Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Bromo-2-(1-naphthyliminomethyl)phenol

Xi-Shi Tai,[a]* Jie Yin[b] and Yi-Min Feng[a]

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, People's Republic of China

Correspondence e-mail: taixishi@lzu.edu.cn

Received 9 January 2007
Accepted 10 January 2007

Key indicators

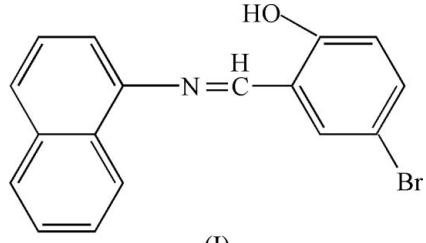
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.012 Å
R factor = 0.066
wR factor = 0.171
Data-to-parameter ratio = 13.4

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

The conformation of the title compound, $C_{17}H_{12}BrNO$, is dictated by an intramolecular O—H···N hydrogen bond.

Comment

As part of our ongoing studies (Tai *et al.*, 2005) on the synthesis, characterization and properties of Schiff base ligands and their metal complexes, we now report the synthesis and structural characterization of the title compound, (I) (Fig. 1).



(I)

In the molecule of (I), the C11═N1 [1.298 (9) Å] and C13—O1 [1.363 (9) Å] bond lengths are those expected for a double and single bond, respectively. The dihedral angle between the mean planes of the C1–C4/C9/C10 and C12–C17 benzene rings is 53.1 (4)°. An intramolecular O—H···N hydrogen bond (Table 1) helps to establish the molecular conformation.

Experimental

5-Bromosalicylaldehyde (10 mmol) was added to a solution of 1-naphthylamine (10 mmol) in 10 ml of CH_3CH_2OH. The mixture was

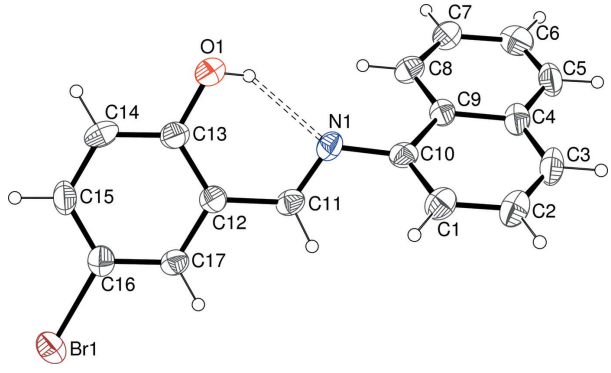


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). The intramolecular hydrogen bond is indicated by a double dashed line.

continuously stirred for 3 h at refluxing temperature, evaporating some ethanol; the product was then collected by filtration and dried *in vacuo* (yield 86%). Elemental analysis calculated for $C_{17}H_{12}BrNO$: C 60.57, H 3.68, N 4.29%; found: C 60.46, H 3.38, N 4.50%. Single crystals of (I) were obtained by evaporation of an ethanol solution after two weeks.

Crystal data

$C_{17}H_{12}BrNO$
M_r = 326.19
Monoclinic, $P2_1/c$
a = 25.467 (7) Å
b = 4.3831 (13) Å
c = 12.587 (4) Å
β = 90.238 (5)°
V = 1405.0 (7) Å^3
Z = 4
D_x = 1.542 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.566, T_{max} = 0.622
5365 measured reflections
2444 independent reflections
1574 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.171
S = 1.11
2444 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 6.3049P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 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	2.02	2.666 (7)	135

The H atoms were geometrically placed (O—H = 0.82 Å, C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (20671073), NingXia Natural Gas Transferring Key Laboratory (2004007), the Science and Technology Foundation of Weifang and Weifang University for a research grant.

References

Bruker (2000). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Tai, X.-S., Liu, W.-Y., Liu, Y.-Z. & Li, Y.-Z. (2005). *Acta Cryst.* E**61**, o389–o390.