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N,*N*′-Bis(3,4-dimethoxybenzylidene)ethylenediamine

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.056
wR factor = 0.152
Data-to-parameter ratio = 17.6

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

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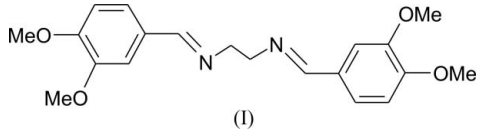
The molecule of the title compound, $C_{20}H_{24}N_2O_4$, has crystallographic inversion symmetry. In the crystal structure, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds into a three-dimensional structure.

Comment

Ethylenediamine and its derivatives play an important role in developing molecular architectures in coordination chemistry (Brown *et al.*, 2001; Dapporto *et al.*, 2000). Similarly, the condensation products of ethylenediamine with aldehydes, *i.e.* Schiff bases, form an interesting class of ligands for transition metal complexes (Goswami & Eichhorn, 1999; Henson *et al.*, 1999). Recently, we have reported a Schiff base compound derived from the condensation of ethylenediamine with 2-nitrobenzaldehyde, which has been structurally characterized (Li *et al.*, 2005). As an extension of this work, the crystal structure of the title compound, (I), has been determined.



(I)

In (I) (Fig. 1), two 3,4-dimethoxybenzylidene groups are bridged by the ethylenediamine fragment *via* two C=N double bonds in a roughly linear geometry. The torsion angle C6—C7—C9—N1 of 172.34 (15)° indicates an extended configuration. The molecule is disposed about a centre of inversion at the mid-point of the central C—C bond. The C9=N1 bond length of 1.260 (2) Å is comparable to the corresponding values of 1.250 (2) Å observed in bis(2-nitrobenzaldehyde)ethylenediamine (Li *et al.*, 2005). All other bond lengths are within normal ranges (Allen *et al.*, 1987).

In the crystal packing, the molecules are linked *via* weak intermolecular C—H···O hydrogen bonds, forming a three-dimensional structure (Table 1 and Fig. 2).

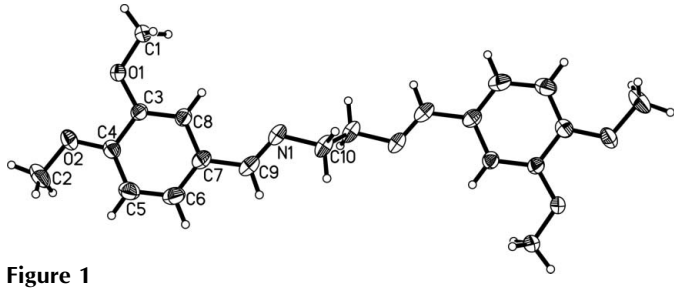


Figure 1
The structure of centrosymmetric (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry code (1 − *x*, 2 − *y*, 1 − *z*).

Experimental

Ethylenediamine (1 mmol, 60 mg) and 3,4-dimethoxybenzaldehyde (2 mmol, 332 mg) were dissolved in methanol (10 ml) at 323 K. The mixture was stirred for 10 min to give a clear and colourless solution. After the solution had been allowed to stand in air for 8 d, colourless crystals formed, in about 87% yield, on slow evaporation of the solvent. Analysis found: C 67.35, H 6.91, N 7.85%; $C_{20}H_{24}N_2O_4$ requires C 67.39, H 6.79, N 7.86%.

Crystal data

$C_{20}H_{24}N_2O_4$
M_r = 356.41
Monoclinic, $P2_1/c$
a = 13.126 (3) Å
b = 8.531 (2) Å
c = 8.393 (2) Å
β = 97.125 (4)°
V = 932.6 (4) Å^3
Z = 2
D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2443 reflections
θ = 2.7–23.0°
μ = 0.09 mm^{-1}
T = 292 (2) K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.897, T_{max} = 0.995
10357 measured reflections
2111 independent reflections
1415 reflections with $I > 2\sigma(I)$
R_{int} = 0.142
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.152
S = 0.94
2111 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2C···O1^{i}	0.96	2.56	3.490 (2)	164
C1—H1B···O2^{ii}	0.96	2.57	3.521 (2)	171

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

The H atoms were included in calculated positions and refined using a riding-model approximation, with aromatic C—H = 0.93 Å, methylene C—H = 0.97 Å and methyl C—H = 0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and methylene, and 1.5U_{eq}(C) for methyl H atoms. The high value of R_{int} is due to the weak precision of single-crystal reflection data.

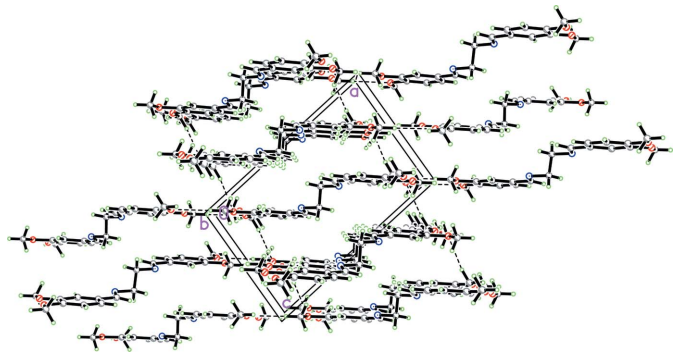


Figure 2
The crystal packing of (I), viewed along the b axis. Dashed lines show intermolecular C—H···O hydrogen bonds.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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: *SHELXL97*.

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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.
Brown, D. A., Errington, W., Glass, W. K., Haase, W., Kemp, T. J., Nimir, H., Ostrovsky, S. M. & Werner, R. (2001). *Inorg. Chem.* **40**, 5962–5971.
Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dapporto, P., Formica, M., Fusi, V., Micheloni, M., Paoli, P., Pontellini, R., Romani, P. & Rossi, P. (2000). *Inorg. Chem.* **39**, 2156–2163.
Goswami, N. & Eichhorn, D. M. (1999). *Inorg. Chem.* **38**, 4329–4333.
Henson, N. J., Hay, P. J. & Redondo, A. (1999). *Inorg. Chem.* **38**, 1618–1626.
Li, Y.-G., Zhu, H.-L., Chen, X.-Z. & Song, Y. (2005). *Acta Cryst.* E**61**, o4156–o4157.
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.