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# 1-[(5-*tert*-Butyl-2-hydroxyphenyl)-iminomethyl]-2-napthol

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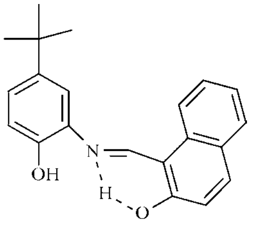
In the crystal structure of the title compound, $C_{21}H_{21}NO_2$, strong N—H···O and O—H···O hydrogen bonds exist. The keto–amine form is favoured over the enol–imine form in the tautomerism. Six-membered chelate rings formed by intramolecular hydrogen bonds increase the stability of the whole molecule. Intermolecular hydrogen bonds link adjacent units together, forming an infinite one-dimensional chain parallel to the *a* axis.

## Comment

Schiff bases have been widely used as ligands in the formation of transition metal complexes (Elmali *et al.*, 1998). Although many structures of transition metal complexes with Schiff base ligands have been determined, a relatively small number of free Schiff bases have been structurally characterized (Ünver *et al.*, 2005). Schiff bases with an OH group in the position *ortho* to the imine group are of interest mainly because of the existence of either O—H···N or N—H···O hydrogen bonds and tautomerism between the enol–imine and keto–amine forms (Ünver *et al.*, 2005; Hökelek *et al.*, 2000; Mondal *et al.*, 2002). These Schiff bases usually have the keto–amine form and show photochromism, because the H atom from the phenol group is reversibly transferred to the imine N atom (Hadjoudis *et al.*, 1987; Elmali *et al.*, 1998; Elmali & Eleman, 1998). We report here the structure of the title compound, (I).



(I)

In the title compound (Fig. 1), either atom O1 or O2 may be hydrogen bonded to H1*A*, but the distance between O1 and H1*A* [2.10 (2) Å] is significantly longer than the O2···H1*A* distance [1.77 (2) Å]. The N1—H1*A*···O2 hydrogen bond in (I) completes a six-membered ring (C11/C12/C13/O2/H1*A*/N1), which creates greater π-delocalization with the naphthalene ring system, increasing the stability of this compound.

The C14═C15 bond length [1.338 (3) Å] in the title compound is shorter than the expected value (1.40 Å). The C13═O2 bond length [1.275 (2) Å] is consistent with an O═C double bond. The corresponding bond lengths in a substituted naphthalenone are 1.351 (5) and 1.274 (4) Å, respectively (Hökelek *et al.*, 2000). The reason for the shortening of the C13═O2 and C14═C15 bond lengths in (I) may

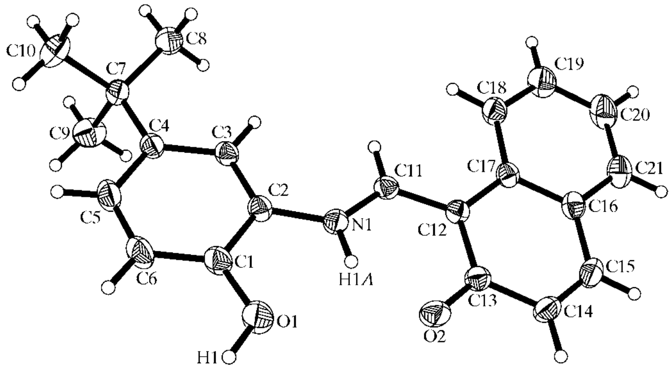


**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids.

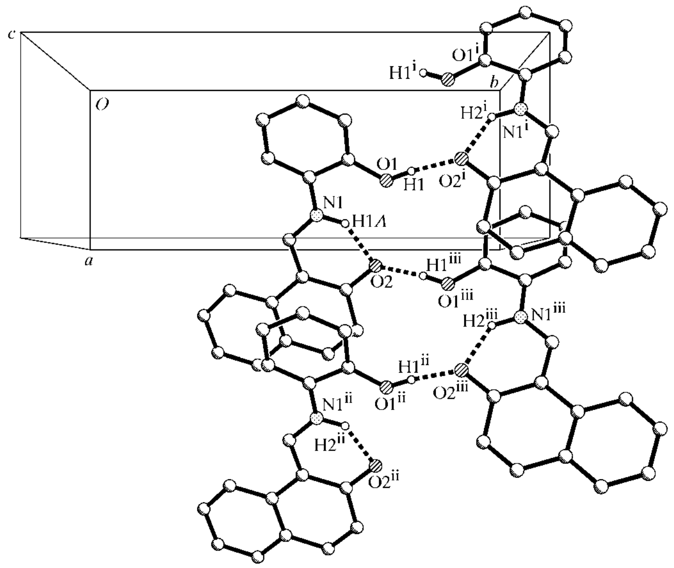


**Figure 2**
The one-dimensional hydrogen-bonded chain parallel to the *a* axis. Some H atoms and *tert*-butyl groups have been omitted for clarity. [Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 2$; (ii) $x + 1, y, z$; (iii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 2$.]

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be the quinoidal structure (keto–amine form), as in the naphthalimine reported by Đilović *et al.* (2005).

The N1—C11—C12 angle [122.65 (14)°] is close to 120°, while the C2—N1—C11 angle is 130.69 (14)°, thus decreasing the planarity of the whole molecule. The C1–C7 and O2/C11–C21 planes are inclined at an angle of 13.15 (7)°; this angle increases to 56.9° when a similar ligand is coordinated to a copper(II) ion (Ünver, 2002).

The O2···N1 distance of 2.5257 (19) Å is clearly indicative of a strong intermolecular hydrogen bond (Table 1); this distance is significantly shorter than the sum (3.07 Å) of the van der Waals radii for N and O atoms. At the same time, the N1—C11 distance of 1.309 (2) Å is slightly longer than a C═N double bond. All these bond lengths reveal that the keto tautomer (N—H···O) is favoured over the enol tautomer (O—H···N).

Other intermolecular hydrogen bonds also exist in the crystal structure. Atom O1 is hydrogen bonded to O2$^{i}$ (see Table 1 for symmetry code) from an adjacent molecule, which links adjacent units, forming a one-dimensional chain parallel to the *a* axis (Fig. 2).

In addition to hydrogen bonds, the crystal packing of (I) is also stabilized by $\pi$-stacking interactions between the naphthalene ring system (C12–C21) and the benzene ring in a neighbouring molecule [C1$^{ii}$–C6$^{ii}$; symmetry code: (ii) $x + 1$, $y$, $z$]. The distance between the centroids of the corresponding rings is 4.287 (16) Å.

## Experimental

2-Hydroxy-1-naphthaldehyde (0.172 g, 1 mmol) and 2-amino-4-*tert*-butylphenol (0.165 g, 1 mmol) were dissolved in ethanol (20 ml) and the solution was refluxed for 2 h. The resulting red product was recrystallized from methanol and dried in a vacuum (yield 0.300 g, 85%; m.p. 513–515 K). Elemental analysis found: C 78.99, H 7.12, N 4.37%; calculated for $C_{21}H_{21}NO_2$: C 78.97, H 6.63, N 4.39%. Crystals were obtained from methanol at room temperature by slow evaporation for about a week. After a period of time, the crystals deteriorated into a red powder.

### *Crystal data*

$C_{21}H_{21}NO_2$
$M_r = 319.39$
Orthorhombic, $P2_12_12_1$
$a = 6.1882$ (6) Å
$b = 15.9350$ (15) Å
$c = 17.2295$ (16) Å
$V = 1699.0$ (3) Å$^3$
$Z = 4$
$D_x = 1.249$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm$^{-1}$
$T = 294$ (2) K
Block, red
0.26 × 0.20 × 0.16 mm

### *Data collection*

Bruker CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.975$, $T_{\max} = 0.987$
11475 measured reflections
2343 independent reflections
2039 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 27.9°$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.089$
$S = 1.06$
2343 reflections
229 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.13$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0126 (17)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.90 (3) | 1.69 (3) | 2.5846 (18) | 174 (3) |
| N1—H1$A$···O2 | 0.91 (2) | 1.77 (2) | 2.5257 (19) | 139 (2) |

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

H atoms attached to N or O atoms were located in a difference Fourier synthesis and were refined freely. Other H atoms were positioned geometrically and were constrained to ride on their parent atoms [C—H = 0.93 (aromatic H) or 0.96 Å (methyl H); $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(aromatic C) or 1.5$U_{\rm eq}$(methyl C)].

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3047). Services for accessing these data are described at the back of the journal.

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