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2,2′-[1,2-Phenylenebis(nitrilomethylidyne)]-bis(5-methylphenol)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.117
Data-to-parameter ratio = 21.2

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

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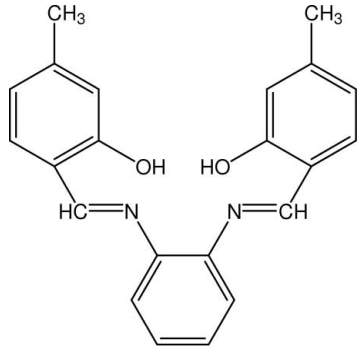
The crystal structure of the title compound, $C_{22}H_{20}N_2O_2$, is stabilized by C—H···O, C—H···π and π–π interactions. The central benzene ring forms dihedral angles of 58.55 (6) and 4.02 (6)° with the terminal benzene rings.

Comment

Some Schiff base compounds exhibit various pharmacological activities, *e.g.* anticancer (Dao *et al.*, 2000), anti-HIV (Sriram *et al.*, 2006), antibacterial and antifungal (Karthikeyan *et al.*, 2006). In addition, some of them may be used as analytical reagents for the determination of trace elements (Eltayeb & Ahmed, 2005*a*,*b*). Recently we have reported the crystal structures of 1-{2-[2-hydroxy-1-naphthyl)methyleneamino]-phenyliminiomethyl}-2-naphtholate methanol hemisolvate (Eltayeb *et al.*, 2007*a*) and 6,6′-dimethyl-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenol (Eltayeb *et al.*, 2007*b*). In this paper, we report the crystal structure of the title compound, (I), obtained by the reaction of *o*-phenylenediamine and 4-methylsalicylaldehyde.



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). The dihedral angles between the planes defined by *A* (C1–C6), *B* (C8–C13) and *C* (C15–C20) are 58.55 (6) (*A*/*B*), 61.04 (6) (*A*/*C*) and 4.02 (6)° (*B*/*C*). Intramolecular O—H···N hydrogen bonds generate *S*(6) ring motifs (Table 1 and Fig.1) (Bernstein *et al.*, 1995).

The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds and C—H···π interactions involving the C1–C6 benzene ring (centroid *Cg*1). In addition, the crystal packing is stabilized by π–π interactions between the C8–C13 (centroid *Cg*2) and C15–C20 (centroid *Cg*3) benzene rings with a $Cg2\cdots Cg3^{i}$ distance of 3.6914 (8) Å [symmetry code (i) is given in Table 1]. The molecules are stacked into columns along the *a* axis (Fig. 2).

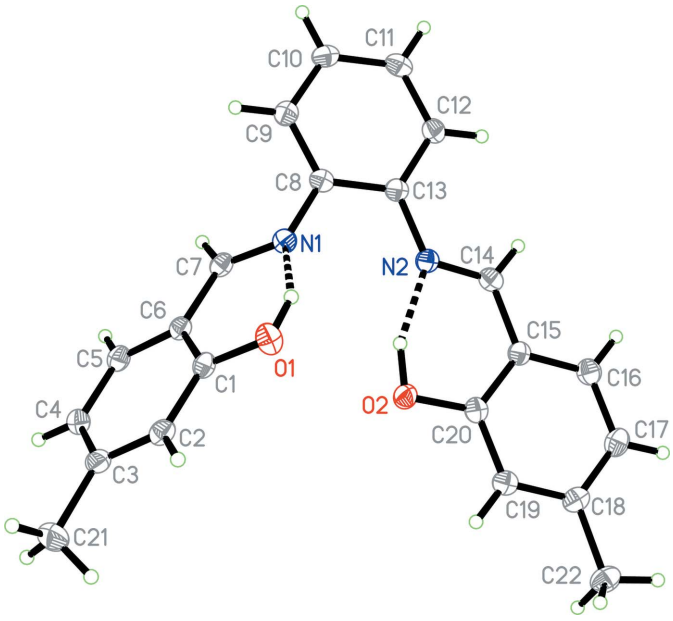


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are shown as dashed lines.

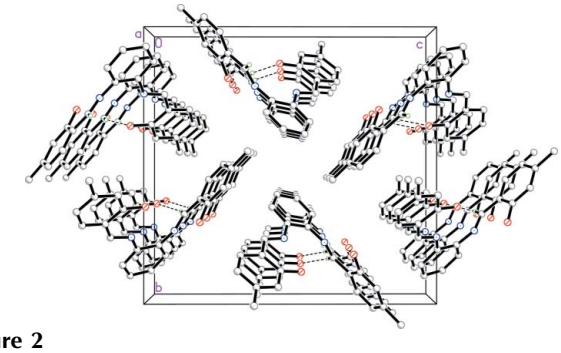


Figure 2
The crystal packing of (I), viewed down the *a* axis. H atoms not involved in intermolecular hydrogen bonding (dashed lines) have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.96 (2)	1.73 (2)	2.599 (1)	149 (2)
O2—H2B···N2	0.95 (2)	1.67 (2)	2.558 (1)	155 (2)
C7—H7A···O2^{i}	0.93	2.40	3.250 (2)	152
C12—H12A···$Cg1^{ii}$	0.93	2.78	3.643 (2)	156
C22—H22B···$Cg1^{iii}$	0.96	2.92	3.446 (1)	116

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

Experimental

To a solution of *o*-phenylenediamine (0.172 g, 1.6 mmol) in ethanol (20 ml) was added 4-methylsalicylaldehyde (0.444 g, 3.2 mmol). The mixture was refluxed with stirring for 30 min. The resultant orange solution was filtered and orange crystals suitable for X-ray diffraction analysis formed after one week on slow evaporation of the solvent at room temperature (yield 0.35 g, 63.63%; m.p. 410–412 K).

Crystal data

$C_{22}H_{20}N_2O_2$
M_r = 344.40
Monoclinic, $P2_1/c$
a = 6.0782 (2) Å
b = 16.5573 (6) Å
c = 17.4989 (6) Å
β = 90.348 (2)°
V = 1761.03 (11) Å^3
Z = 4
D_x = 1.299 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100.0 (1) K
Needle, orange
0.46 × 0.11 × 0.09 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.855, T_{max} = 0.992
22113 measured reflections
5201 independent reflections
3751 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 30.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
S = 1.05
5201 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.5205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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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