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4-Methyl-2-[(4-nitrophenylimino)methyl]phenol

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The title compound, $C_{14}H_{12}N_2O_3$, crystallizes with two molecules in the asymmetric unit. The molecular structure is stabilized by intramolecular O—H···N interactions, generating an *S*(6) motif. The crystal packing is stabilized by intermolecular C—H···O interactions.

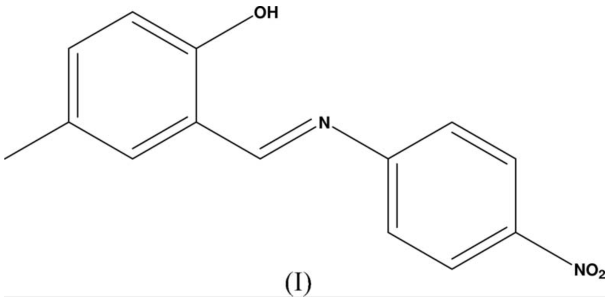
Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.086
wR factor = 0.202
Data-to-parameter ratio = 16.8

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

Comment

The development of receptors for recognizing cation, anion and neutral species has attracted much attention in molecular recognition studies and supramolecular chemistry (Gale, 2000). These molecular receptors are designed to bind and sense selectively cationic, anionic and neutral guests through macroscopic physical responses, where the binding events are converted into an electrochemical or fluorescence signal or colorimetric change detectable by the naked eye (Suksai & Tuntulani, 2003). Aromatic nitro compounds containing suitable binding groups attract increasing interest for the selective and sensitive colorimetric detection of cations and anions (Kato *et al.*, 2001). As the title compound, (I), is of much importance, we have solved the crystal structure using the technique of X-ray diffraction.



(I)

Compound (I) crystallizes in the monoclinic system with two molecules in the asymmetric unit (Fig. 1). The bond lengths and angles are comparable with the literature values (Allen *et al.*, 1987). The sums of the bond angles around atoms N2 and N4 (360°) indicate sp^2 hydribization. Atoms O1 and C1 deviate by 0.028 (2) and 0.046 (3) Å, respectively, from the C2-benzene ring; C15 deviates by 0.013 (4) Å from the C16-benzene ring. Atom O4 lies in the plane of the C16–C21 ring. The torsion angles C11—C12—N2—O2 [−3.2 (2)°] and C11—C12—N2—O3 [176.9 (1)°] in molecule *A*, and C25—C26—N4—O5 [−179.0 (3)°] and C25—C26—N4—O6 [1.7 (4)°] in molecule *B*, indicate that the nitro groups are coplanar with the benzene rings C9–C14 and C23–C28, respectively. The dihedral angle between the two benzene rings in molecule *A* is 46.9 (1)°, while in molecule *B* it is 5.9 (1)°, and this difference

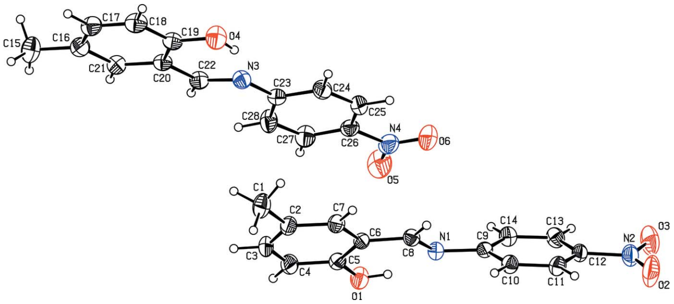


Figure 1
The asymmetric unit of(I), showing 30% probability displacement ellipsoids.

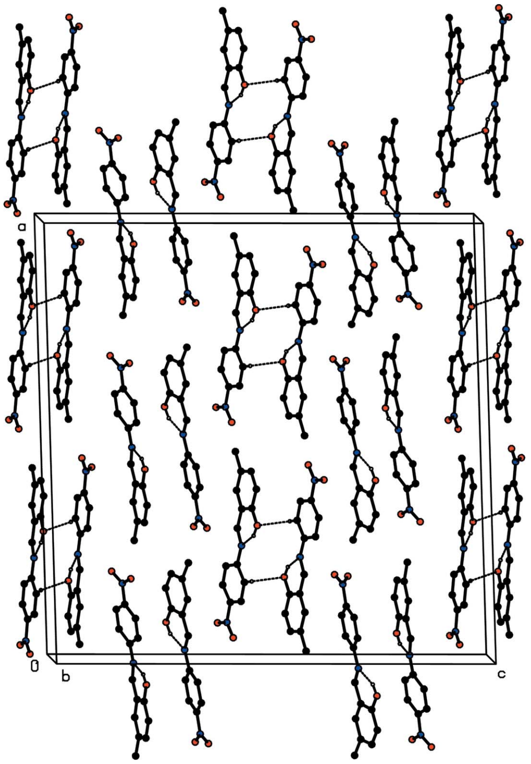


Figure 2
The molecular packing of (I), viewed approximately down the *b* axis. For clarity, H atoms not involved in hydrogen bonding (dashed lines) have been omitted.

is correlated with the difference in the torsion angles C8—N1—C9—C14 [−140.9 (2)°] and C22—N3—C23—C24 [172.8 (2)°] in molecules *A* and *B*, respectively.

The structure of (I) is stabilized by strong O—H···N intramolecular interactions, generating *S*(6) motifs (Bernstein *et al.*, 1995; Table 1). The crystal packing is highly stabilized by C—H···O intermolecular interactions (observed only for molecule *A*), generating a centrosymmetric dimer with an $R_2^2(16)$ ring.

Experimental

Compound (I) was synthesized by Schiff base condensation between 4-nitroaniline and 5-methylsalicylaldehyde. A methanolic solution (20 ml) of 4-nitroaniline (0.51 g, 3.68 mmol) was added dropwise to a stirred solution of 5-methylsalicylaldehyde (0.50 g, 3.68 mmol) in methanol (20 ml) and the mixture was stirred for 1 h. After stirring, the solution was heated to reflux for 20 min and then cooled to room temperature. The resulting crystalline solid was filtered off and washed with cold methanol. The microcrystalline compound was recrystallized from ethanol and crystals of (I) suitable for X-ray diffraction were obtained on slow evaporation (yield 90%; m.p. 417 K).

Crystal data

$C_{14}H_{12}N_2O_3$
$M_r = 256.26$
Monoclinic, $C2/c$
$a = 28.698$ (2) Å
$b = 6.0051$ (5) Å
$c = 28.574$ (2) Å
$\beta = 92.318$ (2)°
$V = 4920.3$ (6) Å^3
$Z = 16$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
27143 measured reflections
5813 independent reflections
4304 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.086$
$wR(F^2) = 0.202$
$S = 1.20$
5813 reflections
345 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.23$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.87	2.599 (3)	147
O4—H4*A*···N3	0.82	1.89	2.617 (3)	147
C24—H24···O4$^{\rm i}$	0.93	2.54	3.399 (3)	154

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

All H-atoms were refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H, O—H = 0.83 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(O) for the OH group, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for CH_3 atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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