Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(2-nitrobenzylidene)ethylenediamine

Yu-Guang Li,[a,b] Hai-Liang Zhu,[a]* Xin-Zhi Chen[a] and Yu Song[a]

[a]Department of Chemistry, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China, and [b]Department of Chemistry, Huazhong University of Science and Technology, Wuhan 430074, People's Republic of China

Correspondence e-mail: hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.154
Data-to-parameter ratio = 15.3

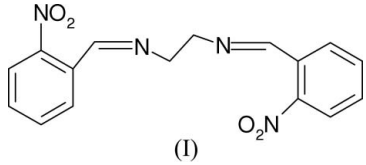
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 October 2005
Accepted 11 November 2005
Online 16 November 2005

The molecule of the title compound, $C_6H_{14}N_4O_4$, possesses a crystallographically imposed centre of symmetry. In the crystal packing, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds into a sheet-like structure parallel to the $(10\bar{2})$ plane.

Comment

Schiff base compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and molecular architectures. Recently, we have reported two Schiff base compounds with 2-nitrobenzaldehyde, which have been structurally characterized (Shao, You, Xiong *et al.*, 2004; Shao, You, Fan *et al.*, 2004). As an extension of work on the structural characterization of these Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

In (I), two 2-nitrobenzaldehyde groups are bridged by ethylenediamine *via* two C═N double bonds in a roughly linear geometry. The molecule possesses C_i symmetry (Fig. 1). The C7═N2 bond length of 1.250 (2) Å is shorter than the values of 1.261 (2) and 1.263 (2) Å observed in the Schiff base compounds described above, suggesting the presence of a weaker C—H···O intramolecular hydrogen interaction. All other bond lengths are within normal ranges (Allen *et al.*, 1987). The torsion angle C5—C6—C7—N2 is −36.3°. The

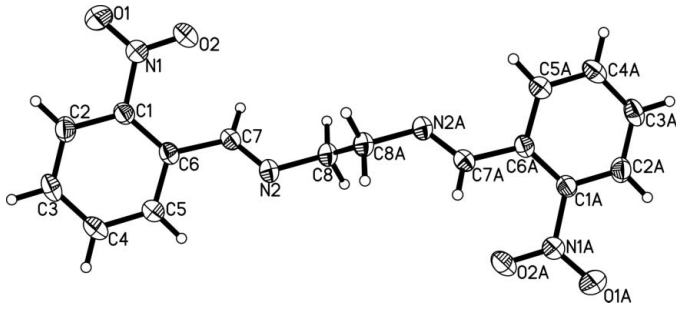


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Suffix A denotes the symmetry operator (2 − *x*, 1 − *y*, 1 − *z*).

benzene rings of the two 2-nitrobenzaldehyde groups are parallel by symmetry.

In the crystal packing, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds, forming a sheet-like structure running parallel to the (10$\bar{2}$) plane (Table 1 and Fig. 2).

Experimental

Ethylenediamine (1 mmol, 60 mg) and 2-nitrobenzaldehyde (2 mmol, 302 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. The solution was kept in air for 8 d, and yellow block-shaped crystals formed on slow evaporation of the solvent.

Crystal data

$C_{16}H_{14}N_4O_4$
$M_r = 326.31$
Monoclinic, $P2_1/c$
$a = 7.4255$ (10) Å
$b = 15.497$ (2) Å
$c = 7.0806$ (10) Å
$\beta = 108.648$ (2)°
$V = 772.00$ (18) Å^3
$Z = 2$
$D_x = 1.404$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1412 reflections
$\theta = 2.6$–$24.1°$
$\mu = 0.10$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.975$, $T_{max} = 0.979$
4450 measured reflections
1671 independent reflections
1319 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.0°$
$h = -9 \rightarrow 7$
$k = -19 \rightarrow 19$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.154$
$S = 1.05$
1671 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.2476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2	0.93	2.36	2.689 (3)	101
C5—H5···O1^{i}	0.93	2.50	3.229 (3)	135

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

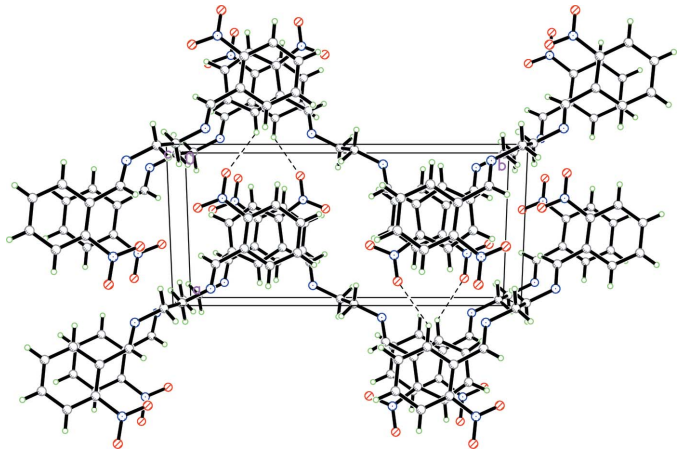


Figure 2
The crystal packing of (I), viewed along the *c* axis. Dashed lines show intermolecular C—H···O hydrogen bonds.

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

ZHU thanks the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, and the Natural Science Foundation of Hubei Province, People's Republic of China, for research grant No. 2003ABB010.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Shao, S.-Ch., You, Zh.-L., Fan, Sh.-H., Tang, L.-L., Xiong, Zh.-D. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, o2183–o2184.
Shao, S.-Ch., You, Zh.-L., Xiong, Zh.-D., Chen, B. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, o2187–o2188.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.