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6,6′-Dimethyl-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenol

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.057
wR factor = 0.169
Data-to-parameter ratio = 37.4

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

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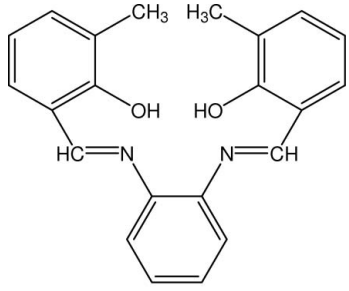
The crystal structure of the title compound, $C_{22}H_{20}N_2O_2$, is stabilized by intramolecular O—H···N hydrogen bonds and intermolecular C—H···O and C—H···π interactions.

Comment

A number of Schiff bases exhibit a variety of pharmacological activities: anticancer (Dao *et al.*, 2000), anti-HIV (Sriram *et al.*, 2006), antibacterial and antifungal (Karthikeyan *et al.*, 2006). In addition, some Schiff bases may be used as analytical reagents for the determination of trace elements (Eltayeb & Ahmed, 2005*a*,*b*).



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). The dihedral angles between the benzene rings C1–C6 and C8–C13, C1–C6 and C15–C20, and C8–C13 and C15–C20 are 49.04 (5), 39.45 (5) and 12.44 (5)°, respectively (Fig. 1). The intramolecular O—H···N interactions generate *S*(6) ring motifs (Table 1) (Bernstein *et al.*, 1995). The crystal structure is further stabilized by intermolecular C—H···O and C—H···π interactions (Table 1).

Experimental

To a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (20 ml) was added 3-methylsalicylaldehyde (0.5 ml, 4 mmol). The mixture was refluxed with stirring for 0.5 h. The resultant orange solution was filtered and allowed to evaporate slowly at room temperature to produce X-ray quality crystals of (I). (Yield 0.55 g, 79.94%, m.p. 380–381 K).

Crystal data

$C_{22}H_{20}N_2O_2$
M_r = 344.40
Monoclinic, $P2_1/c$
a = 10.7922 (4) Å
b = 7.7650 (3) Å
c = 23.3440 (8) Å
β = 116.789 (2)°
V = 1746.30 (11) Å^3
Z = 4
D_x = 1.310 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
Needle, orange
0.42 × 0.21 × 0.12 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.880, T_{max} = 0.990
45277 measured reflections
9156 independent reflections
6376 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 37.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.169
S = 1.04
9156 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0906P)^2 + 0.125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.95 (2)	1.74 (2)	2.611 (1)	151 (2)
O2—H2A···N2	0.90 (2)	1.75 (2)	2.591 (1)	154 (2)
C17—H17A···O1^{i}	0.93	2.58	3.298 (2)	134
C21—H21C···$Cg1^{ii}$	0.96	2.87	3.673 (1)	141

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ is the centroid of the C8–C13 ring.

O-bound H atoms were located in difference maps and refined isotropically. The remaining H atoms were positioned geometrically and treated as riding, with C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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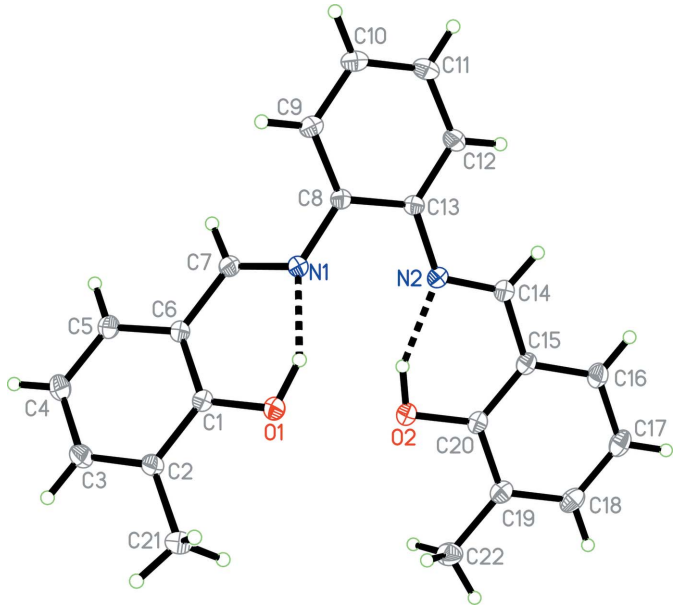

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are shown as dashed lines.

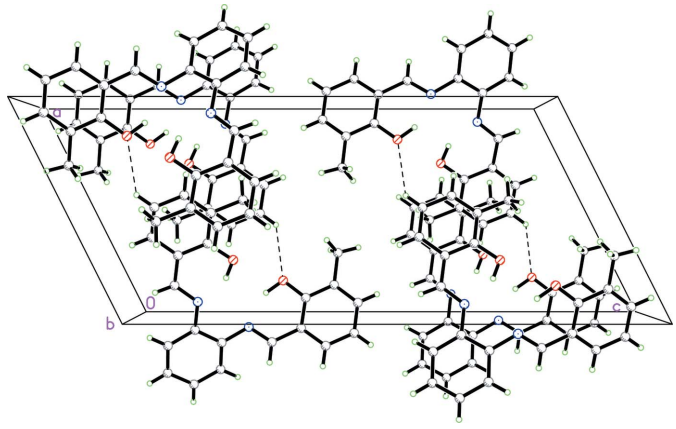

Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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