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# 3-Ethylsulfinyl-5-iodo-2-phenyl-1-benzofuran

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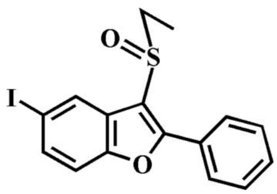
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.028; $wR$ factor = 0.068; data-to-parameter ratio = 18.8.

In the title compound, $C_{16}H_{13}IO_2S$, the phenyl ring is rotated out of the benzofuran plane, as indicated by the dihedral angle of 32.56 (6)°. The crystal structure is stabilized by an I$\cdots$O halogen interaction [3.200 (2) Å].

## Related literature

For the crystal structures of similar 2-aryl-3-ethylsulfinyl-5-halo-1-benzofuran derivatives, see: Choi *et al.* (2010*a*,*b*). For the pharmacological activity of benzofuran compounds, see: Aslam *et al.* (2006); Galal *et al.* (2009); Khan *et al.* (2005). For natural products with benzofuran rings, see: Akgul & Anil (2003); Soekamto *et al.* (2003). For a review of halogen bonding, see: Politzer *et al.* (2007).



## Experimental

### *Crystal data*

$C_{16}H_{13}IO_2S$
$M_r$ = 396.22
Orthorhombic, $Pbca$
$a$ = 11.7297 (4) Å
$b$ = 7.4560 (2) Å
$c$ = 34.0313 (9) Å
$V$ = 2976.26 (15) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 2.29 mm$^{-1}$
$T$ = 296 K
0.02 × 0.02 × 0.02 mm

### *Data collection*

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{\rm min}$ = 0.954, $T_{\rm max}$ = 0.967
14370 measured reflections
3415 independent reflections
3106 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.027

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.068
$S$ = 1.15
3415 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.97 e Å$^{-3}$

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2264).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1814 [ **doi:10.1107/S1600536810024190** ]

# 3-Ethylsulfinyl-5-iodo-2-phenyl-1-benzofuran

**P. J. Seo, H. D. Choi, B. W. Son** and **U. Lee**

## Comment

The compounds involving benzofuran skeleton show various pharmacological properties such as antifungal (Aslam *et al.*, 2006), antitumor and antiviral (Galal *et al.*, 2009), antimicrobial (Khan *et al.*, 2005) activities.

These compounds widely occur in nature (Akgul & Anil, 2003; Soekamto *et al.*, 2003). As a part of our ongoing studies of the effect of side chain substituents on the solid state structures of 2-aryl-3-ethylsulfinyl-5-halo-1-benzofuran analogues (Choi*et al.*, 2010*a*,*b*), we report the crystal structure of the title compound (Fig. 1).

The benzofuran unit is essentially planar, with a mean deviation of 0.005 (2) Å from the least-squares plane defined by the nine constituent atoms. The dihedral angle formed by the benzofuran plane and the phenyl ring is 32.56 (6)°. The crystal packing (Fig. 2) is stabilized by I···O halogen–bonding interactions between the iodine and the oxygen of the S═O unit [$I\cdots O2^{i}$ = 3.200 (2) Å; $C4–I\cdots O2^{i}$ = 176.44 (8)°] (Politzer *et al.*, 2007).

## Experimental

77% 3-chloroperoxybenzoic acid (247 mg, 1.1 mmol) was added in small portions to a stirred solution of 3-ethylsulfanyl-5-iodo-2-phenyl-1-benzofuran (380 mg, 1.0 mmol) in dichloromethane (30 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 at reduced pressure. The residue was purified by column chromatography (hexane-ethyl acetate, 1:1 v/v) to afford the title compound as a colourless solid [yield 79%, m.p. 419-420 K; $R_f$ = 0.5 (hexane-ethyl acetate, 1:1 v/v)]. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a 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 aryl, 0.97 Å for methylene and 0.96 Å for methyl H atoms. $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl and methylene H atoms, and $1.5U_{eq}(C)$ for methyl H atoms.

## Figures

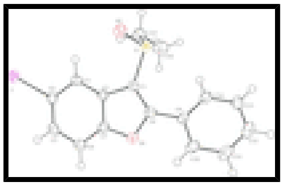

Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

Fig. 2. I···O interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) - $x$ + 1, - $y$, - $z$ + 1 .]

### 3-Ethylsulfinyl-5-iodo-2-phenyl-1-benzofuran

#### *Crystal data*

$C_{16}H_{13}IO_2S$

$M_r$ = 396.22

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a$ = 11.7297 (4) Å

$b$ = 7.4560 (2) Å

$c$ = 34.0313 (9) Å

$V$ = 2976.26 (15) Å$^3$

$Z$ = 8

$F$(000) = 1552

$D_x$ = 1.769 Mg m$^{-3}$

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

Cell parameters from 8139 reflections

$\theta$ = 2.4–27.5°

$\mu$ = 2.29 mm$^{-1}$

$T$ = 296 K

Block, colourless

0.02 × 0.02 × 0.02 mm

#### *Data collection*

Bruker SMART APEXII CCD diffractometer

Radiation source: rotating anode

graphite multilayer

Detector resolution: 10.0 pixels mm$^{-1}$

$\varphi$ and $\omega$ scans

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

$T_{\min}$ = 0.954, $T_{\max}$ = 0.967

14370 measured reflections

3415 independent reflections

3106 reflections with $I > 2\sigma(I)$

$R_{\text{int}}$ = 0.027

$\theta_{\max}$ = 27.5°, $\theta_{\min}$ = 2.1°

$h = -15 \rightarrow 9$

$k = -8 \rightarrow 9$

$l = -43 \rightarrow 44$

#### *Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.028

$wR(F^2)$ = 0.068

$S$ = 1.15

3415 reflections

182 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

$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 3.2745P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max}$ = 0.002

$\Delta\rho_{\max}$ = 0.55 e Å$^{-3}$

$\Delta\rho_{\min}$ = −0.97 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 $F^2 > 2\sigma(F^2)$ 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* | $U_{\text{iso}}$*/$U_{\text{eq}}$ |
|---|---|---|---|---|
| I | 0.337055 (15) | 0.11075 (3) | 0.528788 (5) | 0.03128 (7) |
| S | 0.56486 (5) | 0.15154 (8) | 0.360798 (17) | 0.02225 (13) |
| O1 | 0.23461 (14) | 0.2567 (2) | 0.35329 (5) | 0.0259 (4) |
| O2 | 0.58668 (16) | −0.0183 (3) | 0.38324 (6) | 0.0318 (4) |
| C1 | 0.4196 (2) | 0.2055 (3) | 0.36723 (7) | 0.0217 (5) |
| C2 | 0.3566 (2) | 0.1963 (3) | 0.40373 (7) | 0.0212 (5) |
| C3 | 0.3845 (2) | 0.1631 (3) | 0.44285 (7) | 0.0239 (5) |
| H3 | 0.4594 | 0.1420 | 0.4506 | 0.029* |
| C4 | 0.2959 (2) | 0.1628 (4) | 0.46975 (7) | 0.0261 (5) |
| C5 | 0.1832 (2) | 0.1945 (4) | 0.45888 (8) | 0.0296 (6) |
| H5 | 0.1263 | 0.1937 | 0.4779 | 0.036* |
| C6 | 0.1550 (2) | 0.2274 (4) | 0.41965 (8) | 0.0288 (6) |
| H6 | 0.0802 | 0.2483 | 0.4118 | 0.035* |
| C7 | 0.2435 (2) | 0.2273 (3) | 0.39332 (7) | 0.0244 (5) |
| C8 | 0.34345 (19) | 0.2429 (3) | 0.33829 (7) | 0.0219 (5) |
| C9 | 0.3539 (2) | 0.2680 (3) | 0.29579 (7) | 0.0226 (5) |
| C10 | 0.2650 (2) | 0.2139 (3) | 0.27091 (8) | 0.0289 (5) |
| H10 | 0.1990 | 0.1639 | 0.2814 | 0.035* |
| C11 | 0.2760 (3) | 0.2353 (4) | 0.23078 (8) | 0.0353 (6) |
| H11 | 0.2171 | 0.1990 | 0.2143 | 0.042* |
| C12 | 0.3734 (3) | 0.3100 (4) | 0.21470 (8) | 0.0346 (6) |
| H12 | 0.3802 | 0.3226 | 0.1876 | 0.042* |
| C13 | 0.4609 (3) | 0.3660 (4) | 0.23919 (8) | 0.0320 (6) |
| H13 | 0.5261 | 0.4176 | 0.2286 | 0.038* |
| C14 | 0.4512 (2) | 0.3451 (3) | 0.27951 (7) | 0.0273 (5) |
| H14 | 0.5101 | 0.3829 | 0.2958 | 0.033* |
| C15 | 0.6250 (2) | 0.3317 (4) | 0.38974 (8) | 0.0314 (6) |
| H15A | 0.5900 | 0.3315 | 0.4156 | 0.038* |
| H15B | 0.7060 | 0.3106 | 0.3931 | 0.038* |
| C16 | 0.6077 (3) | 0.5131 (4) | 0.37097 (10) | 0.0434 (7) |
| H16A | 0.6474 | 0.5172 | 0.3463 | 0.065* |
| H16B | 0.6369 | 0.6047 | 0.3880 | 0.065* |
| H16C | 0.5278 | 0.5327 | 0.3666 | 0.065* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I | 0.03590 (12) | 0.03674 (12) | 0.02121 (10) | 0.00703 (7) | 0.00679 (6) | 0.00190 (7) |
| S | 0.0199 (3) | 0.0276 (3) | 0.0193 (3) | 0.0033 (2) | 0.0005 (2) | 0.0016 (2) |
| O1 | 0.0206 (8) | 0.0319 (9) | 0.0251 (8) | 0.0007 (7) | −0.0023 (7) | 0.0016 (7) |
| O2 | 0.0311 (10) | 0.0325 (10) | 0.0318 (10) | 0.0093 (8) | 0.0016 (8) | 0.0083 (8) |
| C1 | 0.0209 (11) | 0.0235 (12) | 0.0208 (11) | −0.0001 (9) | 0.0002 (9) | 0.0007 (9) |
| C2 | 0.0212 (11) | 0.0198 (12) | 0.0226 (11) | 0.0016 (9) | 0.0029 (9) | 0.0022 (9) |
| C3 | 0.0223 (12) | 0.0251 (12) | 0.0242 (12) | 0.0042 (10) | 0.0013 (9) | 0.0007 (10) |
| C4 | 0.0301 (13) | 0.0252 (12) | 0.0231 (12) | 0.0039 (10) | 0.0038 (10) | 0.0010 (10) |
| C5 | 0.0262 (13) | 0.0328 (15) | 0.0299 (13) | 0.0005 (11) | 0.0081 (10) | −0.0004 (11) |
| C6 | 0.0192 (12) | 0.0349 (14) | 0.0322 (14) | 0.0021 (10) | −0.0003 (10) | 0.0002 (11) |
| C7 | 0.0242 (11) | 0.0233 (12) | 0.0256 (12) | 0.0008 (10) | −0.0012 (10) | 0.0024 (10) |
| C8 | 0.0199 (11) | 0.0208 (11) | 0.0250 (12) | −0.0001 (9) | −0.0018 (9) | 0.0003 (9) |
| C9 | 0.0256 (12) | 0.0204 (12) | 0.0217 (12) | 0.0026 (9) | −0.0043 (9) | 0.0008 (9) |
| C10 | 0.0313 (14) | 0.0251 (13) | 0.0304 (13) | −0.0039 (11) | −0.0077 (11) | 0.0032 (10) |
| C11 | 0.0465 (17) | 0.0304 (14) | 0.0289 (13) | −0.0046 (12) | −0.0144 (12) | 0.0017 (11) |
| C12 | 0.0563 (18) | 0.0251 (13) | 0.0226 (12) | 0.0014 (13) | −0.0035 (12) | 0.0027 (10) |
| C13 | 0.0372 (15) | 0.0298 (14) | 0.0291 (13) | 0.0016 (11) | 0.0048 (11) | 0.0067 (11) |
| C14 | 0.0282 (13) | 0.0269 (13) | 0.0269 (13) | −0.0005 (10) | −0.0055 (10) | 0.0043 (10) |
| C15 | 0.0236 (12) | 0.0421 (16) | 0.0284 (13) | −0.0054 (12) | −0.0048 (10) | −0.0047 (12) |
| C16 | 0.0392 (16) | 0.0340 (16) | 0.057 (2) | −0.0074 (13) | −0.0056 (15) | −0.0078 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| I—C4 | 2.102 (2) | C8—C9 | 1.464 (3) |
| I—O2$^i$ | 3.200 (2) | C9—C14 | 1.393 (4) |
| S—O2 | 1.500 (2) | C9—C10 | 1.402 (3) |
| S—C1 | 1.764 (2) | C10—C11 | 1.381 (4) |
| S—C15 | 1.809 (3) | C10—H10 | 0.9300 |
| O1—C8 | 1.379 (3) | C11—C12 | 1.384 (4) |
| O1—C7 | 1.384 (3) | C11—H11 | 0.9300 |
| C1—C8 | 1.359 (3) | C12—C13 | 1.386 (4) |
| C1—C2 | 1.447 (3) | C12—H12 | 0.9300 |
| C2—C7 | 1.392 (3) | C13—C14 | 1.385 (4) |
| C2—C3 | 1.393 (3) | C13—H13 | 0.9300 |
| C3—C4 | 1.385 (3) | C14—H14 | 0.9300 |
| C3—H3 | 0.9300 | C15—C16 | 1.510 (4) |
| C4—C5 | 1.393 (4) | C15—H15A | 0.9700 |
| C5—C6 | 1.397 (4) | C15—H15B | 0.9700 |
| C5—H5 | 0.9300 | C16—H16A | 0.9600 |
| C6—C7 | 1.372 (4) | C16—H16B | 0.9600 |
| C6—H6 | 0.9300 | C16—H16C | 0.9600 |
| C4—I—O2$^i$ | 176.44 (8) | C14—C9—C8 | 121.0 (2) |
| O2—S—C1 | 107.1 (1) | C10—C9—C8 | 119.8 (2) |
| O2—S—C15 | 106.4 (1) | C11—C10—C9 | 119.6 (3) |

| | | | |
|---|---|---|---|
| C1—S—C15 | 98.0 (1) | C11—C10—H10 | 120.2 |
| C8—O1—C7 | 106.4 (2) | C9—C10—H10 | 120.2 |
| C8—C1—C2 | 107.2 (2) | C10—C11—C12 | 121.0 (3) |
| C8—C1—S | 126.3 (2) | C10—C11—H11 | 119.5 |
| C2—C1—S | 126.1 (2) | C12—C11—H11 | 119.5 |
| C7—C2—C3 | 119.8 (2) | C11—C12—C13 | 119.6 (3) |
| C7—C2—C1 | 105.1 (2) | C11—C12—H12 | 120.2 |
| C3—C2—C1 | 135.1 (2) | C13—C12—H12 | 120.2 |
| C4—C3—C2 | 117.1 (2) | C14—C13—C12 | 120.1 (3) |
| C4—C3—H3 | 121.4 | C14—C13—H13 | 120.0 |
| C2—C3—H3 | 121.4 | C12—C13—H13 | 120.0 |
| C3—C4—C5 | 122.5 (2) | C13—C14—C9 | 120.5 (2) |
| C3—C4—I | 117.4 (2) | C13—C14—H14 | 119.8 |
| C5—C4—I | 120.2 (2) | C9—C14—H14 | 119.8 |
| C4—C5—C6 | 120.6 (2) | C16—C15—S | 112.5 (2) |
| C4—C5—H5 | 119.7 | C16—C15—H15A | 109.1 |
| C6—C5—H5 | 119.7 | S—C15—H15A | 109.1 |
| C7—C6—C5 | 116.4 (2) | C16—C15—H15B | 109.1 |
| C7—C6—H6 | 121.8 | S—C15—H15B | 109.1 |
| C5—C6—H6 | 121.8 | H15A—C15—H15B | 107.8 |
| C6—C7—O1 | 125.8 (2) | C15—C16—H16A | 109.5 |
| C6—C7—C2 | 123.7 (2) | C15—C16—H16B | 109.5 |
| O1—C7—C2 | 110.4 (2) | H16A—C16—H16B | 109.5 |
| C1—C8—O1 | 110.8 (2) | C15—C16—H16C | 109.5 |
| C1—C8—C9 | 133.4 (2) | H16A—C16—H16C | 109.5 |
| O1—C8—C9 | 115.7 (2) | H16B—C16—H16C | 109.5 |
| C14—C9—C10 | 119.2 (2) | | |

| | | | |
|---|---|---|---|
| O2—S—C1—C8 | −128.5 (2) | C1—C2—C7—O1 | −0.8 (3) |
| C15—S—C1—C8 | 121.5 (2) | C2—C1—C8—O1 | −0.7 (3) |
| O2—S—C1—C2 | 43.2 (2) | S—C1—C8—O1 | 172.33 (17) |
| C15—S—C1—C2 | −66.8 (2) | C2—C1—C8—C9 | −179.8 (3) |
| C8—C1—C2—C7 | 0.9 (3) | S—C1—C8—C9 | −6.8 (4) |
| S—C1—C2—C7 | −172.14 (19) | C7—O1—C8—C1 | 0.2 (3) |
| C8—C1—C2—C3 | 179.7 (3) | C7—O1—C8—C9 | 179.5 (2) |
| S—C1—C2—C3 | 6.7 (4) | C1—C8—C9—C14 | −33.4 (4) |
| C7—C2—C3—C4 | 0.0 (4) | O1—C8—C9—C14 | 147.5 (2) |
| C1—C2—C3—C4 | −178.7 (3) | C1—C8—C9—C10 | 146.6 (3) |
| C2—C3—C4—C5 | −0.2 (4) | O1—C8—C9—C10 | −32.5 (3) |
| C2—C3—C4—I | 179.54 (19) | C14—C9—C10—C11 | 1.0 (4) |
| C3—C4—C5—C6 | 0.4 (4) | C8—C9—C10—C11 | −179.0 (2) |
| I—C4—C5—C6 | −179.4 (2) | C9—C10—C11—C12 | −0.2 (4) |
| C4—C5—C6—C7 | −0.3 (4) | C10—C11—C12—C13 | −0.7 (5) |
| C5—C6—C7—O1 | 180.0 (2) | C11—C12—C13—C14 | 0.8 (4) |
| C5—C6—C7—C2 | 0.1 (4) | C12—C13—C14—C9 | 0.0 (4) |
| C8—O1—C7—C6 | −179.5 (3) | C10—C9—C14—C13 | −0.9 (4) |
| C8—O1—C7—C2 | 0.4 (3) | C8—C9—C14—C13 | 179.1 (2) |
| C3—C2—C7—C6 | 0.0 (4) | O2—S—C15—C16 | −179.1 (2) |
| C1—C2—C7—C6 | 179.1 (2) | C1—S—C15—C16 | −68.5 (2) |
| C3—C2—C7—O1 | −179.8 (2) | | |

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

**Fig. 1**

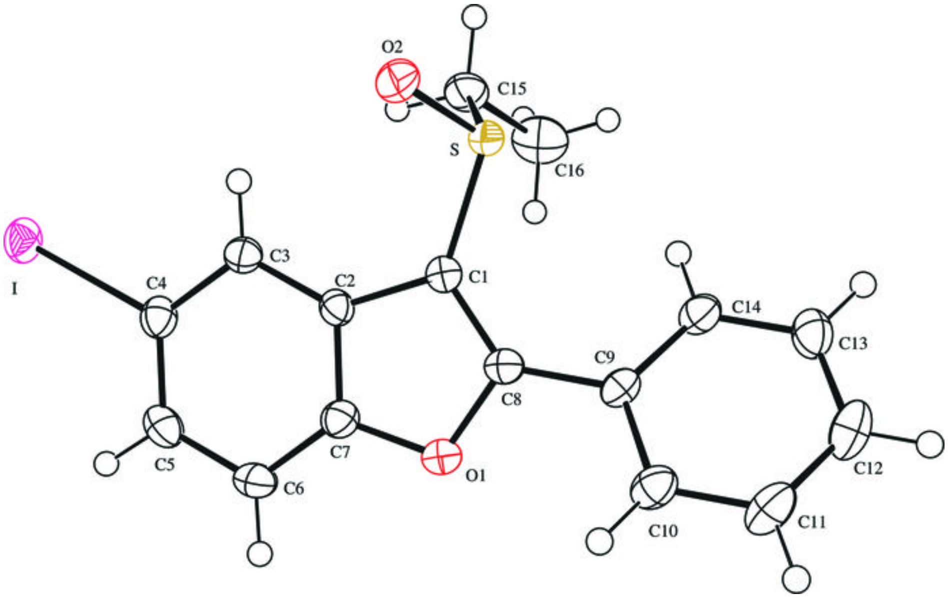

**Fig. 2**