

2-Methyl-3-(methylsulfinyl)naphtho[1,2-*b*]furanHong Dae Choi,^a Hyun Mi Woo,^a
Pil Ja Seo,^a Byeng Wha Son^b and
Uk Lee^{b*}^aDepartment of Chemistry, Dongeui University,
San 24 Kaya-dong Busanjin-ku, Busan 614-714,
Republic of Korea, and ^bDepartment of
Chemistry, Pukyong National University, 599-1
Daeyeon 3-dong Nam-ku, Busan 608-737,
Republic of Korea

Correspondence e-mail: uklee@pknu.ac.kr

The title compound, C₁₄H₁₂O₂S, was prepared by the
oxidation of 2-methyl-3-(methylsulfonyl)naphtho[1,2-*b*]furan
using *m*-chloroperbenzoic acid. The crystal structure contains
aromatic π - π stacking, C—H \cdots O and C—H \cdots π interactions.Received 2 August 2006
Accepted 14 August 2006

Comment

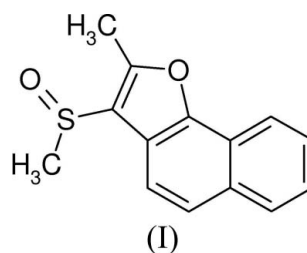
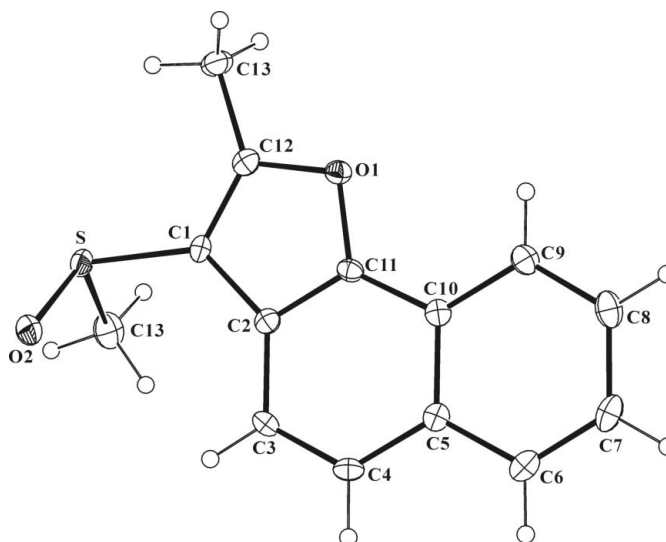
This work follows on from our previous report on 2-methyl-1-
(methylsulfinyl)naphtho[2,1-*b*]furan (Choi *et al.*, 2006). In the
isomeric title compound, (I), the naphtho[1,2-*b*]furan unit is
again nearly planar, with a mean deviation of 0.028 Å from the
least-squares plane defined by the 13 constituent atoms.Similar to the 2-methyl-1-(methylsulfinyl) isomer, the
crystal structure of (I) exhibits aromatic π - π stacking of the
naphtho units along the *a* axis (Fig. 2), with alternate inter-
plane separations of 3.34 (1) and 3.37 (1) Å. In the former
case, the shortest separation between ring centroids is
Cg2 \cdots Cg1ⁱ = 3.61 Å, where Cg1 is the centroid of the C5–C10

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

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ (C—C) = 0.004 Å
R factor = 0.069
wR factor = 0.146
Data-to-parameter ratio = 16.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

ring and Cg2 is the centroid of the C2–C5/C10/C11 ring (symmetry code as in Fig. 2). In the latter, the shortest separation between ring centroids is $Cg3 \cdots Cg3^{ii} = 3.86 \text{ \AA}$, where Cg3 is the centroid of the O1/C1/C2/C11/C12 ring. C–H $\cdots\pi$ interactions also exist between these two molecules, with $H14C \cdots Cg1^{ii} = 3.08 \text{ \AA}$ (symmetry code as in Fig. 2).

As observed for the 2-methyl-1-(methylsulfinyl) isomer, C–H \cdots O interactions are formed to atom O2, with $H4 \cdots O2^{iii} = 2.65 \text{ \AA}$ and $H7 \cdots O2^{iv} = 2.50 \text{ \AA}$ [symmetry codes: (iii) $\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$; (iv) $\frac{1}{2} - x, \frac{1}{2} + y, -\frac{1}{2} - z$]. Atom O1 does not make any such contacts.

Experimental

Compound (I) was prepared according to the method described for the previously reported isomer (Choi *et al.*, 2006), using 2-methyl-3-(methylsulfonyl)naphtho[1,2-*b*]furan (Choi *et al.*, 1999) instead of 2-methyl-1-(methylsulfonyl)naphtho[2,1-*b*]furan. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetone solution [yield 86%, m.p. 406–407 K; $R_f = 0.53$ (EtOAc)].

Crystal data

$C_{14}H_{12}O_2S$	$Z = 4$
$M_r = 244.30$	$D_x = 1.368 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.1443$ (4) \AA	$\mu = 0.26 \text{ mm}^{-1}$
$b = 15.8684$ (8) \AA	$T = 120$ (2) K
$c = 9.5313$ (5) \AA	Block, colourless
$\beta = 105.684$ (1) $^\circ$	$0.45 \times 0.40 \times 0.38 \text{ mm}$
$V = 1185.93$ (10) \AA^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2592 independent reflections
φ and ω scans	2119 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.083$
10083 measured reflections	$\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.5124P]$
$R[F^2 > 2\sigma(F^2)] = 0.069$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.20$	$\Delta\rho_{max} = 0.44 \text{ e \AA}^{-3}$
2592 reflections	$\Delta\rho_{min} = -0.41 \text{ e \AA}^{-3}$
156 parameters	
H-atom parameters constrained	

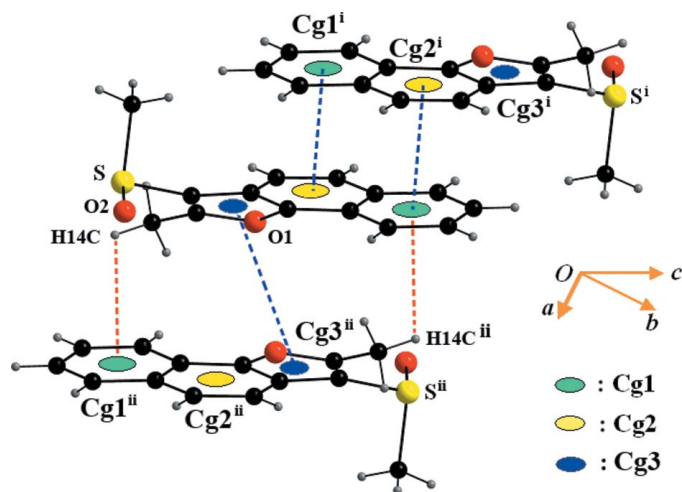


Figure 2

The π – π and C–H $\cdots\pi$ interactions in (I). Cg denotes the centroid of each ring. [Symmetry codes: (i) $1 - x, -y, -z$; (ii) $-x, -y, -z$].

All H atoms were placed in idealised positions and refined using a riding model, with C–H = 0.93 \AA and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H, and C–H = 0.96 \AA and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H. Both methyl groups were allowed to rotate about their local threefold axes.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

References

- Brandenburg, K. (1998). *DIAMOND*. Version 2.1. Crystal Impact GbR, Bonn, Germany.
- Bruker (1997). *SMART* and *SAINTE*. Versions 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
- Choi, H. D., Seo, P. J. & Son, B. W. (1999). *J. Korean Chem. Soc.* **43**, 237–240.
- Choi, H. D., Woo, H. M., Seo, P. J., Son, B. W. & Lee, U. (2006). *Acta Cryst.* **E62**, o3881–o3882.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.