

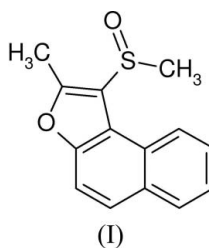
2-Methyl-1-(methylsulfinyl)naphtho[2,1-*b*]furanHong Dae Choi,^a Hyun Mi Woo,^a
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Key indicators

Single-crystal X-ray study
T = 120 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.065
wR factor = 0.151
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title compound, $\text{C}_{14}\text{H}_{12}\text{O}_2\text{S}$, was prepared by the
oxidation of 2-methyl-1-(methylsulfonyl)naphtho[2,1-*b*]furan
using *m*-chloroperbenzoic acid. The crystal structure contains
aromatic π - π stacking, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.Received 2 August 2006
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Comment

Naphthofuran compounds are important heterocyclic ring
systems in organic chemistry, and their derivatives exhibit
interesting biological properties (Bilger *et al.*, 1987; Hagiwara
et al., 1999, 2001). Although the presence of several structural
isomers for naphthofurans is possible, a useful method for the
synthesis of naphthofuran derivatives is the base-catalyzed
dehydrative cyclization of appropriate *o*-alkoxybenzoylarene
derivatives (Park & Jeong, 2005).With our ongoing interest in the syntheses and structures of
naphthofurans and naphthodifurans (Choi *et al.*, 1999, 2006),
we report here the crystal structure of the title compound, (I)
(Fig. 1), which was obtained by the oxidation of 2-methyl-1-
(methylsulfonyl)naphtho[2,1-*b*]furan using *m*-chloro-
perbenzoic acid. The bond lengths and angles are within
normal ranges. The naphtho[2,1-*b*]furan unit is nearly planar,
with a mean deviation of 0.092 \AA from the least-squares plane
defined by the 13 constituent atoms.The crystal structure of (I) exhibits aromatic π - π stacking
of naphtho units along the *a* axis. Adjacent naphtho[2,1-
b]furan groups are arranged in a centrosymmetric manner,
with alternate interplane separations of 3.36 (1) and 3.42 (1) \AA
(Fig. 2). In the former case, the shortest separation between
ring centroids is $\text{Cg}2\cdots\text{Cg}2^i = 3.67 \text{ \AA}$, where *Cg*2 is the
centroid of the C2/C3/C8-C11 ring (symmetry code as in
Fig. 2). In the latter, the shortest separation between ring
centroids is $\text{Cg}3\cdots\text{Cg}3^{ii} = 3.55 \text{ \AA}$, where *Cg*3 is the centroid of
the O1/C1/C2/C11/C12 ring. $\text{C}-\text{H}\cdots\pi$ interactions also exist
in this region, with $\text{H}13\text{A}\cdots\text{Cg}1^{iii} = 2.91 \text{ \AA}$ (symmetry code as
in Fig. 2). Between stacks, $\text{C}-\text{H}\cdots\text{O}$ interactions are formed
to atom O2, with $\text{H}7\cdots\text{O}2^{iii} = 2.54 \text{ \AA}$ [symmetry code: (iii)
 $\frac{1}{2} - x, \frac{1}{2} + y, -\frac{1}{2} - z$]. Atom O1 does not make any such
contacts.

Experimental

m-Chloroperbenzoic acid (77%, 695 mg, 3.1 mmol) was added in small portions to a stirred solution of 2-methyl-1-(methylsulfanyl)naphtho[2,1-*b*]furan (Choi *et al.*, 1999) (684 mg, 3.0 mmol) in dichloromethane (30 ml) at 273 K. After being stirred at room temperature for 1 h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (EtOAc) to afford (I) as a white solid. Crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone solution [yield 88%, m.p. 413–414 K; $R_f = 0.62$ (EtOAc)].

Crystal data

$C_{14}H_{12}O_2S$	$Z = 4$
$M_r = 244.30$	$D_x = 1.418 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.3158 (7) \text{ \AA}$	$\mu = 0.27 \text{ mm}^{-1}$
$b = 13.798 (1) \text{ \AA}$	$T = 120 (2) \text{ K}$
$c = 10.3969 (8) \text{ \AA}$	Block, colourless
$\beta = 106.389 (1)^\circ$	$0.45 \times 0.43 \times 0.40 \text{ mm}$
$V = 1144.50 (15) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	2495 independent reflections
φ and ω scans	2067 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.095$
9694 measured reflections	$\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 1.6525P]$
$R[F^2 > 2\sigma(F^2)] = 0.066$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.151$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.13$	$\Delta\rho_{max} = 0.59 \text{ e \AA}^{-3}$
2495 reflections	$\Delta\rho_{min} = -0.44 \text{ e \AA}^{-3}$
155 parameters	
H-atom parameters constrained	

All H atoms were placed in idealised positions and refined using a riding model, with C–H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H, and C–H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H. Methyl group C14 was allowed to rotate about its local threefold axis.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

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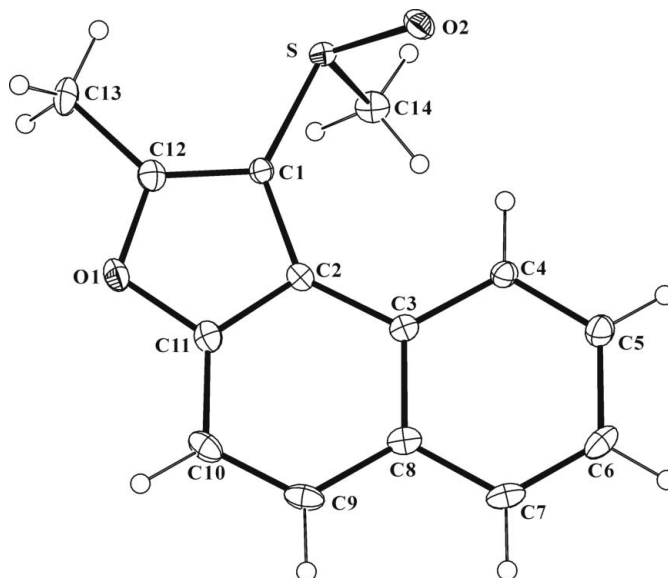


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

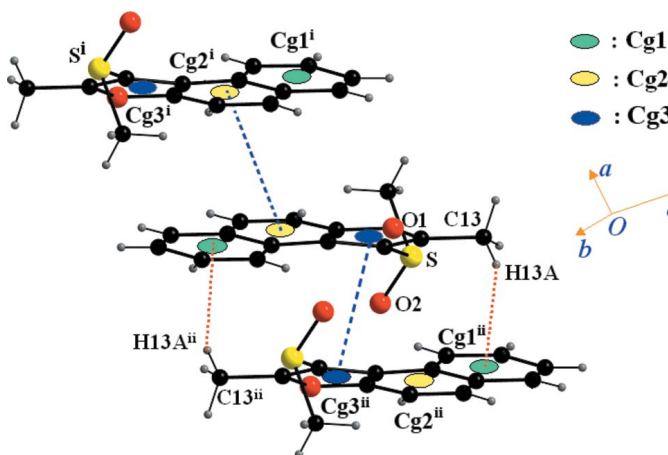


Figure 2
The π – π and C–H... π interactions in (I). Cg denotes the centroid of each ring. [Symmetry codes: (i) $1 - x, 2 - y, -z$; (ii) $-x, 2 - y, -z$].

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