Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(1,3-Benzothiazol-2-yl)-2-naphthol

Zhi-Qiang Huang, Zhi-Qiang Du,* Guan-Sheng Du and Jun Yan

Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China

Correspondence e-mail: duzq@zju.edu.cn

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.112
Data-to-parameter ratio = 13.8

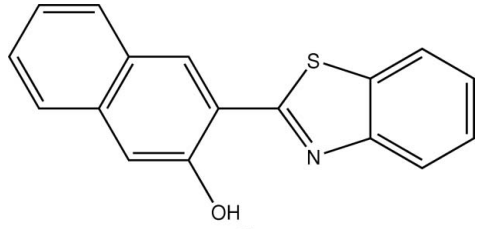
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 April 2006
Accepted 16 April 2006

The molecule of the title compound, $C_{17}H_{11}NOS$, is planar, the dihedral angle between the benzothiazole and 2-naphthol systems being 3.44 (6)°. The face-to-face separation of 3.48 (2) Å indicates π–π stacking between parallel benzothiazole systems.

Comment

The title compound, (I), is an intermediate of photochromic compounds (Deligeorgiev *et al.*, 2002). We report here the molecular structure of (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule is planar, the dihedral angle between the benzothiazole and 2-naphthol mean planes being 3.44 (6)°. Intramolecular hydrogen bonding occurs between the benzothiazole and naphthol ring systems (Table 1).

The parallel benzothiazole systems partially overlap each other (Fig. 2). The face-to-face separation of 3.48 (2) Å indicates the existence of π–π stacking.

Experimental

The title compound was prepared according to the procedure described by Deligeorgiev *et al.* (2002). It was synthesized by reaction of 2-hydroxy-3-naphthalenecarboxylic acid and 2-aminothiophenol in boiling toluene. Single crystals of (I) were obtained by recrystallization from toluene solution.

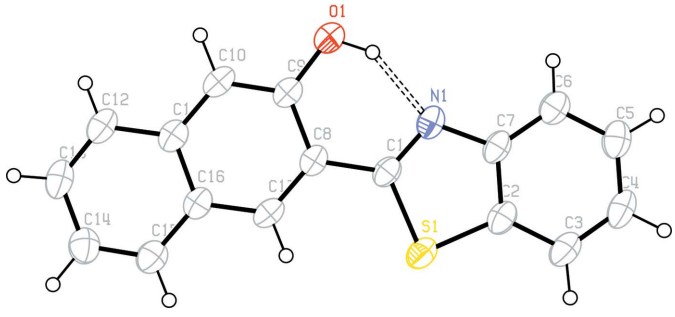


Figure 1
The molecular structure of (I), with 40% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonding.

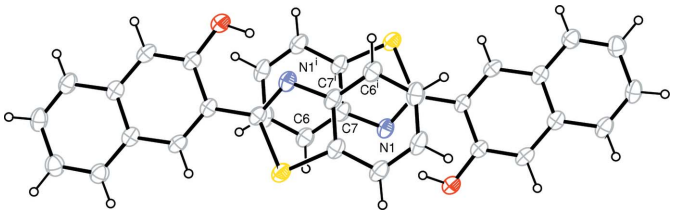


Figure 2
The π–π stacking in (I) [symmetry code: (i) $1-x, -y, 2-z$].

Crystal data

$C_{17}H_{11}NOS$
$M_r = 277.33$
Monoclinic, $P2_1/n$
$a = 6.3634\ (9)$ Å
$b = 8.5293\ (12)$ Å
$c = 23.588\ (3)$ Å
$\beta = 95.120\ (3)^\circ$
$V = 1275.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.445$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.25$ mm^{-1}
$T = 295\ (2)$ K
Prism, pale yellow
$0.34 \times 0.27 \times 0.22$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.931$, $T_{max} = 0.945$
6746 measured reflections
2497 independent reflections
1755 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.112$
$S = 0.86$
2497 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ 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	1.88	2.612 (2)	149

H atoms bonded to C atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The hydroxy H atom was located in a difference Fourier map and refined as riding in its as-found relative position (O—H = 0.82 Å), with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The work was supported by the National Natural Science Foundation of China (grant No. 20376071). The authors thank Professor Long-Guan Zhu for his kind assistance in preparing the CIF.

References

Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02a) and *SMART* (Version 5.618). Bruker AXS Inc., Madison, Wisconsin, USA.
Deligeorgiev, T., Minkovska, S., Jejiazkova, B. & Rakovsky, S. (2002). *Dyes Pigments*, **53**, 101–108.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.