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4-{[1-(1-Adamantyl)ethyl]iminomethyl}phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.086
Data-to-parameter ratio = 10.3

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

The title compound, $C_{19}H_{25}NO$, a Schiff base, crystallized in the phenol–imine tautomeric form. The C═N bond length is 1.270 (3) Å and the bond length between the C atom of the aromatic ring and the C atom of the imine group is 1.460 (4) Å, which corresponds to a conjugated C═N group. In the crystal structure, a one-dimensional chain is formed *via* a strong intermolecular O—H···N hydrogen bond.

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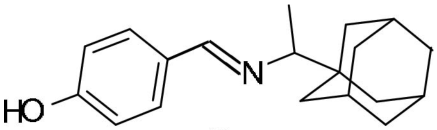
Comment

Schiff bases form an important class of compounds and find varied applications. These include uses as catalysts and stabilizers, in polymers, pigments and dyes, in photography, and in various biological systems. Some Schiff bases have also been used as analytical reagents, as inhibitors against corrosion and as flocculants. Additionally, Schiff bases find applications in many other fields of fundamental and applied research (Dhar & Taploo, 1982; Dey, 1974; Hodnett & Dunn, 1970; Ming *et al.*, 1997; Bi & Liu, 1996; Wei *et al.*, 1998). Fernández-G *et al.* (2001) reported the characterization of several Schiff base ligands resulting from the condensation of salicylaldehyde, 2-hydroxy-1-naphthaldehyde and 3-hydroxy-2-naphthaldehyde with 1-adamantanamine and 1-adamantanemethylamine. It has been reported that, in the solid state, some Schiff bases can exist either as keto–amine or as phenol–imine tautomers. We report here the structure of the title Schiff base, (I), obtained by the condensation of rimantadine and 4-hydroxybenzaldehyde.



(I)

The molecular structure of (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. In the solid state, (I) exists in the phenol–imine tautomeric form, with a C4—O1 bond of 1.360 (3) Å and an O—H distance of 0.91 Å. This configuration is similar to the situation found in *N*-(1-adamantyl)salicylaldamine and 2-[(1-adamantyl)iminomethyl]-3-naphthol (Fernández-G *et al.*, 2001), but not in 1-[(1-adamantanemethylamino)methylene]-2-(1*H*)-naphthalenone (Fernández-G *et al.*, 2001), which exists as the keto–amine tautomer.

The C═N bond length of 1.270 (3) Å and C1—C7 bond length of 1.460 (4) Å correspond to a conjugated C═N group (Fernández-G *et al.*, 2001). The C atoms of the adamantane moiety have sp^3-hybridized orbitals, with C—C—C angles in

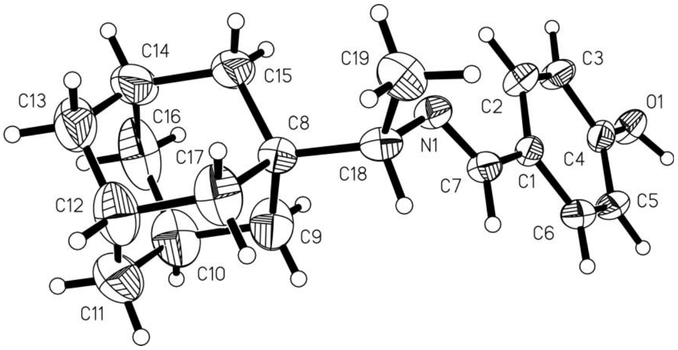


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

the range 106.2 (4)–115.7 (2)°.

In the crystal structure of (I), a one-dimensional chain structure is formed *via* a strong intermolecular hydrogen bond involving hydroxy atom O1 and atom N1 of a symmetry-related molecule (details are given in Table 2 and Fig. 2).

Experimental

A mixture of rimantadine (0.18 g, 1.0 mmol) and 4-hydroxybenzaldehyde (0.13 g, 1.0 mmol) in absolute methanol (30 ml) was stirred and refluxed on a water bath for 4 h. The solution was cooled to room temperature. Light-yellow single crystals, suitable for X-ray diffraction, were obtained by slow evaporation after 5 d. Yield 0.18 g (62%). M.p: 452–453 K. Analysis calculated for $C_{19}H_{25}NO$: C 80.52, H 8.89, N 4.94%; found: C 80.49, H 8.85, N 4.91%. IR (KBr, cm^{-1}): ν 1634 (*s*, C═N), 3444, 1284 (Ar–OH). ^{1}H NMR ($CDCl_3$): δ 8.07 (*s*, 1H, –CH═N–), 6.60–7.46 (*s*, 4H, C_6H_4), 2.82 (*m*, 1H, CH), 9.81 (*w*, 1H, Ar–OH), 1.55–2.00 (*w*, 15H, $C_{10}H_{15}$), 1.20 (*s*, 3H, –CH_3).

Crystal data

$C_{19}H_{25}NO$
$M_r = 283.40$
Orthorhombic, $Pna2_1$
$a = 12.706$ (3) Å
$b = 11.141$ (2) Å
$c = 11.552$ (2) Å
$V = 1635.4$ (6) Å^3
$Z = 4$
$D_x = 1.151$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 3577 reflections
$\theta = 2.4$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.33 × 0.32 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.977$, $T_{\max} = 0.981$
3578 measured reflections

1968 independent reflections
1004 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 27.5°$
$h = -16 \rightarrow 16$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.086$
$S = 1.09$
1968 reflections
192 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0083 (9)

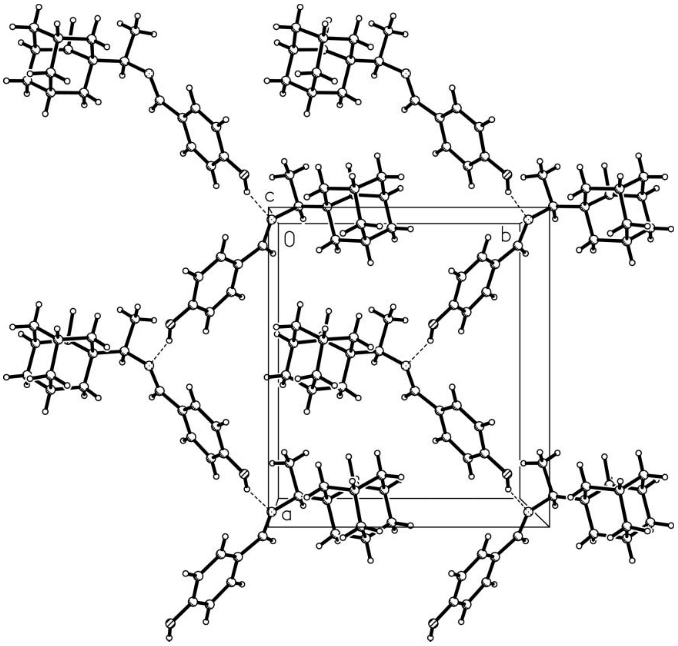


Figure 2
The molecular packing of (I), viewed along the *c* axis. Broken lines indicate the O—H···N hydrogen-bonding interactions (see Table 2 for details).

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.360 (3)	C1—C7	1.460 (4)
N1—C7	1.270 (3)	C8—C18	1.553 (4)
N1—C18	1.472 (4)		
C7—N1—C18	117.6 (3)	N1—C18—C19	108.4 (3)
N1—C7—C1	125.7 (3)	N1—C18—C8	110.3 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1$^{\rm i}$	0.91	1.88	2.778 (3)	168

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

The hydroxy H atom was initially located in a difference Fourier map. The bond distance was fixed at 0.91 Å and $U_{\rm iso}$(H) was refined. The other H atoms were constrained to an ideal geometry, with C—H distances of 0.96 Å and $U_{\rm iso}$(H) = 1.5 or 1.2$U_{\rm eq}$(C). In the absence of significant anomalous dispersion effects, 1780 Friedel pairs were merged.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL/PC*.

o1772 Feng *et al.* • $C_{19}H_{25}NO$ *Acta Cryst.* (2005). E**61**, o1771–o1773

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Acta Cryst. (2005). E**61**, o1771–o1773 Feng *et al.* • $C_{19}H_{25}NO$ **o1773**