

2,4,5,6-Tetramethyl-3-phenylsulfinyl-1-benzofuran

Pil Ja Seo,^a Hong Dae Choi,^a Byung Wha Son^b and Uk Lee^{b*}

^aDepartment of Chemistry, Donggeui University, San 24 Kaya-dong Busanjin-gu, Busan 614-714, Republic of Korea, and ^bDepartment of Chemistry, Pukyong National University, 599-1 Daeyeon 3-dong, Nam-gu, Busan 608-737, Republic of Korea

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

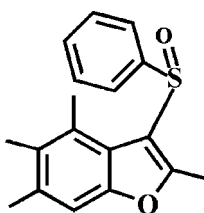
Received 3 May 2011; accepted 19 May 2011

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.058; wR factor = 0.155; data-to-parameter ratio = 18.1.

In the title compound, $\text{C}_{18}\text{H}_{18}\text{O}_2\text{S}$, the phenyl ring makes a dihedral angle of $87.47(6)^\circ$ with the mean plane of the benzofuran fragment. In the crystal, molecules are linked by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the biological activity of benzofuran compounds, see: Aslam *et al.* (2009); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For structural studies of related 2-methyl-3-phenylsulfinyl-1-benzofuran derivatives, see: Choi *et al.* (2008a,b,c).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{18}\text{O}_2\text{S}$
 $M_r = 298.38$
 Monoclinic, $P2_1/c$

$a = 14.2611(5)$ Å
 $b = 6.0661(2)$ Å
 $c = 17.2436(7)$ Å

$\beta = 99.740(2)^\circ$
 $V = 1470.23(9)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.22$ mm⁻¹
 $T = 173$ K
 $0.29 \times 0.20 \times 0.14$ mm

Data collection

Bruker SMART APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.622$, $T_{\max} = 0.746$

25036 measured reflections
 3397 independent reflections
 2888 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.155$
 $S = 1.04$
 3397 reflections

188 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 1.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.56$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the C2–C7 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O2}^{\text{i}}$	0.95	2.35	3.286 (3)	169
$\text{C10}-\text{H10A}\cdots\text{O2}^{\text{ii}}$	0.98	2.56	3.517 (3)	167
$\text{C12}-\text{H12C}\cdots\text{Cg}^{\text{iii}}$	0.98	2.66	3.482 (3)	142

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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: JJ2090).

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supplementary materials

Acta Cryst. (2011). E67, o1512 [doi:10.1107/S1600536811018952]

2,4,5,6-Tetramethyl-3-phenylsulfinyl-1-benzofuran

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Comment

Recently, a series of compounds containing the benzofuran ring system have been shown to exhibit significant pharmacological properties such as antibacterial, antifungal, antitumor, antiviral, and antimicrobial activities (Aslam *et al.*, 2009, Galal *et al.*, 2009, Khan *et al.*, 2005). These types of compounds occur in a wide range of natural products (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our study of the substituent effect on the solid state structures of 2-methyl-3-phenylsulfinyl-1-benzofuran analogues (Choi *et al.*, 2008*a,b,c*), we report herein the crystal structure of the title compound, C₁₈H₁₈O₂S.

In the title compound (Fig. 1), the benzofuran unit is essentially planar, with a mean deviation of 0.017 (1) Å from the least-squares plane defined by the nine constituent atoms. The phenyl ring makes a dihedral angle of 87.47 (6)° with the mean plane of the benzofuran fragment. Crystal packing is stabilized by weak intermolecular C—H⋯O hydrogen bonds (Table 1 & Fig. 2) and weak C—H⋯Cg π -ring interactions (Table 1 & Fig 3; Cg is the centroid of the C2–C7 benzene ring).

Experimental

77% 3-chloroperoxybenzoic acid (247 mg, 1.1 mmol) was added in small portions to a stirred solution of 2,4,5,6-tetramethyl-3-phenylsulfonyl-1-benzofuran (310 mg, 1.1 mmol) in dichloromethane (40 mL) at 273 K. After being stirred at room temperature for 4h, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated at reduced pressure. The residue was purified by column chromatography (hexane-ethyl acetate, 2:1 v/v) to afford the title compound as a colorless solid [yield 74%, m.p. 438–439 K; R_f = 0.51 (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 compound in ethyl acetate at room temperature.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aryl and 0.99 Å for methyl H atoms. $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl and $1.5U_{eq}(C)$ for methyl H atoms.

Figures

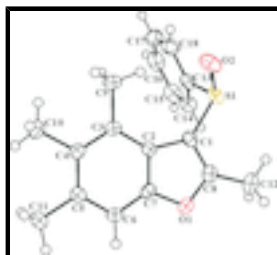


Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

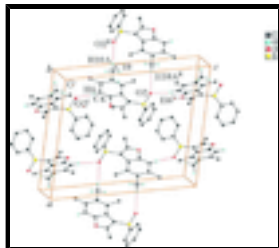


Fig. 2. A view of the weak C—H...O interactions (dotted lines) in the crystal packing of the title compound. [Symmetry codes: (i) $x, -y + 1/2, z - 1/2$; (ii) $-x, -y + 1, -z + 1$; (iv) $x, -y + 1/2, z + 1/2$.]

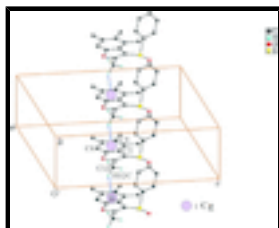


Fig. 3. A view of the weak C—H...Cg π -ring intermolecular interactions (dotted lines) in the crystal packing of the title compound. [Symmetry codes: (iii) $x, y - 1, z$.]

2,4,5,6-Tetramethyl-3-phenylsulfinyl-1-benzofuran

Crystal data

$C_{18}H_{18}O_2S$

$M_r = 298.38$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 14.2611$ (5) Å

$b = 6.0661$ (2) Å

$c = 17.2436$ (7) Å

$\beta = 99.740$ (2)°

$V = 1470.23$ (9) Å³

$Z = 4$

$F(000) = 632$

$D_x = 1.348$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7044 reflections

$\theta = 2.4$ – 27.5 °

$\mu = 0.22$ mm⁻¹

$T = 173$ K

Block, colourless

$0.29 \times 0.20 \times 0.14$ mm

Data collection

Bruker SMART APEXII CCD diffractometer

Radiation source: rotating anode graphite multilayer

Detector resolution: 10.0 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2009)

$T_{\min} = 0.622$, $T_{\max} = 0.746$

25036 measured reflections

3397 independent reflections

2888 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\max} = 27.6$ °, $\theta_{\min} = 1.5$ °

$h = -18 \rightarrow 17$

$k = -7 \rightarrow 7$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$$R[F^2 > 2\sigma(F^2)] = 0.058$$

$$wR(F^2) = 0.155$$

$$S = 1.04$$

3397 reflections

188 parameters

0 restraints

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 1.9351P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 1.20 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.28526 (4)	0.15501 (10)	0.58076 (4)	0.03155 (19)
O1	0.27241 (11)	0.1859 (3)	0.35463 (10)	0.0271 (4)
O2	0.19888 (14)	0.1527 (3)	0.61794 (11)	0.0420 (5)
C1	0.25752 (15)	0.2287 (4)	0.48136 (13)	0.0251 (5)
C2	0.20419 (15)	0.4077 (3)	0.43714 (12)	0.0219 (4)
C3	0.14688 (15)	0.5842 (4)	0.45266 (12)	0.0225 (4)
C4	0.10995 (15)	0.7234 (4)	0.39007 (13)	0.0233 (4)
C5	0.12764 (15)	0.6842 (4)	0.31306 (13)	0.0239 (4)
C6	0.18162 (15)	0.5044 (4)	0.29734 (13)	0.0245 (5)
H6	0.1930	0.4739	0.2457	0.029*
C7	0.21775 (15)	0.3723 (3)	0.36019 (13)	0.0230 (4)
C8	0.29453 (16)	0.1033 (4)	0.42877 (14)	0.0275 (5)
C9	0.12387 (18)	0.6209 (4)	0.53373 (14)	0.0302 (5)
H9A	0.1379	0.4866	0.5651	0.045*
H9B	0.0563	0.6572	0.5297	0.045*
H9C	0.1624	0.7428	0.5592	0.045*
C10	0.04905 (17)	0.9172 (4)	0.40466 (15)	0.0317 (5)
H10A	-0.0180	0.8728	0.3956	0.048*
H10B	0.0581	1.0374	0.3687	0.048*
H10C	0.0675	0.9672	0.4591	0.048*
C11	0.08671 (18)	0.8332 (4)	0.24575 (14)	0.0320 (5)
H11A	0.1034	0.7760	0.1967	0.048*
H11B	0.1128	0.9819	0.2555	0.048*
H11C	0.0173	0.8384	0.2413	0.048*

supplementary materials

C12	0.35458 (14)	-0.0982 (3)	0.43559 (11)	0.0378 (6)
H12A	0.3646	-0.1510	0.4901	0.057*
H12B	0.4162	-0.0636	0.4205	0.057*
H12C	0.3226	-0.2129	0.4007	0.057*
C13	0.35299 (11)	0.3951 (3)	0.61796 (9)	0.0275 (5)
C14	0.43833 (10)	0.4325 (2)	0.59220 (10)	0.0327 (5)
H14	0.4567	0.3431	0.5521	0.039*
C15	0.49648 (19)	0.6014 (5)	0.62557 (17)	0.0423 (7)
H15	0.5556	0.6278	0.6088	0.051*
C16	0.4686 (2)	0.7322 (5)	0.68343 (17)	0.0456 (7)
H16	0.5083	0.8495	0.7059	0.055*
C17	0.3838 (2)	0.6929 (5)	0.70828 (17)	0.0452 (7)
H17	0.3647	0.7840	0.7476	0.054*
C18	0.32583 (18)	0.5214 (5)	0.67638 (15)	0.0370 (6)
H18	0.2679	0.4914	0.6947	0.044*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0337 (3)	0.0300 (3)	0.0297 (3)	-0.0058 (2)	0.0016 (2)	0.0081 (2)
O1	0.0258 (8)	0.0250 (8)	0.0309 (9)	0.0009 (6)	0.0059 (7)	-0.0045 (6)
O2	0.0397 (10)	0.0523 (12)	0.0347 (10)	-0.0122 (9)	0.0086 (8)	0.0101 (8)
C1	0.0245 (11)	0.0244 (10)	0.0256 (11)	-0.0046 (8)	0.0017 (8)	0.0033 (8)
C2	0.0219 (10)	0.0221 (10)	0.0213 (10)	-0.0044 (8)	0.0024 (8)	0.0005 (8)
C3	0.0207 (10)	0.0256 (10)	0.0217 (10)	-0.0055 (8)	0.0052 (8)	-0.0042 (8)
C4	0.0194 (10)	0.0244 (10)	0.0269 (11)	-0.0021 (8)	0.0062 (8)	-0.0016 (8)
C5	0.0204 (10)	0.0266 (10)	0.0238 (11)	-0.0028 (8)	0.0017 (8)	0.0010 (8)
C6	0.0252 (11)	0.0294 (11)	0.0194 (10)	-0.0028 (8)	0.0049 (8)	-0.0032 (8)
C7	0.0200 (10)	0.0226 (10)	0.0264 (11)	-0.0017 (8)	0.0037 (8)	-0.0051 (8)
C8	0.0225 (11)	0.0236 (10)	0.0355 (12)	-0.0035 (8)	0.0025 (9)	0.0002 (9)
C9	0.0330 (12)	0.0349 (12)	0.0245 (11)	-0.0019 (9)	0.0102 (9)	-0.0039 (9)
C10	0.0283 (12)	0.0305 (12)	0.0373 (13)	0.0050 (9)	0.0085 (10)	-0.0017 (10)
C11	0.0336 (13)	0.0339 (12)	0.0274 (12)	0.0009 (10)	0.0017 (10)	0.0054 (10)
C12	0.0329 (13)	0.0263 (12)	0.0535 (16)	0.0031 (10)	0.0051 (12)	0.0010 (11)
C13	0.0255 (11)	0.0303 (11)	0.0249 (11)	-0.0017 (9)	-0.0013 (9)	0.0069 (9)
C14	0.0273 (12)	0.0362 (13)	0.0342 (13)	-0.0013 (10)	0.0041 (10)	0.0017 (10)
C15	0.0318 (14)	0.0471 (16)	0.0460 (16)	-0.0116 (11)	0.0011 (12)	0.0062 (12)
C16	0.0509 (17)	0.0362 (14)	0.0429 (16)	-0.0085 (12)	-0.0119 (13)	0.0010 (12)
C17	0.0554 (18)	0.0440 (15)	0.0322 (14)	0.0096 (13)	-0.0046 (12)	-0.0070 (12)
C18	0.0327 (13)	0.0504 (15)	0.0271 (12)	0.0049 (11)	0.0024 (10)	0.0034 (11)

Geometric parameters (\AA , $^\circ$)

S1—O2	1.482 (2)	C10—H10A	0.9800
S1—C1	1.751 (2)	C10—H10B	0.9800
S1—C13	1.8046 (18)	C10—H10C	0.9800
O1—C8	1.359 (3)	C11—H11A	0.9800
O1—C7	1.386 (3)	C11—H11B	0.9800
C1—C8	1.357 (3)	C11—H11C	0.9800

C1—C2	1.463 (3)	C12—H12A	0.9800
C2—C7	1.390 (3)	C12—H12B	0.9800
C2—C3	1.400 (3)	C12—H12C	0.9800
C3—C4	1.401 (3)	C13—C18	1.372 (3)
C3—C9	1.506 (3)	C13—C14	1.3830
C4—C5	1.413 (3)	C14—C15	1.381 (3)
C4—C10	1.508 (3)	C14—H14	0.9500
C5—C6	1.388 (3)	C15—C16	1.385 (4)
C5—C11	1.508 (3)	C15—H15	0.9500
C6—C7	1.376 (3)	C16—C17	1.370 (5)
C6—H6	0.9500	C16—H16	0.9500
C8—C12	1.486 (3)	C17—C18	1.384 (4)
C9—H9A	0.9800	C17—H17	0.9500
C9—H9B	0.9800	C18—H18	0.9500
C9—H9C	0.9800		
O2—S1—C1	111.05 (11)	C4—C10—H10B	109.5
O2—S1—C13	106.72 (10)	H10A—C10—H10B	109.5
C1—S1—C13	99.25 (9)	C4—C10—H10C	109.5
C8—O1—C7	106.22 (17)	H10A—C10—H10C	109.5
C8—C1—C2	107.1 (2)	H10B—C10—H10C	109.5
C8—C1—S1	117.52 (18)	C5—C11—H11A	109.5
C2—C1—S1	135.31 (18)	C5—C11—H11B	109.5
C7—C2—C3	118.7 (2)	H11A—C11—H11B	109.5
C7—C2—C1	103.83 (19)	C5—C11—H11C	109.5
C3—C2—C1	137.4 (2)	H11A—C11—H11C	109.5
C2—C3—C4	117.98 (19)	H11B—C11—H11C	109.5
C2—C3—C9	121.1 (2)	C8—C12—H12A	109.5
C4—C3—C9	120.9 (2)	C8—C12—H12B	109.5
C3—C4—C5	121.3 (2)	H12A—C12—H12B	109.5
C3—C4—C10	119.6 (2)	C8—C12—H12C	109.5
C5—C4—C10	119.2 (2)	H12A—C12—H12C	109.5
C6—C5—C4	120.6 (2)	H12B—C12—H12C	109.5
C6—C5—C11	118.4 (2)	C18—C13—C14	121.16 (15)
C4—C5—C11	121.0 (2)	C18—C13—S1	120.72 (16)
C7—C6—C5	116.7 (2)	C14—C13—S1	117.72 (6)
C7—C6—H6	121.6	C15—C14—C13	119.12 (16)
C5—C6—H6	121.6	C15—C14—H14	120.4
C6—C7—O1	124.1 (2)	C13—C14—H14	120.4
C6—C7—C2	124.6 (2)	C14—C15—C16	120.0 (2)
O1—C7—C2	111.25 (19)	C14—C15—H15	120.0
C1—C8—O1	111.6 (2)	C16—C15—H15	120.0
C1—C8—C12	133.8 (2)	C17—C16—C15	120.1 (3)
O1—C8—C12	114.61 (19)	C17—C16—H16	119.9
C3—C9—H9A	109.5	C15—C16—H16	119.9
C3—C9—H9B	109.5	C16—C17—C18	120.4 (3)
H9A—C9—H9B	109.5	C16—C17—H17	119.8
C3—C9—H9C	109.5	C18—C17—H17	119.8
H9A—C9—H9C	109.5	C13—C18—C17	119.2 (2)
H9B—C9—H9C	109.5	C13—C18—H18	120.4

supplementary materials

C4—C10—H10A	109.5	C17—C18—H18	120.4
O2—S1—C1—C8	-132.93 (19)	C8—O1—C7—C6	179.6 (2)
C13—S1—C1—C8	115.04 (18)	C8—O1—C7—C2	-0.6 (2)
O2—S1—C1—C2	50.2 (3)	C3—C2—C7—C6	2.6 (3)
C13—S1—C1—C2	-61.8 (2)	C1—C2—C7—C6	-178.8 (2)
C8—C1—C2—C7	-1.7 (2)	C3—C2—C7—O1	-177.22 (18)
S1—C1—C2—C7	175.39 (19)	C1—C2—C7—O1	1.4 (2)
C8—C1—C2—C3	176.5 (2)	C2—C1—C8—O1	1.4 (2)
S1—C1—C2—C3	-6.4 (4)	S1—C1—C8—O1	-176.26 (14)
C7—C2—C3—C4	-3.2 (3)	C2—C1—C8—C12	179.9 (2)
C1—C2—C3—C4	178.8 (2)	S1—C1—C8—C12	2.2 (4)
C7—C2—C3—C9	175.6 (2)	C7—O1—C8—C1	-0.6 (2)
C1—C2—C3—C9	-2.4 (4)	C7—O1—C8—C12	-179.34 (18)
C2—C3—C4—C5	1.7 (3)	O2—S1—C13—C18	6.54 (19)
C9—C3—C4—C5	-177.1 (2)	C1—S1—C13—C18	121.94 (17)
C2—C3—C4—C10	-179.1 (2)	O2—S1—C13—C14	179.34 (9)
C9—C3—C4—C10	2.1 (3)	C1—S1—C13—C14	-65.26 (9)
C3—C4—C5—C6	0.7 (3)	C18—C13—C14—C15	-0.62 (19)
C10—C4—C5—C6	-178.5 (2)	S1—C13—C14—C15	-173.38 (18)
C3—C4—C5—C11	179.3 (2)	C13—C14—C15—C16	-0.7 (3)
C10—C4—C5—C11	0.1 (3)	C14—C15—C16—C17	0.7 (4)
C4—C5—C6—C7	-1.4 (3)	C15—C16—C17—C18	0.6 (4)
C11—C5—C6—C7	180.0 (2)	C14—C13—C18—C17	1.9 (3)
C5—C6—C7—O1	179.54 (19)	S1—C13—C18—C17	174.44 (19)
C5—C6—C7—C2	-0.3 (3)	C16—C17—C18—C13	-1.9 (4)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C2—C7 benzene ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C6—H6 \cdots O2 ⁱ	0.95	2.35	3.286 (3)	169.
C10—H10A \cdots O2 ⁱⁱ	0.98	2.56	3.517 (3)	167.
C12—H12C \cdots Cg ⁱⁱⁱ	0.98	2.66	3.482 (3)	142.

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

Fig. 1

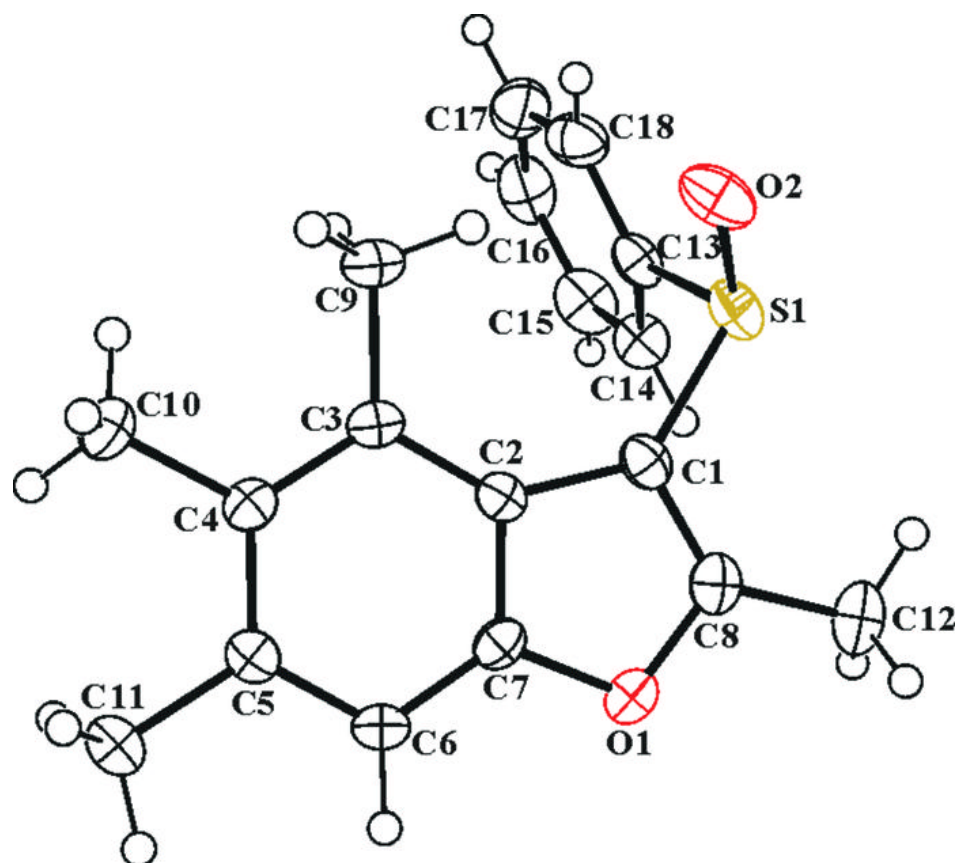


Fig. 2

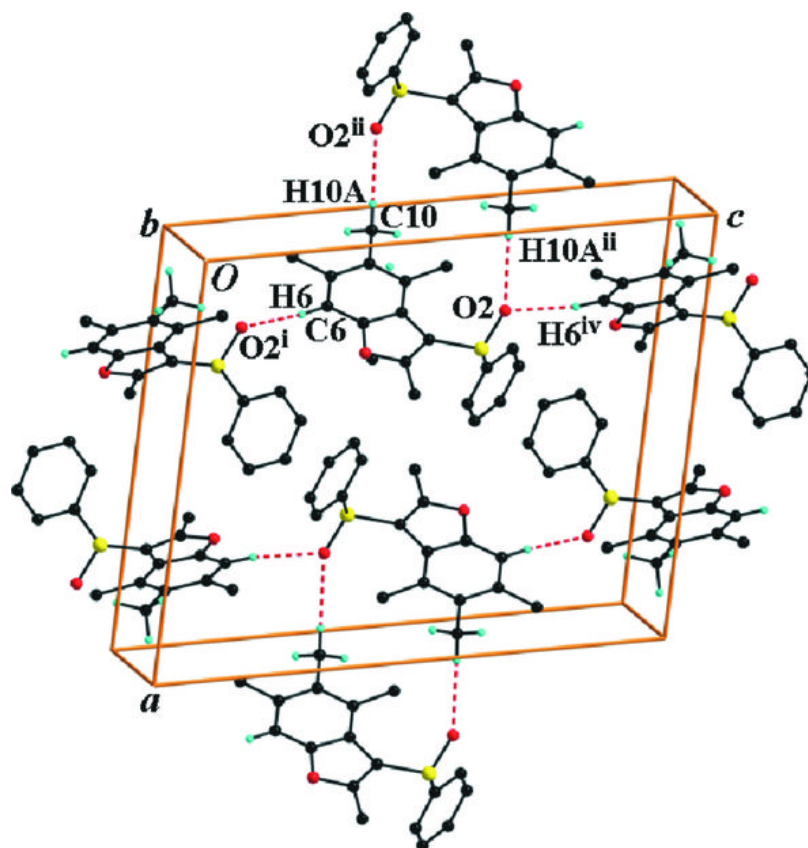


Fig. 3

