å conforms to the value for a single bond. The dihedral angle between the planes of the nitro group and the benzene ring is 6.7 (2)°. The N1—C8—C8^{i}—N1^{i} torsion angle [symmetry code: (i) 2 − *x*, −*y*, 2 − *z*] is 180°, as the inversion centre bisects the C8—C8^{i} bond. The benzene rings of the molecules at (*x*, *y*, *z*) and (2 − *x*, −*y*, 1 − *z*) are stacked with a centroid–centroid separation of 3.696 (3) Å, indicating π–π interactions. The crystal packing is further stabilized by intermolecular C—H···O hydrogen bonds, as illustrated in Fig. 2 (Table 1).

Experimental

1,2-Diaminoethane (0.1 mmol, 6.0 mg) and 4-nitrobenzaldehyde (0.2 mmol, 30.2 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. After keeping the solution in air for 8 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$C_{16}H_{14}N_4O_4$
M_r = 326.31
Monoclinic, $P2_1/n$
a = 9.156 (6) Å
b = 7.233 (5) Å
c = 11.516 (7) Å
β = 97.494 (9)°
V = 756.1 (9) Å^3
Z = 2
D_x = 1.433 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 807 reflections
θ = 2.7–25.1°
μ = 0.11 mm^{-1}
T = 273 (2) K
Block, yellow
0.15 × 0.12 × 0.08 mm

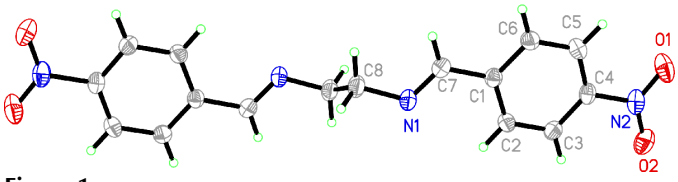


Figure 1
The structure of (I), showing the atom-numbering scheme for the contents of the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.992
4208 measured reflections
1635 independent reflections
1092 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.0°
$h = -11 \rightarrow 11$
$k = -7 \rightarrow 9$
$l = -10 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.133
S = 1.00
1635 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{ii}	0.93	2.41	3.220 (3)	146

Symmetry codes: (ii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C).

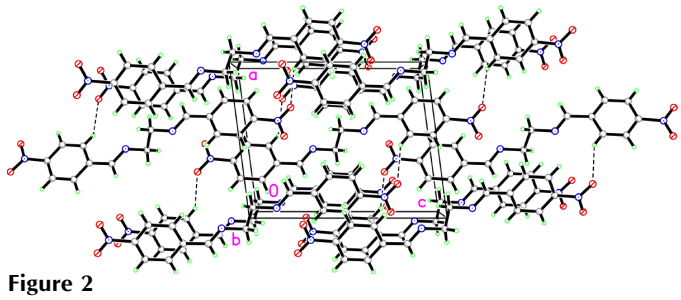


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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