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6,6′-Dimethoxy-2,2′-(hexane-1,6-diyldinitrilodimethylidyne)diphenol

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The title compound, $C_{22}H_{28}N_2O_4$, is a potential multidentate azomethine ligand. The asymmetric unit contains two half-molecules, each molecule lying on a centre of symmetry. The molecules are linked into sheets and a three-dimensional network by C—H···O hydrogen bonds and van der Waals forces.

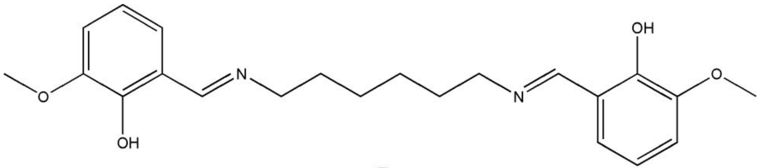
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.073
wR factor = 0.277
Data-to-parameter ratio = 14.3

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

Comment

Schiff base salicylaldehyde derivatives have multicoordinate atoms (N and O), which can not only act as the effective organic ligand, but also exhibit a wide variety of antimicrobial activity (Key, 1974; Hodnett *et al.*, 1970; Dhar *et al.*, 1982). As part of our investigation of the reactions between 3-methoxysalicylaldehyde with diamines, we report here the crystal structure of a salicylaldehyde derivative Schiff base, (I) (Fig. 1), which was obtained by the reaction of 3-methoxysalicylaldehyde with hexane-1,6-diamine and has a *trans* configuration (*E*,*E*).



(I)

The asymmetric unit contains two half-molecules, each molecule lying on a centre of symmetry. The molecules are linked into a sheet parallel to the (100) plane through C—H···O hydrogen bonds (Fig. 2 and Table 1) and another sheet parallel to the (100) plane by van der Waals forces (Fig. 3). The alternate combination of the two (100) planes results in the formation of a three-dimensional network.

Experimental

A solution of 3-methoxysalicylaldehyde (20 mmol) and hexane-1,6-diamine (10 mmol) in ethanol (30 ml) was stirred for 8 h and then filtered. The solution was allowed to stand, yielding, by slow evaporation, yellow crystals of (I) suitable for X-ray structure analysis.

Crystal data

$C_{22}H_{28}N_2O_4$
M_r = 384.46
Monoclinic, $P2_1/c$
a = 21.834 (11) Å
b = 8.420 (4) Å
c = 11.203 (6) Å
β = 91.778 (9)°
V = 2058.6 (19) Å^3
Z = 4
D_x = 1.240 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, yellow
0.52 × 0.48 × 0.15 mm

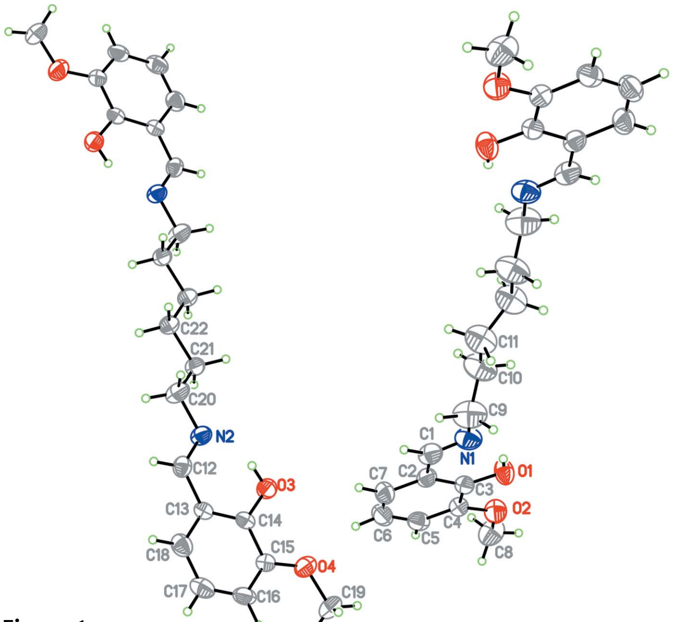


Figure 1
The structures of the two independent centrosymmetric molecules of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. In the N1 molecule unlabelled atoms are related to labelled atoms by ($1 - x$, $-y$, $1 - z$). In the N2 molecule unlabelled atoms are related to labelled atoms by ($-x$, $-y.1 - z$).

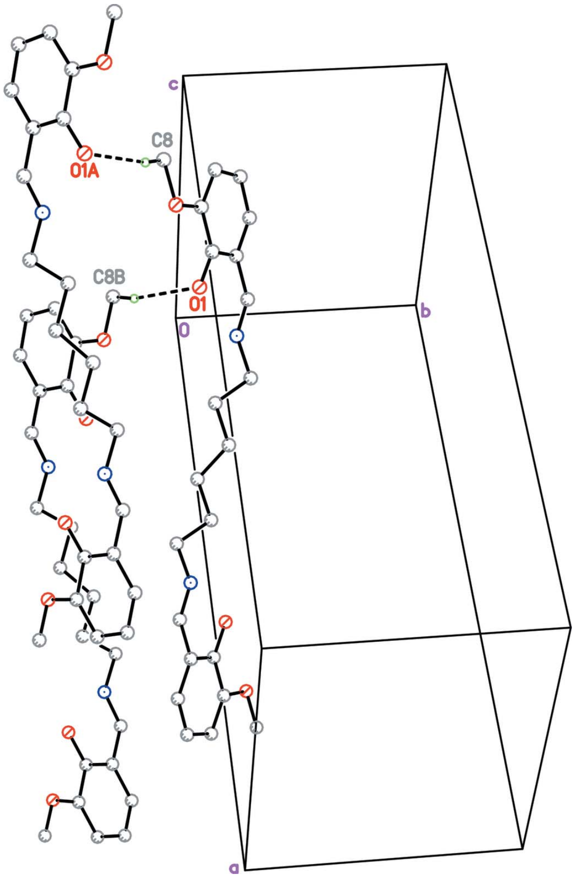


Figure 2
Part of the crystal struture of (I), showing the formation of a hydrogen-bonded sheet built from C—H···O interactions (dashed lines). For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry code: (A) x, $-\frac{1}{2} - y$, $\frac{1}{2} + z$; (B) x, $-\frac{1}{2} - y$, $-\frac{1}{2} + z$].

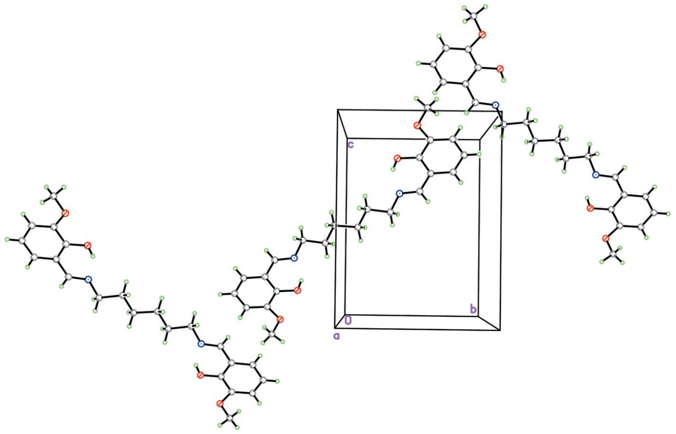


Figure 3
The crystal struture of (I), showing the formation of a sheet by van der Waals forces.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.957$, $T_{\max} = 0.987$
10347 measured reflections
3621 independent reflections
1223 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.102$
$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.277$
$S = 1.02$
3621 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 1.1443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O1$^{\rm i}$	0.96	2.67	3.616 (8)	169

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

All H atoms were located in difference Fourier maps, then repositioned geometrically and treated as riding atoms, with C—H distances of 0.93 (aryl), 0.96 (methyl) and 0.82 Å (hydroxy), and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aryl or $1.5U_{\rm eq}({\rm C,O})$ for methyl and hydroxy groups.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); 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*.

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