Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Phenyl-1-(phenylsulfinyl)naphtho-[2,1-*b*]furan

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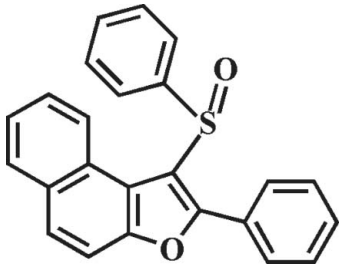
Received 25 May 2009; accepted 26 May 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.106; data-to-parameter ratio = 12.9.

In the title compound, $C_{24}H_{16}O_2S$, the O atom and the phenyl group of the phenylsulfinyl substituent lie on opposite sides of the plane of the naphthofuran fragment; the phenyl ring is almost perpendicular to this plane [82.34 (5)°]. The 2-phenyl ring is rotated out of the naphthofuran plane making a dihedral angle of 48.21 (6)°. The crystal structure shows π–π interactions between the central benzene rings of adjacent molecules [centroid–centroid distance = 3.516 (3) Å], as well as non-classical C—H···O hydrogen bonds.

Related literature

For the crystal structures of similar naphtho[2,1-*b*]furan derivatives, see: Choi *et al.* (2007, 2008). For the biological and pharmacological activity of naphthofuran compounds, see: Goel & Dixit (2004); Hagiwara *et al.* (1999); Piloto *et al.* (2005).



Experimental

Crystal data

$C_{24}H_{16}O_2S$
M_r = 368.43
Triclinic, $P\overline{1}$
a = 9.2262 (7) Å
b = 10.3430 (8) Å
c = 10.4296 (8) Å
α = 78.298 (1)°
β = 86.849 (1)°
γ = 67.506 (1)°
V = 900.15 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
6736 measured reflections
3140 independent reflections
2602 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.06
3140 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.95	2.59	3.488 (3)	158
C18—H18···O2^{ii}	0.95	2.57	3.323 (3)	137

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2587).

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supporting information

Acta Cryst. (2009). E**65**, o1443 [doi:10.1107/S1600536809019977]

2-Phenyl-1-(phenylsulfinyl)naphtho[2,1-*b*]furan

Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee

S1. Comment

The naphthofuran ring system has attracted widespread interest in view of their biological and pharmacological activities (Goel & Dixit, 2004; Hagiwara *et al.*, 1999; Piloto *et al.*, 2005). This work is related to our communications on the synthesis and structures of naphtho[2,1-b]furan analogues, *viz*. 2-methyl-1-(phenylsulfinyl)naphtho[2,1-b]furan (Choi *et al.*, 2007) and 2-methyl-1-(phenylsulfonyl)naphtho[2,1-b]furan (Choi *et al.*, 2008). We present the crystal structure of the title compound (I), 2-phenyl-1-(phenylsulfinyl)naphtho[2,1-b]furan (Fig. 1).

The naphthofuran unit is essentially planar, with a mean deviation of 0.015 (2) Å from the least-squares plane defined by the thirteen constituent atoms. The dihedral angle in (I) formed by the plane of the naphthofuran ring and the plane of 2-phenyl ring is 48.21 (6)°, and the phenyl ring (C19-C24) with 82.34 (5)° lies toward the naphthofuran plane. The crystal packing (Fig. 2) is stabilized by aromatic π–π interactions between the central benzene rings from the adjacent molecules. The Cg···Cg^{iii} distance is 3.516 (3) Å (Cg is the centroide of the C2/C3/C8/C9/C10/C11 benzene ring, symmetry code as in Fig. 2). The molecular packing is further stabilized by weak non-classical intermolecular C–H···O hydrogen bonds, the first between an aromatic H atom of the naphthofuran fragment and the S═O unit, the second between an aromatic H atom of 2-phenyl ring and the S═O unit, respectively (Table 1 and Fig. 2; symmetry code as in Fig. 2).

S2. Experimental

The 77% 3-chloroperoxybenzoic acid (77%, 247 mg, 1.1 mmol) was added in small portions to a stirred solution of 2-phenyl-1-(phenylsulfanyl)naphtho[2,1-b]furan (352 mg, 1.0 mmol) in dichloromethane (30 mL) at 273 K. After being stirred at room temperature for 3h, 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 (hexane-ethyl acetate, 2:1 v/v) to afford the title compound as a colorless solid [yield 81%, m.p. 462-463 K; R_f = 0.54 (hexane-ethyl acetate, 2:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title χompound in benzene at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C–H = 0.95 Å for aromatic H atoms and with Uiso(H) = 1.2Ueq (C) for aromatic H atoms.

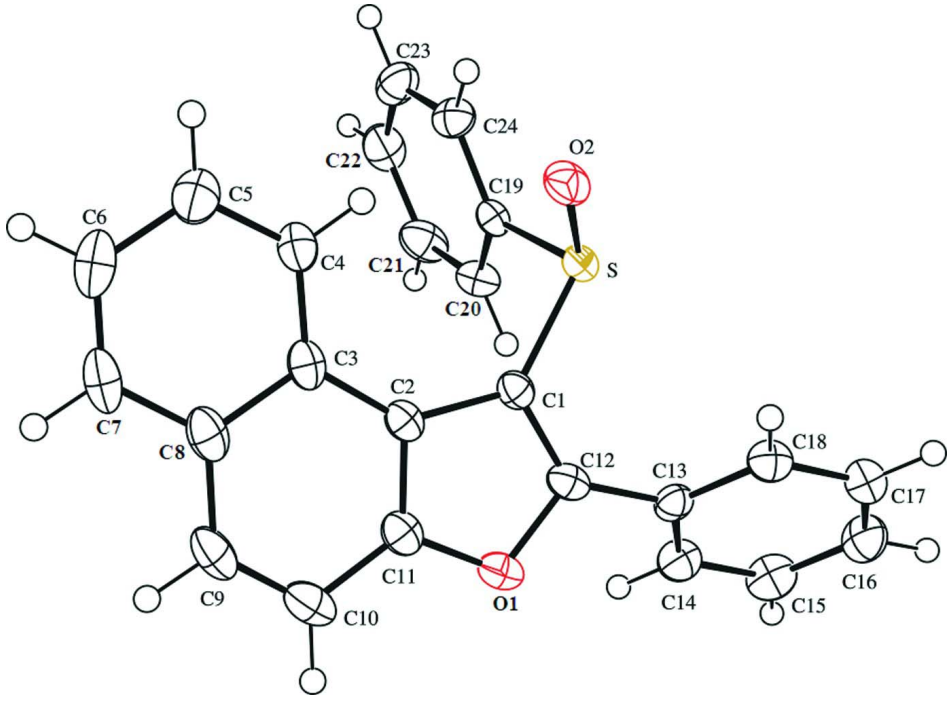

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

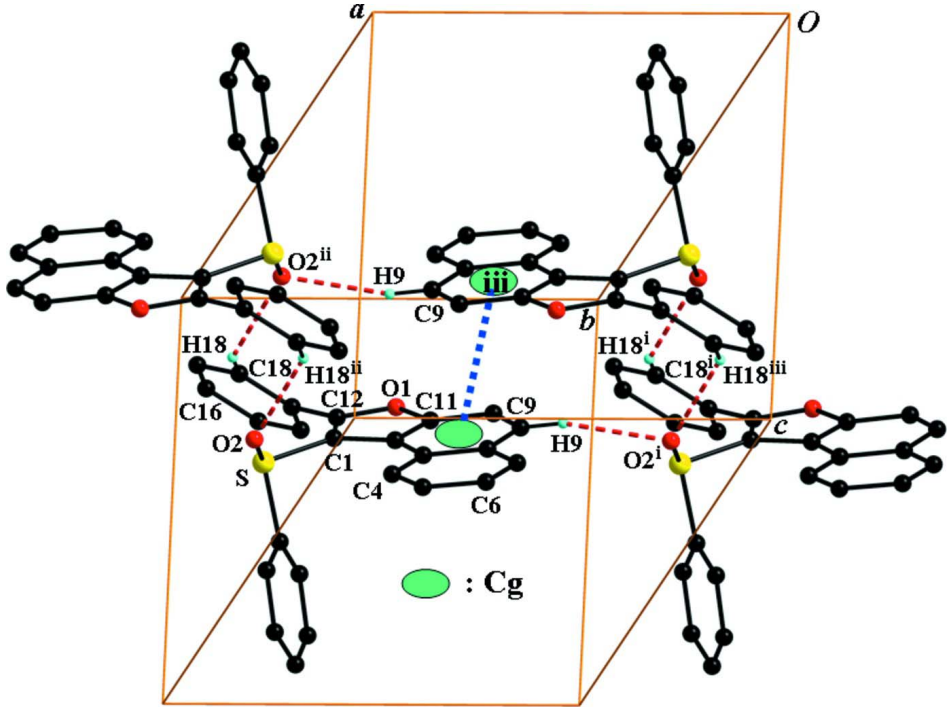

Figure 2

The π–π and C–H···O interactions (dotted lines) in the title compound. Cg denotes the ring centroids. [Symmetry code: (i) x - 1, y, z; (ii) -x + 2, -y + 1, -z + 1; (iii) -x + 1, -y + 1, -z + 1.]

2-Phenyl-1-(phenylsulfinyl)naphtho[2,1-b]furan

Crystal data

$C_{24}H_{16}O_2S$
$M_r = 368.43$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.2262$ (7) Å
$b = 10.3430$ (8) Å
$c = 10.4296$ (8) Å
$\alpha = 78.298$ (1)°
$\beta = 86.849$ (1)°
$\gamma = 67.506$ (1)°
$V = 900.15$ (12) Å^3
$Z = 2$
$F(000) = 384$
$D_x = 1.359$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3903 reflections
$\theta = 2.2$–$28.1°$
$\mu = 0.20$ mm^{-1}
$T = 173$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
6736 measured reflections
3140 independent reflections
2602 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.106$
$S = 1.06$
3140 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 0.4516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S	0.92526 (5)	0.67298 (6)	0.63521 (5)	0.02249 (16)
O1	0.55628 (15)	0.80588 (16)	0.40427 (15)	0.0287 (4)
O2	1.01571 (15)	0.51840 (16)	0.68794 (15)	0.0304 (4)
C1	0.7484 (2)	0.6976 (2)	0.5575 (2)	0.0217 (4)
C2	0.6230 (2)	0.6466 (2)	0.5980 (2)	0.0225 (5)

C3	0.5963 (2)	0.5480 (2)	0.7043 (2)	0.0247 (5)
C4	0.7034 (2)	0.4667 (2)	0.8087 (2)	0.0288 (5)
H4	0.8013	0.4767	0.8114	0.035*
C5	0.6685 (3)	0.3735 (3)	0.9063 (2)	0.0369 (6)
H5	0.7423	0.3195	0.9760	0.044*
C6	0.5244 (3)	0.3568 (3)	0.9045 (3)	0.0409 (6)
H6	0.5006	0.2928	0.9733	0.049*
C7	0.4196 (3)	0.4323 (3)	0.8042 (3)	0.0367 (6)
H7	0.3231	0.4194	0.8033	0.044*
C8	0.4506 (2)	0.5296 (2)	0.7011 (2)	0.0304 (5)
C9	0.3413 (2)	0.6054 (3)	0.5950 (3)	0.0350 (6)
H9	0.2462	0.5900	0.5946	0.042*
C10	0.3676 (2)	0.6990 (3)	0.4943 (2)	0.0341 (6)
H10	0.2936	0.7499	0.4242	0.041*
C11	0.5109 (2)	0.7163 (2)	0.4998 (2)	0.0265 (5)
C12	0.7040 (2)	0.7901 (2)	0.4412 (2)	0.0240 (5)
C13	0.7758 (2)	0.8777 (2)	0.3541 (2)	0.0245 (5)
C14	0.6902 (3)	1.0219 (2)	0.3089 (2)	0.0310 (5)
H14	0.5843	1.0632	0.3339	0.037*
C15	0.7568 (3)	1.1061 (2)	0.2284 (2)	0.0355 (6)
H15	0.6975	1.2049	0.1987	0.043*
C16	0.9113 (3)	1.0456 (3)	0.1907 (2)	0.0362 (6)
H16	0.9579	1.1031	0.1350	0.043*
C17	0.9966 (3)	0.9026 (3)	0.2340 (2)	0.0332 (5)
H17	1.1020	0.8618	0.2076	0.040*
C18	0.9314 (2)	0.8173 (2)	0.3153 (2)	0.0280 (5)
H18	0.9914	0.7185	0.3448	0.034*
C19	0.8432 (2)	0.7532 (2)	0.7740 (2)	0.0233 (5)
C20	0.7332 (2)	0.8915 (2)	0.7556 (2)	0.0296 (5)
H20	0.6946	0.9429	0.6700	0.036*
C21	0.6802 (3)	0.9539 (3)	0.8632 (3)	0.0376 (6)
H21	0.6040	1.0485	0.8519	0.045*
C22	0.7381 (3)	0.8787 (3)	0.9879 (2)	0.0369 (6)
H22	0.7005	0.9218	1.0617	0.044*
C23	0.8501 (3)	0.7414 (3)	1.0049 (2)	0.0344 (5)
H23	0.8901	0.6904	1.0901	0.041*
C24	0.9038 (2)	0.6785 (2)	0.8972 (2)	0.0286 (5)
H24	0.9817	0.5846	0.9080	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0174 (2)	0.0248 (3)	0.0242 (3)	−0.0081 (2)	−0.00033 (18)	−0.0022 (2)
O1	0.0238 (7)	0.0305 (9)	0.0299 (9)	−0.0084 (6)	−0.0053 (6)	−0.0044 (7)
O2	0.0223 (7)	0.0265 (9)	0.0369 (10)	−0.0036 (6)	−0.0003 (6)	−0.0050 (7)
C1	0.0188 (9)	0.0223 (11)	0.0238 (11)	−0.0064 (8)	0.0017 (8)	−0.0074 (9)
C2	0.0193 (9)	0.0216 (11)	0.0274 (12)	−0.0063 (8)	0.0018 (8)	−0.0095 (9)
C3	0.0232 (10)	0.0224 (11)	0.0308 (12)	−0.0091 (8)	0.0083 (8)	−0.0112 (9)

C4	0.0261 (11)	0.0277 (12)	0.0332 (13)	−0.0113 (9)	0.0050 (9)	−0.0062 (10)
C5	0.0389 (12)	0.0335 (14)	0.0367 (14)	−0.0142 (10)	0.0070 (10)	−0.0046 (11)
C6	0.0474 (14)	0.0377 (15)	0.0431 (16)	−0.0235 (12)	0.0206 (12)	−0.0106 (12)
C7	0.0319 (12)	0.0411 (15)	0.0481 (16)	−0.0229 (11)	0.0184 (11)	−0.0193 (12)
C8	0.0244 (10)	0.0321 (13)	0.0389 (14)	−0.0115 (9)	0.0105 (9)	−0.0172 (11)
C9	0.0197 (10)	0.0421 (15)	0.0493 (16)	−0.0135 (10)	0.0068 (10)	−0.0207 (12)
C10	0.0211 (10)	0.0397 (14)	0.0417 (15)	−0.0075 (10)	−0.0035 (9)	−0.0158 (11)
C11	0.0225 (10)	0.0256 (12)	0.0316 (13)	−0.0071 (9)	0.0020 (8)	−0.0104 (9)
C12	0.0207 (9)	0.0244 (11)	0.0257 (12)	−0.0053 (8)	−0.0019 (8)	−0.0085 (9)
C13	0.0281 (10)	0.0268 (12)	0.0196 (11)	−0.0105 (9)	−0.0003 (8)	−0.0064 (9)
C14	0.0325 (11)	0.0265 (13)	0.0302 (13)	−0.0064 (9)	0.0002 (9)	−0.0072 (10)
C15	0.0466 (13)	0.0213 (12)	0.0367 (14)	−0.0115 (10)	−0.0019 (10)	−0.0036 (10)
C16	0.0468 (13)	0.0354 (14)	0.0331 (14)	−0.0249 (11)	0.0010 (10)	−0.0027 (11)
C17	0.0305 (11)	0.0376 (14)	0.0325 (13)	−0.0144 (10)	0.0019 (9)	−0.0064 (11)
C18	0.0290 (11)	0.0247 (12)	0.0282 (12)	−0.0075 (9)	−0.0010 (9)	−0.0051 (9)
C19	0.0208 (10)	0.0268 (12)	0.0257 (12)	−0.0128 (9)	0.0000 (8)	−0.0045 (9)
C20	0.0261 (10)	0.0292 (13)	0.0314 (13)	−0.0080 (9)	−0.0063 (9)	−0.0045 (10)
C21	0.0298 (12)	0.0363 (14)	0.0453 (16)	−0.0060 (10)	−0.0018 (10)	−0.0173 (12)
C22	0.0374 (13)	0.0480 (16)	0.0337 (14)	−0.0202 (11)	0.0059 (10)	−0.0199 (12)
C23	0.0453 (13)	0.0397 (14)	0.0251 (13)	−0.0252 (11)	−0.0016 (10)	−0.0027 (10)
C24	0.0335 (11)	0.0244 (12)	0.0288 (13)	−0.0137 (9)	−0.0030 (9)	−0.0009 (9)

Geometric parameters (Å, º)

S—O2	1.4926 (15)	C12—C13	1.464 (3)
S—C1	1.7690 (19)	C13—C14	1.388 (3)
S—C19	1.801 (2)	C13—C18	1.402 (3)
O1—C12	1.376 (2)	C14—C15	1.377 (3)
O1—C11	1.380 (3)	C14—H14	0.9500
C1—C12	1.356 (3)	C15—C16	1.391 (3)
C1—C2	1.455 (3)	C15—H15	0.9500
C2—C11	1.373 (3)	C16—C17	1.375 (3)
C2—C3	1.426 (3)	C16—H16	0.9500
C3—C4	1.407 (3)	C17—C18	1.381 (3)
C3—C8	1.431 (3)	C17—H17	0.9500
C4—C5	1.369 (3)	C18—H18	0.9500
C4—H4	0.9500	C19—C24	1.380 (3)
C5—C6	1.406 (3)	C19—C20	1.383 (3)
C5—H5	0.9500	C20—C21	1.381 (3)
C6—C7	1.357 (4)	C20—H20	0.9500
C6—H6	0.9500	C21—C22	1.389 (4)
C7—C8	1.414 (3)	C21—H21	0.9500
C7—H7	0.9500	C22—C23	1.382 (3)
C8—C9	1.423 (3)	C22—H22	0.9500
C9—C10	1.355 (4)	C23—C24	1.386 (3)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.406 (3)	C24—H24	0.9500
C10—H10	0.9500		

O2—S—C1	110.64 (9)	C1—C12—C13	133.87 (18)
O2—S—C19	106.60 (9)	O1—C12—C13	115.97 (18)
C1—S—C19	98.59 (9)	C14—C13—C18	119.2 (2)
C12—O1—C11	106.29 (16)	C14—C13—C12	120.17 (18)
C12—C1—C2	107.88 (17)	C18—C13—C12	120.62 (19)
C12—C1—S	119.06 (15)	C15—C14—C13	120.8 (2)
C2—C1—S	132.80 (16)	C15—C14—H14	119.6
C11—C2—C3	119.15 (18)	C13—C14—H14	119.6
C11—C2—C1	104.07 (19)	C14—C15—C16	119.7 (2)
C3—C2—C1	136.75 (18)	C14—C15—H15	120.2
C4—C3—C2	124.79 (18)	C16—C15—H15	120.2
C4—C3—C8	118.6 (2)	C17—C16—C15	119.9 (2)
C2—C3—C8	116.6 (2)	C17—C16—H16	120.1
C5—C4—C3	120.9 (2)	C15—C16—H16	120.1
C5—C4—H4	119.5	C16—C17—C18	121.0 (2)
C3—C4—H4	119.5	C16—C17—H17	119.5
C4—C5—C6	120.6 (2)	C18—C17—H17	119.5
C4—C5—H5	119.7	C17—C18—C13	119.4 (2)
C6—C5—H5	119.7	C17—C18—H18	120.3
C7—C6—C5	119.8 (2)	C13—C18—H18	120.3
C7—C6—H6	120.1	C24—C19—C20	121.2 (2)
C5—C6—H6	120.1	C24—C19—S	118.22 (16)
C6—C7—C8	121.5 (2)	C20—C19—S	120.25 (17)
C6—C7—H7	119.2	C21—C20—C19	119.0 (2)
C8—C7—H7	119.2	C21—C20—H20	120.5
C7—C8—C9	121.0 (2)	C19—C20—H20	120.5
C7—C8—C3	118.5 (2)	C20—C21—C22	120.2 (2)
C9—C8—C3	120.5 (2)	C20—C21—H21	119.9
C10—C9—C8	122.5 (2)	C22—C21—H21	119.9
C10—C9—H9	118.8	C23—C22—C21	120.2 (2)
C8—C9—H9	118.8	C23—C22—H22	119.9
C9—C10—C11	116.1 (2)	C21—C22—H22	119.9
C9—C10—H10	122.0	C22—C23—C24	119.8 (2)
C11—C10—H10	122.0	C22—C23—H23	120.1
C2—C11—O1	111.62 (17)	C24—C23—H23	120.1
C2—C11—C10	125.1 (2)	C19—C24—C23	119.5 (2)
O1—C11—C10	123.3 (2)	C19—C24—H24	120.3
C1—C12—O1	110.10 (18)	C23—C24—H24	120.3

O2—S—C1—C12	−136.67 (16)	C9—C10—C11—C2	−0.1 (3)
C19—S—C1—C12	111.89 (17)	C9—C10—C11—O1	179.1 (2)
O2—S—C1—C2	50.0 (2)	C2—C1—C12—O1	1.4 (2)
C19—S—C1—C2	−61.5 (2)	S—C1—C12—O1	−173.45 (13)
C12—C1—C2—C11	−0.5 (2)	C2—C1—C12—C13	178.2 (2)
S—C1—C2—C11	173.40 (17)	S—C1—C12—C13	3.3 (3)
C12—C1—C2—C3	177.6 (2)	C11—O1—C12—C1	−1.8 (2)
S—C1—C2—C3	−8.5 (4)	C11—O1—C12—C13	−179.21 (17)

C11—C2—C3—C4	178.0 (2)	C1—C12—C13—C14	−129.7 (3)
C1—C2—C3—C4	0.1 (4)	O1—C12—C13—C14	47.0 (3)
C11—C2—C3—C8	−0.6 (3)	C1—C12—C13—C18	50.2 (3)
C1—C2—C3—C8	−178.5 (2)	O1—C12—C13—C18	−133.2 (2)
C2—C3—C4—C5	−179.5 (2)	C18—C13—C14—C15	−0.8 (3)
C8—C3—C4—C5	−0.9 (3)	C12—C13—C14—C15	179.1 (2)
C3—C4—C5—C6	0.0 (3)	C13—C14—C15—C16	0.6 (4)
C4—C5—C6—C7	0.9 (4)	C14—C15—C16—C17	−0.1 (4)
C5—C6—C7—C8	−0.8 (4)	C15—C16—C17—C18	−0.3 (4)
C6—C7—C8—C9	178.5 (2)	C16—C17—C18—C13	0.1 (3)
C6—C7—C8—C3	−0.2 (3)	C14—C13—C18—C17	0.5 (3)
C4—C3—C8—C7	1.1 (3)	C12—C13—C18—C17	−179.4 (2)
C2—C3—C8—C7	179.70 (19)	O2—S—C19—C24	16.08 (18)
C4—C3—C8—C9	−177.6 (2)	C1—S—C19—C24	130.73 (17)
C2—C3—C8—C9	1.0 (3)	O2—S—C19—C20	−170.04 (16)
C7—C8—C9—C10	−179.7 (2)	C1—S—C19—C20	−55.39 (18)
C3—C8—C9—C10	−1.1 (3)	C24—C19—C20—C21	−1.9 (3)
C8—C9—C10—C11	0.6 (3)	S—C19—C20—C21	−175.57 (17)
C3—C2—C11—O1	−179.15 (17)	C19—C20—C21—C22	0.6 (3)
C1—C2—C11—O1	−0.6 (2)	C20—C21—C22—C23	0.6 (4)
C3—C2—C11—C10	0.1 (3)	C21—C22—C23—C24	−0.5 (3)
C1—C2—C11—C10	178.7 (2)	C20—C19—C24—C23	2.0 (3)
C12—O1—C11—C2	1.5 (2)	S—C19—C24—C23	175.80 (15)
C12—O1—C11—C10	−177.8 (2)	C22—C23—C24—C19	−0.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.95	2.59	3.488 (3)	158
C18—H18···O2^{ii}	0.95	2.57	3.323 (3)	137

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$.