Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Methylsulfinyl-2-phenylnaphtho[2,1-*b*]furan

Hong Dae Choi,[a] Pil Ja Seo,[a] Byoung Won Kang,[a] Byeng Wha Son[b] and Uk Lee[b]*

[a]Department of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-ku, Busan 614-714, Republic of Korea, and [b]Department 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

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.114
Data-to-parameter ratio = 15.8

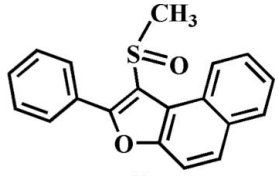
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{19}H_{14}O_2S$, was prepared by oxidation of 1-methylsulfanyl-2-phenylnaphtho[2,1-*b*]furan using 3-chloroperbenzoic acid. The naphthofuran ring system is approximately planar. The crystal structure includes aromatic π–π stacking and C—H$\cdots\pi$ interactions.

Received 1 November 2006
Accepted 13 November 2006

Comment

This work follows on from our previous investigations of isomeric naphtho[2,1-*b*]furan (Choi *et al.*, 2006*a*) and naphtho[1,2-*b*]furan (Choi *et al.*, 2006*b*). The title compound, (I) (Fig. 1), was obtained by oxidation of 1-methylsulfanyl-2-phenylnaphtho[2,1-*b*]furan using 3-chloroperbenzoic acid. The naphthofuran unit is approximately planar (mean deviation of 0.44 Å from the least-squares plane defined by the thirteen constituent atoms) and forms a dihedral angle of 32.91 (4)° with the mean plane of the phenyl ring.



(I)

In the crystal structure, π–π stacking interations are observed between the furan ring and a benzene ring of an adjacent naphthofuran unit, which is almost parallel [dihedral angle 1.38 (3)°] (Fig. 2). The *Cg*1$\cdots$*Cg*2^{iii} distance is 3.75 Å [*Cg*1 and *Cg*2 are the the centroids of the C1/C2/C11/O1/C12 and C3–C8 rings; symmetry code: (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$]. C19—H19*C*$\cdots\pi$ interactions are also observed [H19*C*$\cdots$*Cg*3^{i} = 3.55 Å; *Cg*3 is the centroid of the C13–C18 ring; symmetry code: (i) $-x, 1-y, 1-z$].

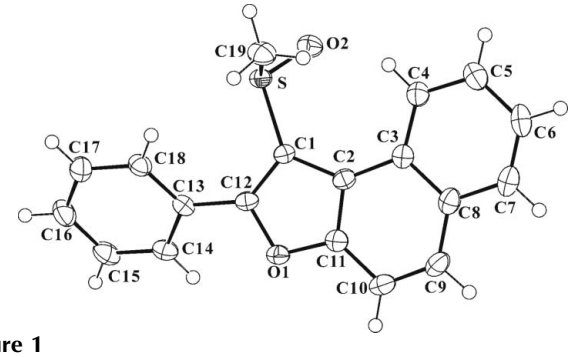


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms.

Experimental

3-Chloroperbenzoic acid (77%, 725 mg, 2.50 mmol) was added in small portions to a stirred solution of 1-methylsulfanyl-2-phenylnaphtho[2,1-*b*]furan (583 mg, 2.60 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. The organic layer was separated, dried over magnesium sulfate, filtered and concentrated *in vacuo*. The residue was purified by column chromatography (1:1 hexane/EtOAc) to afford (I) as a white solid. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution [yield 86%, m.p. 431–432 K; R_f = 0.73 (1:1 hexane/EtOAc)].

Crystal data

$C_{19}H_{14}O_2S$
M_r = 306.36
Monoclinic, $P2_1/n$
a = 10.868 (1) Å
b = 9.410 (1) Å
c = 14.190 (2) Å
β = 94.568 (2)°
V = 1446.6 (3) Å^3
Z = 4
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 173 (2) K
Plate, colourless
0.52 × 0.34 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
8612 measured reflections
3151 independent reflections
2751 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.114
S = 1.09
3151 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 1.0385P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

H atoms were placed in idealized positions and refined using a riding model, with C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and C—H = 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

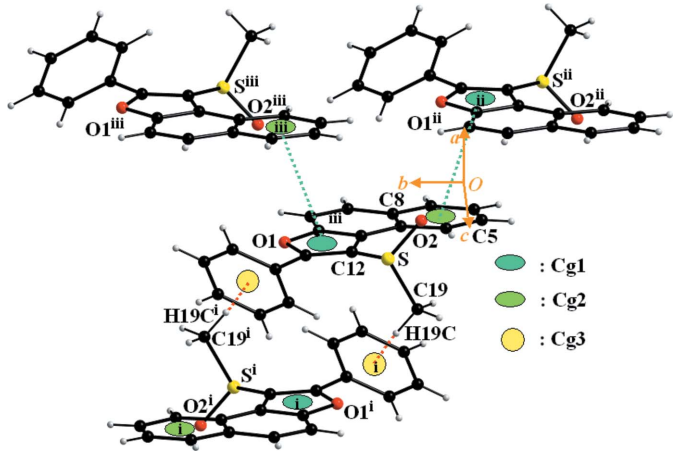


Figure 2
π—π and C—H$\cdots\pi$ interactions in (I). *Cg* denotes ring centroids. [Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.]

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: *ORTEP3* (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 *SAINT*. Versions 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Choi, H. D., Woo, H. M., Seo, P. J., Son, B. W. & Lee, U. (2006*a*). *Acta Cryst.* E**62**, o3881–o3882.
Choi, H. D., Woo, H. M., Seo, P. J., Son, B. W. & Lee, U. (2006*b*). *Acta Cryst.* E**62**, o3883–o3884.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.