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6,6′-Dimethoxy-2,2′-(ethane-1,2-diyldiimino-dimethylene)diphenol

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In the crystal structure of the title compound, $C_{18}H_{24}O_2N_4$, centrosymmetric molecules are linked into a layer *via* C—H···O and O—H···N hydrogen bonds.

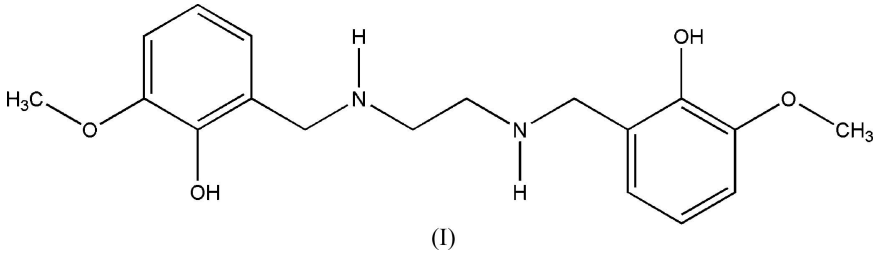
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.136
Data-to-parameter ratio = 14.0

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

Comment

As part of our investigation of crystal structure of ethylenediamine derivatives, we report here the crystal structure of a new ethylenediamine derivative, (I).



(I)

The title molecule has a center of symmetry (Fig. 1). In the crystal structure, molecules are linked *via* C—H···O and O—H···N hydrogen bonds (Table 1), forming a layer extending parallel to the (001) plane (Fig. 2). The hydrogen bonds in the layer form an $R_2^2(8)$ ring (Bernstein *et al.*, 1995). There are no significant intermolecular interactions between the layers.

Experimental

Solutions of *N*,*N*′-bis(2-hydroxy-3-methoxybenzylene)ethylenediamine (10 mmol) in methanol–chloroform (1:1 *v*/*v*, 20 ml) and solid $NaBH_4$ (40 mmol) were mixed. The mixture was stirred at room temperature for 24 h and then filtered. The filtrate was allowed to evaporate slowly, giving single crystals of (I).

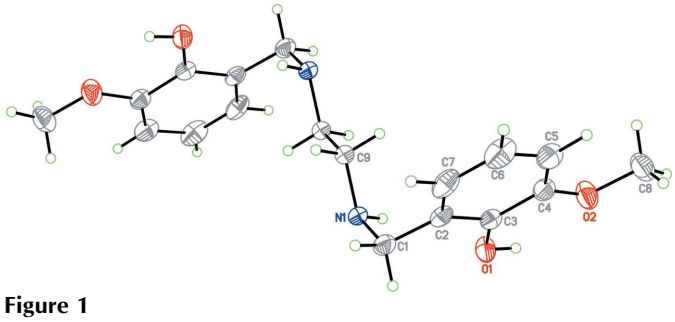


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $1-x, 1-y, 1-z$.

Crystal data

$C_{18}H_{24}N_2O_4$
M_r = 332.39
Orthorhombic, *Pbca*
a = 9.431 (3) Å
b = 10.512 (4) Å
c = 17.414 (6) Å
V = 1726.4 (10) Å^3
Z = 4
D_x = 1.279 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, white
0.56 × 0.54 × 0.32 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.951, T_{max} = 0.972
8220 measured reflections
1525 independent reflections
1104 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.136
S = 1.02
1525 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.7829P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1*C*···O2^{i}	0.97	2.68	3.284 (3)	121
O1—H1···N1^{ii}	0.82	2.02	2.723 (2)	144

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

All H atoms were located in a difference Fourier map and then treated as riding atoms, with C—H = 0.93–0.97 Å, N—H = 0.90 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(aryl and methylene C, and N) and 1.5U_{eq}(methyl C, O).

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*.

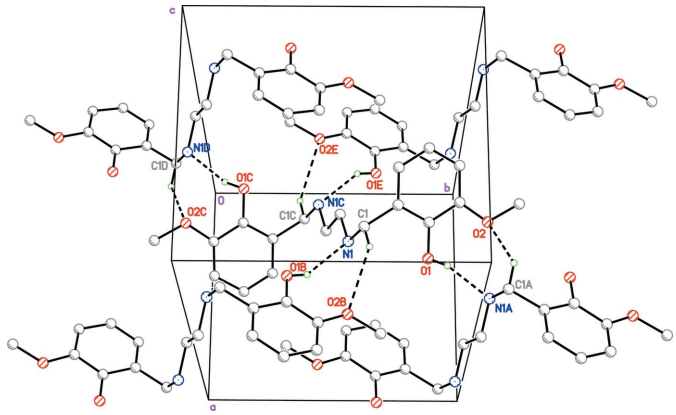


Figure 2
A packing diagram of (I), showing a hydrogen-bonded layer built by C—H···O and O—H···N interactions (dashed lines). For clarity, H atoms not involved in the hydrogen bonds have been omitted. [Symmetry codes: (A) $\frac{3}{2}-x, \frac{1}{2}+y, z$; (B) $\frac{3}{2}-x, -\frac{1}{2}+y, z$; (C) $1-x, 1-y, 1-z$; (D) $-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (E) $-\frac{1}{2}+x, \frac{3}{2}-y, 1-z$.]

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