Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methyl-3-(phenylsulfonyl)naphtho-[1,2-*b*]furan

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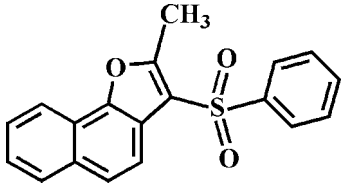
Received 24 December 2007; accepted 10 January 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 13.0.

In the title molecule, $C_{19}H_{14}O_3S$, the phenyl ring forms a dihedral angle of 69.13 (6)° with the plane of the naphthofuran fragment, being slightly tilted towards it. The crystal packing exhibits π–π interactions between the benzene rings from neighbouring molecules [centroid–centroid distance = 3.616 (4) Å] and weak C—H···O and C—H···π interactions.

Related literature

The crystal structure of 2-methyl-3-(methylsulfinyl)naphtho-[1,2-*b*]furan has been reported by Choi *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{14}O_3S$
M_r = 322.36
Orthorhombic, $Pna2_1$
a = 8.198 (4) Å
b = 18.589 (8) Å
c = 10.049 (4) Å
V = 1531.4 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 173 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
8102 measured reflections
2714 independent reflections
2538 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.05
2714 reflections
208 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1125 Friedel pairs
Flack parameter: 0.04 (7)

Table 1
Selected interatomic distances (Å).

*Cg*2 and *Cg*3 are the centroids of the C2–C5/C10/C11 benzene ring and the C5–C10 benzene ring, respectively.

*Cg*2···*Cg*3^{i}	3.616 (4)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z$.

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the O1/C12/C1/C2/C11 furan ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*A*···*Cg*1^{i}	0.98	2.64	3.483 (3)	144
C8—H8···O3^{ii}	0.95	2.51	3.406 (3)	157
C16—H16···O3^{iii}	0.95	2.51	3.430 (3)	164

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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: CV2379).

References

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supplementary materials

Acta Cryst. (2008). E**64**, o452 [**doi:10.1107/S1600536808000895**]

2-Methyl-3-(phenylsulfonyl)naphtho[1,2-*b*]furan

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Comment

As part of our ongoing study of 2-methylnaphtho[1,2-*b*]furan derivatives, the crystal structure of 2-methyl-3-(methylsulfinyl)naphtho[1,2-*b*]furan has been recently reported (Choi *et al.*, 2006). Herein we present the molecular and crystal structure of the title compound, (I).

In (I) (Fig. 1), the naphthofuran unit is essentially planar, with a mean deviation of 0.007 Å from the least-squares plane defined by the thirteen constituent atoms. The crystal packing (Fig. 2) is stabilized by aromatic π—π stacking interactions between adjacent benzene rings. The *Cg*2···*Cg*3^{i} distance is 3.616 (4) Å (Table 1; *Cg*2 and *Cg*3 are the centroids of the C2—C5/C10/C11 benzene ring and the C5—C10 benzene ring, respectively, symmetry code as in Fig. 2). The molecular packing is further stabilized by CH_2—H···π interactions between the methyl group and the furan ring of the naphthofuran unit, with a C13—H13A···*Cg*1^{i} separation of 2.64 Å (Fig. 2 and Table 2; *Cg*1 is the centroid of the O1/C12/C1/C2/C11 furan ring; symmetry code as in Fig. 2). Additionally, the weak hydrogen bonds were observed; one between the benzene H atom of naphthofuran unit and the O atom of sulfonyl group, with a C8—H8···O3^{ii}, a second between the benzene H atom of phenylsulfonyl group and adjacent O atom of sulfonyl group, with a C16—H16···O3^{iii} (Fig. 2 and Table 2; symmetry code as in Fig. 2).

Experimental

3-Chloroperbenzoic acid (77%, 560 mg, 2.5 mmol) was added in small portions to a stirred solution of 2-methyl-3-(phenylsulfanyl)naphtho[1,2-*b*] furan (348 mg, 1.2 mmol) in dichloromethane (40 ml) at 273 K. After being stirred at room temperature for 4 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 (hexane-ethyl acetate, 2:1 *v*/*v*) to afford the title compound as a pale yellow solid [yield 84%, m.p. 412–413 K; R_f = 0.64 (hexane-ethyl acetate, 2:1 *v*/*v*)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a dilute solution of the title compound in acetone at room temperature.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and 0.98 Å for methyl H atoms, respectively, and with U_{iso}(H) = 1.2Ueq(C) for all H atoms.

Figures

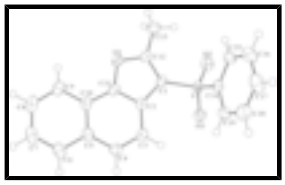


Fig. 1. The molecular structure of the title compound, showing displacement ellipsoides drawn at the 50% probability level.

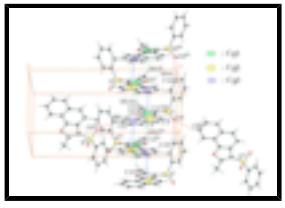


Fig. 2. π—π, C—H···π and C—H···O interactions (dotted lines) in the title compound [symmetry codes: (i) $x - 1/2, -y + 1/2, z$; (ii) $-x + 3/2, y + 1/2, z - 1/2$; (iii) $x - 1, y, z$; (iv) $x + 1/2, -y + 1/2, z$; (v) $x + 1, y, z$; (vi) $-x + 3/2, y - 1/2, z + 1/2$.]

2-Methyl-3-(phenylsulfonyl)naphtho[1,2-*b*]furan

Crystal data

$C_{19}H_{14}O_3S$	$F_{000} = 672$
$M_r = 322.36$	$D_x = 1.398$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 5173 reflections
$a = 8.198$ (4) Å	$\theta = 2.2$–$28.1°$
$b = 18.589$ (8) Å	$\mu = 0.22$ mm^{-1}
$c = 10.049$ (4) Å	$T = 173$ (2) K
$V = 1531.4$ (11) Å^3	Block, yellow
$Z = 4$	0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer	2714 independent reflections
Radiation source: fine-focus sealed tube	2538 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 26.0°$
$T = 173(2)$ K	$\theta_{min} = 2.2°$
φ and ω scans	$h = -7 \rightarrow 10$
Absorption correction: none	$k = -22 \rightarrow 22$
8102 measured reflections	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.1234P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
2714 reflections	$\Delta\rho_{min} = -0.21$ e Å^{-3}
208 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1125 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (7)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
S1	0.44268 (6)	0.07870 (2)	0.60161 (6)	0.02617 (13)
O1	0.51082 (18)	0.27348 (7)	0.46110 (15)	0.0291 (3)
O2	0.3904 (2)	0.09804 (9)	0.73361 (15)	0.0373 (4)
O3	0.58124 (17)	0.03221 (8)	0.58544 (17)	0.0369 (4)
C1	0.4858 (2)	0.15710 (10)	0.5141 (2)	0.0253 (4)
C2	0.5822 (2)	0.16115 (11)	0.3939 (2)	0.0260 (4)
C3	0.6620 (3)	0.11149 (11)	0.3089 (2)	0.0293 (4)
H3	0.6565	0.0612	0.3254	0.035*
C4	0.7466 (3)	0.13772 (11)	0.2031 (2)	0.0314 (5)
H4	0.8012	0.1048	0.1460	0.038*
C5	0.7564 (3)	0.21297 (11)	0.1745 (2)	0.0296 (4)
C6	0.8432 (3)	0.23949 (14)	0.0629 (2)	0.0379 (5)
H6	0.8960	0.2067	0.0045	0.045*
C7	0.8521 (3)	0.31235 (14)	0.0381 (3)	0.0448 (6)
H7	0.9111	0.3293	−0.0370	0.054*
C8	0.7749 (3)	0.36149 (12)	0.1225 (3)	0.0421 (6)
H8	0.7828	0.4115	0.1042	0.051*
C9	0.6884 (3)	0.33880 (11)	0.2309 (2)	0.0342 (5)
H9	0.6355	0.3726	0.2872	0.041*
C10	0.6786 (3)	0.26389 (11)	0.2582 (2)	0.0276 (4)
C11	0.5932 (2)	0.23396 (10)	0.3665 (2)	0.0270 (4)
C12	0.4468 (2)	0.22595 (11)	0.5500 (2)	0.0282 (4)
C13	0.3579 (3)	0.25867 (13)	0.6634 (2)	0.0375 (5)

H13A	0.2672	0.2878	0.6297	0.045*
H13B	0.4325	0.2893	0.7143	0.045*
H13C	0.3154	0.2206	0.7211	0.045*
C14	0.2753 (2)	0.03853 (10)	0.51984 (19)	0.0249 (4)
C15	0.1181 (3)	0.05753 (12)	0.5593 (2)	0.0312 (5)
H15	0.1021	0.0928	0.6265	0.037*
C16	−0.0141 (3)	0.02474 (14)	0.5000 (2)	0.0404 (5)
H16	−0.1217	0.0368	0.5272	0.048*
C17	0.0105 (3)	−0.02571 (14)	0.4009 (3)	0.0469 (6)
H17	−0.0805	−0.0486	0.3604	0.056*
C18	0.1664 (3)	−0.04291 (13)	0.3605 (3)	0.0447 (6)
H18	0.1818	−0.0767	0.2908	0.054*
C19	0.3008 (3)	−0.01150 (11)	0.4204 (2)	0.0327 (5)
H19	0.4082	−0.0241	0.3937	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0274 (2)	0.0262 (2)	0.0250 (2)	−0.00075 (19)	−0.0024 (2)	0.0041 (2)
O1	0.0359 (8)	0.0213 (6)	0.0301 (8)	0.0009 (6)	0.0004 (6)	−0.0021 (6)
O2	0.0459 (9)	0.0419 (8)	0.0241 (8)	−0.0059 (8)	−0.0011 (7)	0.0014 (7)
O3	0.0300 (8)	0.0329 (7)	0.0477 (11)	0.0043 (6)	−0.0026 (7)	0.0125 (8)
C1	0.0254 (9)	0.0224 (9)	0.0282 (11)	−0.0009 (8)	−0.0043 (8)	0.0008 (8)
C2	0.0254 (10)	0.0265 (10)	0.0261 (10)	−0.0022 (8)	−0.0030 (8)	0.0021 (8)
C3	0.0337 (11)	0.0226 (9)	0.0317 (11)	−0.0016 (9)	−0.0024 (9)	−0.0003 (8)
C4	0.0356 (12)	0.0298 (10)	0.0290 (11)	0.0004 (9)	0.0012 (9)	−0.0030 (9)
C5	0.0321 (11)	0.0337 (11)	0.0229 (10)	−0.0027 (9)	−0.0040 (8)	0.0025 (9)
C6	0.0411 (13)	0.0454 (14)	0.0271 (12)	−0.0046 (11)	−0.0001 (9)	0.0043 (9)
C7	0.0469 (14)	0.0538 (15)	0.0337 (13)	−0.0117 (12)	−0.0025 (11)	0.0163 (11)
C8	0.0503 (14)	0.0320 (11)	0.0441 (15)	−0.0122 (10)	−0.0105 (11)	0.0122 (11)
C9	0.0381 (12)	0.0278 (10)	0.0366 (13)	−0.0050 (9)	−0.0084 (9)	0.0021 (9)
C10	0.0295 (11)	0.0272 (10)	0.0260 (10)	−0.0050 (8)	−0.0080 (8)	0.0046 (8)
C11	0.0287 (10)	0.0237 (10)	0.0286 (11)	−0.0013 (8)	−0.0042 (8)	−0.0021 (9)
C12	0.0280 (10)	0.0273 (10)	0.0294 (10)	−0.0001 (9)	−0.0032 (8)	−0.0012 (8)
C13	0.0426 (14)	0.0349 (12)	0.0349 (12)	0.0055 (10)	0.0026 (10)	−0.0042 (10)
C14	0.0282 (10)	0.0235 (9)	0.0229 (11)	−0.0014 (8)	0.0004 (8)	0.0052 (8)
C15	0.0327 (11)	0.0338 (10)	0.0271 (11)	0.0014 (10)	0.0036 (8)	0.0036 (8)
C16	0.0297 (11)	0.0534 (14)	0.0380 (14)	−0.0038 (11)	0.0007 (10)	0.0068 (11)
C17	0.0412 (14)	0.0608 (16)	0.0386 (14)	−0.0207 (13)	−0.0045 (11)	0.0009 (12)
C18	0.0576 (15)	0.0430 (13)	0.0335 (13)	−0.0117 (12)	0.0037 (11)	−0.0098 (11)
C19	0.0354 (12)	0.0311 (11)	0.0316 (11)	−0.0021 (9)	0.0058 (9)	−0.0032 (9)

Geometric parameters (Å, °)

S1—O3	1.437 (2)	C8—C9	1.367 (3)
S1—O2	1.440 (2)	C8—H8	0.9500
S1—C1	1.738 (2)	C9—C10	1.422 (3)
S1—C14	1.765 (2)	C9—H9	0.9500
O1—C12	1.361 (3)	C10—C11	1.409 (3)

O1—C11	1.378 (2)	C12—C13	1.483 (3)
C1—C12	1.368 (3)	C13—H13A	0.9800
C1—C2	1.446 (3)	C13—H13B	0.9800
C2—C11	1.384 (3)	C13—H13C	0.9800
C2—C3	1.418 (3)	C14—C19	1.381 (3)
C3—C4	1.360 (3)	C14—C15	1.394 (3)
C3—H3	0.9500	C15—C16	1.378 (3)
C4—C5	1.430 (3)	C15—H15	0.9500
C4—H4	0.9500	C16—C17	1.383 (4)
C5—C6	1.417 (3)	C16—H16	0.9500
C5—C10	1.417 (3)	C17—C18	1.379 (4)
C6—C7	1.379 (4)	C17—H17	0.9500
C6—H6	0.9500	C18—C19	1.384 (3)
C7—C8	1.398 (4)	C18—H18	0.9500
C7—H7	0.9500	C19—H19	0.9500
Cg2···Cg3^{i}	3.616 (4)		
O3—S1—O2	119.3 (1)	C11—C10—C5	114.7 (2)
O3—S1—C1	106.6 (1)	C11—C10—C9	124.3 (2)
O2—S1—C1	108.5 (1)	C5—C10—C9	121.0 (2)
O3—S1—C14	107.9 (1)	O1—C11—C2	110.6 (2)
O2—S1—C14	107.7 (1)	O1—C11—C10	124.5 (2)
C1—S1—C14	106.1 (1)	C2—C11—C10	124.9 (2)
C12—O1—C11	107.2 (2)	O1—C12—C1	110.2 (2)
C12—C1—C2	107.4 (2)	O1—C12—C13	115.3 (2)
C12—C1—S1	127.1 (2)	C1—C12—C13	134.5 (2)
C2—C1—S1	125.3 (2)	C12—C13—H13A	109.5
C11—C2—C3	119.1 (2)	C12—C13—H13B	109.5
C11—C2—C1	104.6 (2)	H13A—C13—H13B	109.5
C3—C2—C1	136.2 (2)	C12—C13—H13C	109.5
C4—C3—C2	118.2 (2)	H13A—C13—H13C	109.5
C4—C3—H3	120.9	H13B—C13—H13C	109.5
C2—C3—H3	120.9	C19—C14—C15	121.1 (2)
C3—C4—C5	122.4 (2)	C19—C14—S1	120.3 (2)
C3—C4—H4	118.8	C15—C14—S1	118.6 (2)
C5—C4—H4	118.8	C16—C15—C14	119.4 (2)
C6—C5—C10	117.6 (2)	C16—C15—H15	120.3
C6—C5—C4	121.8 (2)	C14—C15—H15	120.3
C10—C5—C4	120.6 (2)	C15—C16—C17	119.8 (2)
C7—C6—C5	120.8 (2)	C15—C16—H16	120.1
C7—C6—H6	119.6	C17—C16—H16	120.1
C5—C6—H6	119.6	C18—C17—C16	120.3 (2)
C6—C7—C8	120.5 (2)	C18—C17—H17	119.9
C6—C7—H7	119.7	C16—C17—H17	119.9
C8—C7—H7	119.7	C17—C18—C19	120.8 (2)
C9—C8—C7	121.1 (2)	C17—C18—H18	119.6
C9—C8—H8	119.4	C19—C18—H18	119.6
C7—C8—H8	119.4	C14—C19—C18	118.5 (2)
C8—C9—C10	119.0 (2)	C14—C19—H19	120.7

C8—C9—H9	120.5	C18—C19—H19	120.7
C10—C9—H9	120.5		
O3—S1—C1—C12	−142.38 (19)	C3—C2—C11—O1	−178.86 (17)
O2—S1—C1—C12	−12.7 (2)	C1—C2—C11—O1	0.0 (2)
C14—S1—C1—C12	102.8 (2)	C3—C2—C11—C10	0.2 (3)
O3—S1—C1—C2	32.34 (19)	C1—C2—C11—C10	179.12 (19)
O2—S1—C1—C2	162.06 (16)	C5—C10—C11—O1	179.07 (18)
C14—S1—C1—C2	−82.51 (18)	C9—C10—C11—O1	−1.2 (3)
C12—C1—C2—C11	−0.1 (2)	C5—C10—C11—C2	0.1 (3)
S1—C1—C2—C11	−175.74 (15)	C9—C10—C11—C2	179.8 (2)
C12—C1—C2—C3	178.5 (2)	C11—O1—C12—C1	−0.2 (2)
S1—C1—C2—C3	2.9 (3)	C11—O1—C12—C13	177.78 (17)
C11—C2—C3—C4	0.0 (3)	C2—C1—C12—O1	0.2 (2)
C1—C2—C3—C4	−178.5 (2)	S1—C1—C12—O1	175.70 (14)
C2—C3—C4—C5	−0.5 (3)	C2—C1—C12—C13	−177.2 (2)
C3—C4—C5—C6	−179.2 (2)	S1—C1—C12—C13	−1.7 (4)
C3—C4—C5—C10	0.9 (3)	O3—S1—C14—C19	−22.04 (19)
C10—C5—C6—C7	0.5 (3)	O2—S1—C14—C19	−152.05 (17)
C4—C5—C6—C7	−179.5 (2)	C1—S1—C14—C19	91.94 (18)
C5—C6—C7—C8	−0.2 (4)	O3—S1—C14—C15	156.92 (16)
C6—C7—C8—C9	−0.4 (4)	O2—S1—C14—C15	26.90 (19)
C7—C8—C9—C10	0.6 (3)	C1—S1—C14—C15	−89.10 (18)
C6—C5—C10—C11	179.43 (18)	C19—C14—C15—C16	1.4 (3)
C4—C5—C10—C11	−0.6 (3)	S1—C14—C15—C16	−177.59 (17)
C6—C5—C10—C9	−0.3 (3)	C14—C15—C16—C17	−1.0 (3)
C4—C5—C10—C9	179.69 (19)	C15—C16—C17—C18	−0.5 (4)
C8—C9—C10—C11	−179.9 (2)	C16—C17—C18—C19	1.6 (4)
C8—C9—C10—C5	−0.3 (3)	C15—C14—C19—C18	−0.2 (3)
C12—O1—C11—C2	0.1 (2)	S1—C14—C19—C18	178.69 (18)
C12—O1—C11—C10	−178.99 (19)	C17—C18—C19—C14	−1.2 (4)

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···Cg1^{i}	0.98	2.64	3.483 (3)	144
C8—H8···O3^{ii}	0.95	2.51	3.406 (3)	157
C16—H16···O3^{iii}	0.95	2.51	3.430 (3)	164

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*; (ii) −*x*+3/2, *y*+1/2, *z*−1/2; (iii) *x*−1, *y*, *z*.

Fig. 1

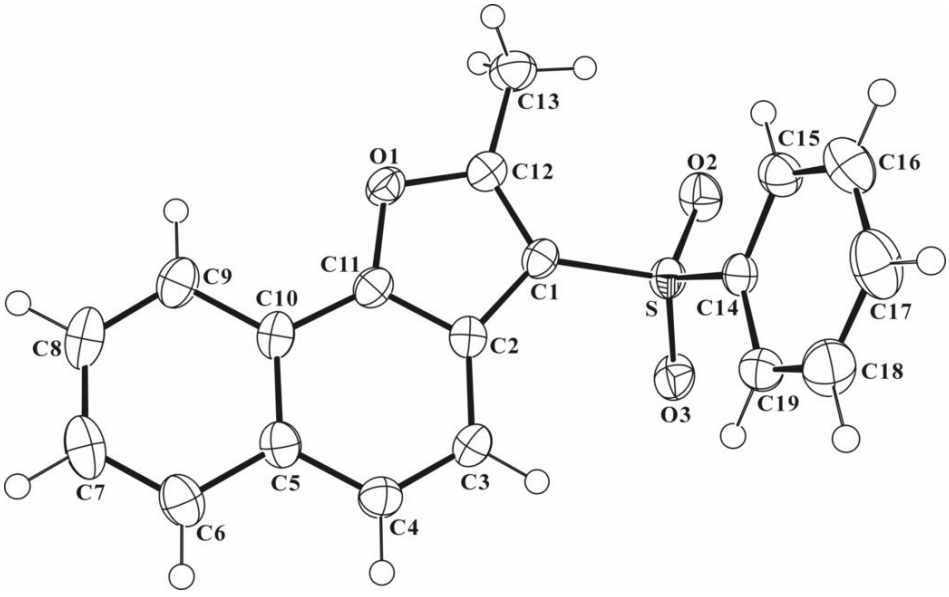
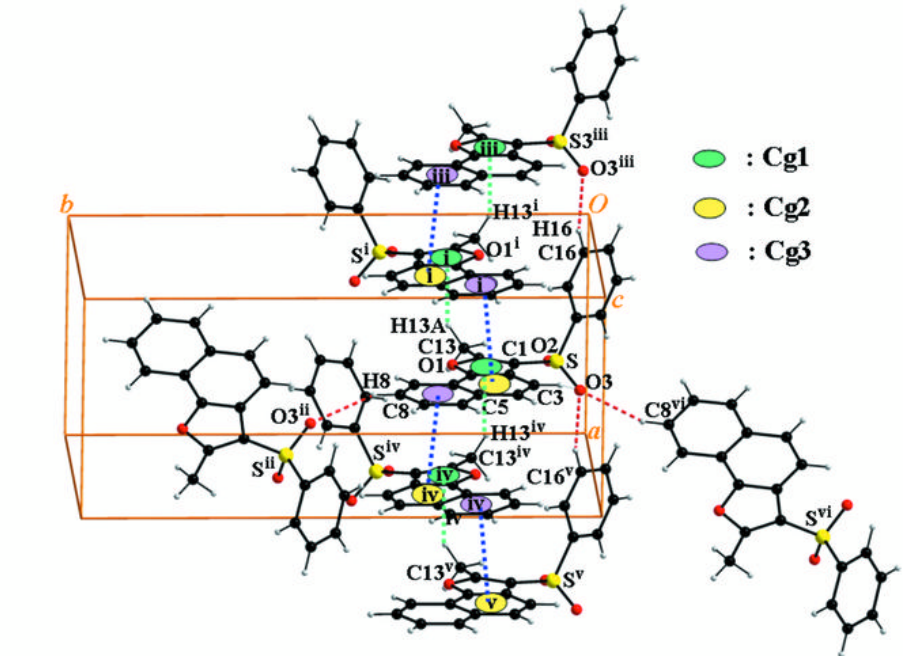

C13
O1
C12
O2
C15
C16
C9
C11
C1
S
C14
C17
C10
C8
C2
O3
C19
C18
C7
C5
C3
C6
C4

Fig. 2


: Cg1
: Cg2
: Cg3
b
O
c
a
S3iii
O3iii
H13i
H16
C16
Si
O1i
H13A
C13
C1
O2
S
O1
H8
C8
C5
C3
O3
O3ii
C8vi
Svi
Siv
Sii
H13iv
C13iv
C16v
C13v
Sv