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2-(1-Naphthyliminomethyl)phenol

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.130
Data-to-parameter ratio = 16.3

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

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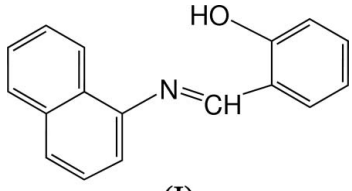
In the molecule of the title compound, $C_{17}H_{13}NO$, the naphthalene ring system is essentially planar. A strong intramolecular O—H···N hydrogen bond results in the formation of a pseudo-six-membered planar ring, which makes a dihedral angle of 2.85 (5)° with the phenol ring.

Comment

Recently, we have reported a few Schiff base compounds and complexes (Cheng *et al.*, 2005; Zhu *et al.*, 2005; You *et al.*, 2004). As an extension of our work on the structural characterization of Schiff base compounds or complexes, a new compound is reported here.



(I)

In the molecule of the title compound, (I), bond lengths and angles (Table 1) are in normal ranges (Allen *et al.*, 1987). The C1═N1 bond length conforms to the value for a double bond. The strong intramolecular O—H···N hydrogen bond (Table 2) results in the formation of a pseudo-six-membered planar ring, *B* (C1/C2/C7/O1/H1/N1) (Fig. 1). The rings *A* (C2–C7), *C* (C8–C11/C16/C17) and *D* (C12–C17) are each planar. The dihedral angles between the rings are *A*/*B* = 2.85 (5)°, *A*/*C* = 68.0 (3)°, *A*/*D* = 67.6 (3)° and *C*/*D* = 0.47 (4)°.

In the crystal packing, the molecules are extended along the *c* axis and stacked along the *a* axis (Fig. 2). Dipole–dipole and van der Waals interactions are effective in the molecular packing.

Experimental

Salicylaldehyde and naphthalidine were available commercially and were used without further purification. Salicylaldehyde (2.0 mmol, 244 mg) was dissolved in methanol (20 ml); to this solution was added a 20 ml solution of naphthalidine (2.0 mmol, 494 mg) with stirring. The suspension was stirred for an additional 20 min and then filtered. After keeping the filtrate in air for 10 d, yellow block-shaped crystals were formed at the bottom of the vessel. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 88.7%). Analysis found: C 82.1, H 5.4, N 5.5%; calculated for $C_{17}H_{13}NO$: C 82.5, H 5.3, N 5.7%.

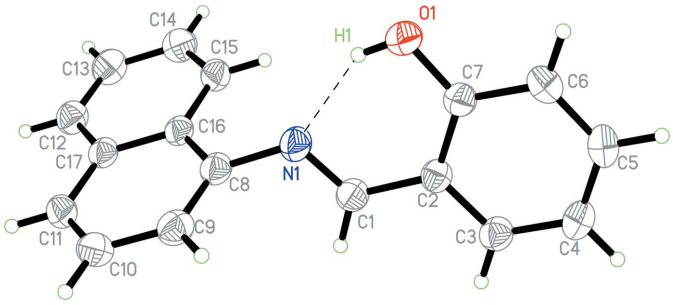


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The O—H···N hydrogen bond is shown as a dashed line.

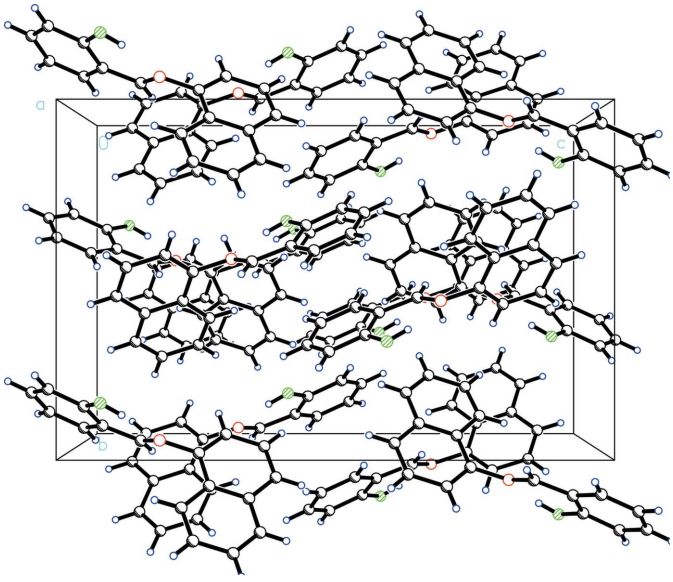


Figure 2
The crystal packing of (I), viewed along the *a* axis.

Crystal data

$C_{17}H_{13}NO$
M_r = 247.28
Orthorhombic, *Pbca*
a = 10.5820 (7) Å
b = 12.5388 (9) Å
c = 19.4250 (13) Å
V = 2577.4 (3) Å^3
Z = 8
D_x = 1.275 Mg m^{-3}
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 292 (2) K
Block, yellow
0.40 × 0.35 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.975
22572 measured reflections
2818 independent reflections
2239 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.130
S = 1.04
2818 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.3644P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.3473 (16)	N1—C8	1.4219 (18)
N1—C1	1.2720 (17)	C1—C2	1.4504 (18)
C1—N1—C8	119.47 (12)	O1—C7—C2	121.62 (12)
N1—C1—C2	122.34 (13)	C9—C8—N1	121.42 (14)
O1—C7—C6	118.81 (13)	C16—C8—N1	117.99 (13)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.89	2.614(s.u.?)	147

H atoms were positioned geometrically, with O—H = 0.82 Å and C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O) or 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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