Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*,*E*)-6,6′-Dimethoxy-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenol

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Received 19 November 2006
Accepted 19 November 2006

Key indicators

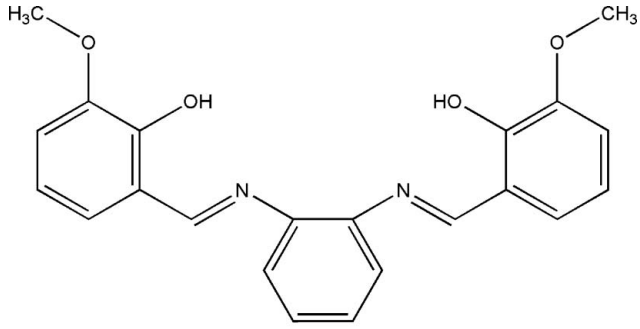
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.063
wR factor = 0.233
Data-to-parameter ratio = 13.2

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

The title compound, $C_{22}H_{20}N_2O_4$, consists of two *o*-vanillin groups connected to a benzene ring *via* two azomethine linkages. The molecule structure is stabilized by intermolecular C—H···O and C—H···N interactions.

Comment

Azomethine compounds exhibit a wide variety of pharmacological activities including antitumour and antimicrobial activity (Modi *et al.*, 1970; Hodnett *et al.*, 1970). In the light of this, we have synthesized and characterized the title compound, (I) (Fig. 1).



(I)

In the crystal structure of (I), molecules are linked into sheets through C—H···O and C—H···N interactions (Table 1

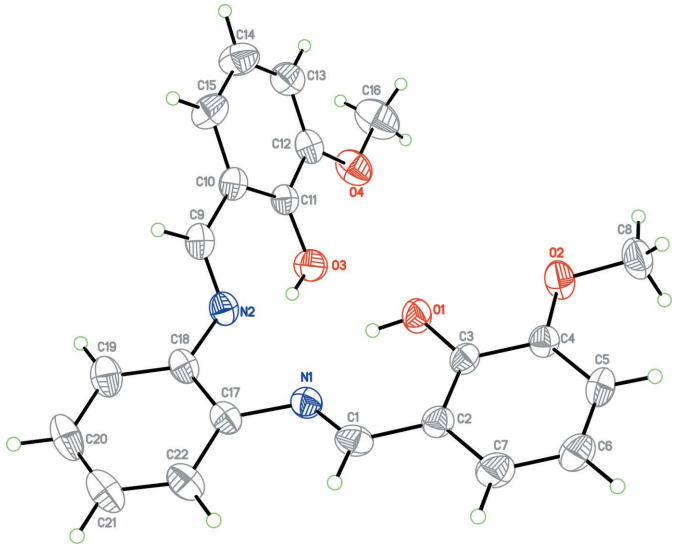


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

and Fig. 2). Neighboring sheets are connected by further C—H···O1 interactions (Fig. 3 and Table 1), thereby linking the molecules into a three-dimensional network involving an $R_2^2(12)$ ring (Bernstein *et al.*, 1995).

Experimental

A solution of *o*-vanillin (20 mmol) and benzene-1,2-diamine (10 mmol) in benzene (30 ml) was stirred for 6 h and then filtered and allowed to stand. Crystals of (I) precipitated from the solution.

Crystal data

$C_{22}H_{20}N_2O_4$
M_r = 376.40
Monoclinic, $P2_1/c$
a = 6.638 (2) Å
b = 16.838 (3) Å
c = 17.137 (3) Å
β = 97.861 (3)°
V = 1897.3 (7) Å^3
Z = 4
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, red
0.65 × 0.13 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.943, T_{max} = 0.992
9506 measured reflections
3339 independent reflections
1566 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.233
S = 1.03
3339 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.8316P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 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
C9—H9···O2^{i}	0.93	2.61	3.058 (5)	110
C8—H8A···O1^{ii}	0.96	2.69	3.413 (6)	133
C6—H6···N2^{iii}	0.93	2.68	3.540 (5)	154
C1—H1A···O4^{iv}	0.93	2.70	3.528 (5)	149

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

All H atoms were located in difference Fourier maps. H atoms bonded to C and O atoms were treated as riding atoms, with C—H distances of 0.93 (aryl), 0.96 (methyl) and 0.82 Å (hydroxy), and with U_{iso}(H) = 1.2 (aryl) or 1.5 (methyl or hydroxy) times U_{eq}(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*.

We acknowledge the financial support of the Huaihai Institute of Technology Science Foundation.

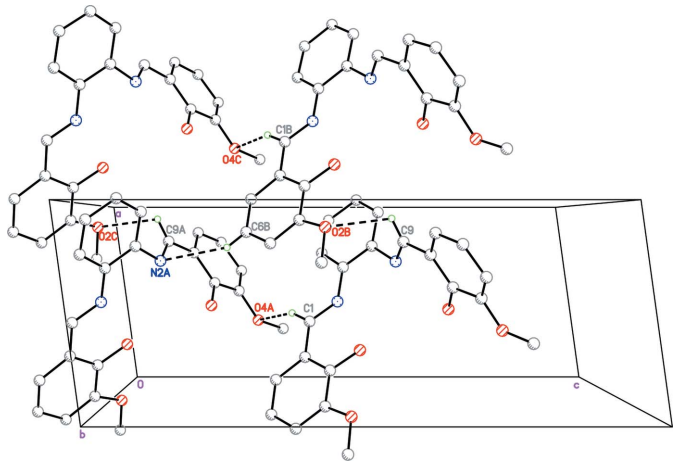


Figure 2
A part of the crystal struture of (I), showing the formation of sheets built from C—H···O and C—H···N interactions. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds [symmetry code: (A) $x, \frac{1}{2}-y, -\frac{1}{2}+z$; (B) $1+x, y, z$; (C) $1+x, \frac{1}{2}-y, -\frac{1}{2}+z$].

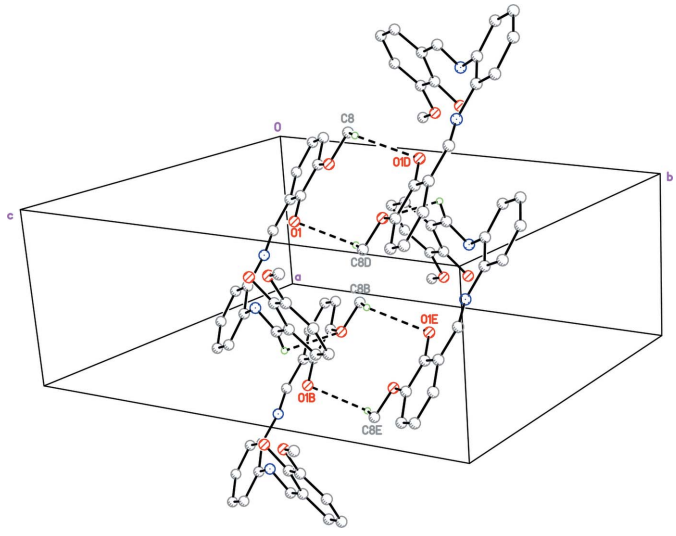


Figure 3
A different view of the crystal structure of (I), showing the formation of a three-dimensional network built from C—H···O hydrogen bonds. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds [symmetry code: (B) $1+x, y, z$; (D) $-x, 1-y, 1-z$; (E) $1-x, 1-y, 1-z$].

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