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3-Iodo-2-methyl-1-phenylsulfonyl-1*H*-indole

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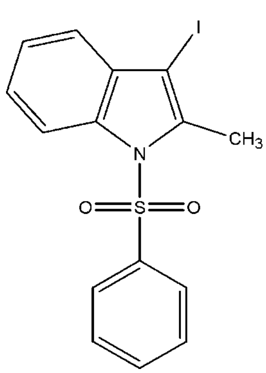
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.144; data-to-parameter ratio = 29.0.

In the title compound, $C_{15}H_{12}INO_2S$, the sulfonyl-bound phenyl ring forms a dihedral angle 82.84 (9)° with the indole ring system. The molecular structure is stabilized by a weak intramolecular C—H···O hydrogen bond. The crystal structure exhibits weak intermolecular C—H···π interactions and π–π interactions between the indole groups [centroid–centroid distance between the five-membered and six-membered rings of the indole group = 3.7617 (18) Å].

Related literature

For the biological properties of indole derivatives, see: Chai *et al.* (2006); Nieto *et al.* (2005). For the structures of closely related compounds, see: Chakkaravarthi *et al.* (2007, 2008).



Experimental

Crystal data

$C_{15}H_{12}INO_2S$
M_r = 397.22
Monoclinic, $P2_1/c$
a = 10.7068 (3) Å
b = 16.2670 (4) Å
c = 8.5147 (2) Å
β = 104.540 (1)°
V = 1435.49 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 295 K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.536, T_{max} = 0.648
21249 measured reflections
5276 independent reflections
3696 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.144
S = 1.06
5276 reflections
182 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −1.56 e Å^{-3}

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

*Cg*3 is the centroid of the C9–C14 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1	0.93	2.29	2.871 (4)	120
C4—H4···$Cg3^{i}$	0.93	2.65	3.517 (5)	156

Symmetry code: (i) $-x+2, -y, -z+2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); 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: GK2346).

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supporting information

Acta Cryst. (2011). E**67**, o632   [doi:10.1107/S1600536811004685]

3-Iodo-2-methyl-1-phenylsulfonyl-1*H*-indole

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S1. Comment

Indole derivatives exhibit antihepatitis B virus (Chai *et al.*, 2006) and antibacterial (Nieto *et al.*, 2005) activities. The geometric parameters of the title molecule (Fig. 1) agree well with the reported similar structures (Chakkaravarthi *et al.* 2007, 2008).

The phenyl ring makes the dihedral angle of 82.84 (9)° with the indole ring system. The sum of the bond angles around N1 [359.4 (2)°] indicates that N1 atom is sp^2 hybridized. The molecular structure is stabilized by weak intramolecular C—H···O hydrogen bond. The crystal structure exhibits weak intermolecular C—H···π (Table 1) and π–π interactions [*Cg*1···*Cg*3 (1 - *x*,-*y*,1 - *z*) 3.7617 (18) Å; *Cg*1 and *Cg*3 are the centroids of the rings N1/C7/C8/C9/C14 and C9—C14, respectively].

S2. Experimental

3-Iodo-2-methylindole (5 g,0.02 mmole) was dissolved in distilled benzene (100 ml).To this, benzenesulfonyl chloride(3.23 ml,0.025 mmol) and 60% aqueous NaOH solution (40 g in 67.0 ml) were added along with tetrabutyl ammonium hydrogensulfate (1.0 g). This two phase system was stirred at room temperature for 2 h. It was then diluted with water (200 ml) and the organic layer was separated. The aqueous layer was extracted with benzene (2x20 ml). The combined organic layer was dried(Na_2SO_4).The benzene was then removed completely and the crude product was recrystallized from methanol (m.p. 395–397 K).

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H and C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for CH_3. The components of the anisotropic displacement parameters in direction of the bond of I1 and C8 were restrained to be equal within an effective standard deviation of 0.001 using the DELU command in *SHELXL* (Sheldrick, 2008).

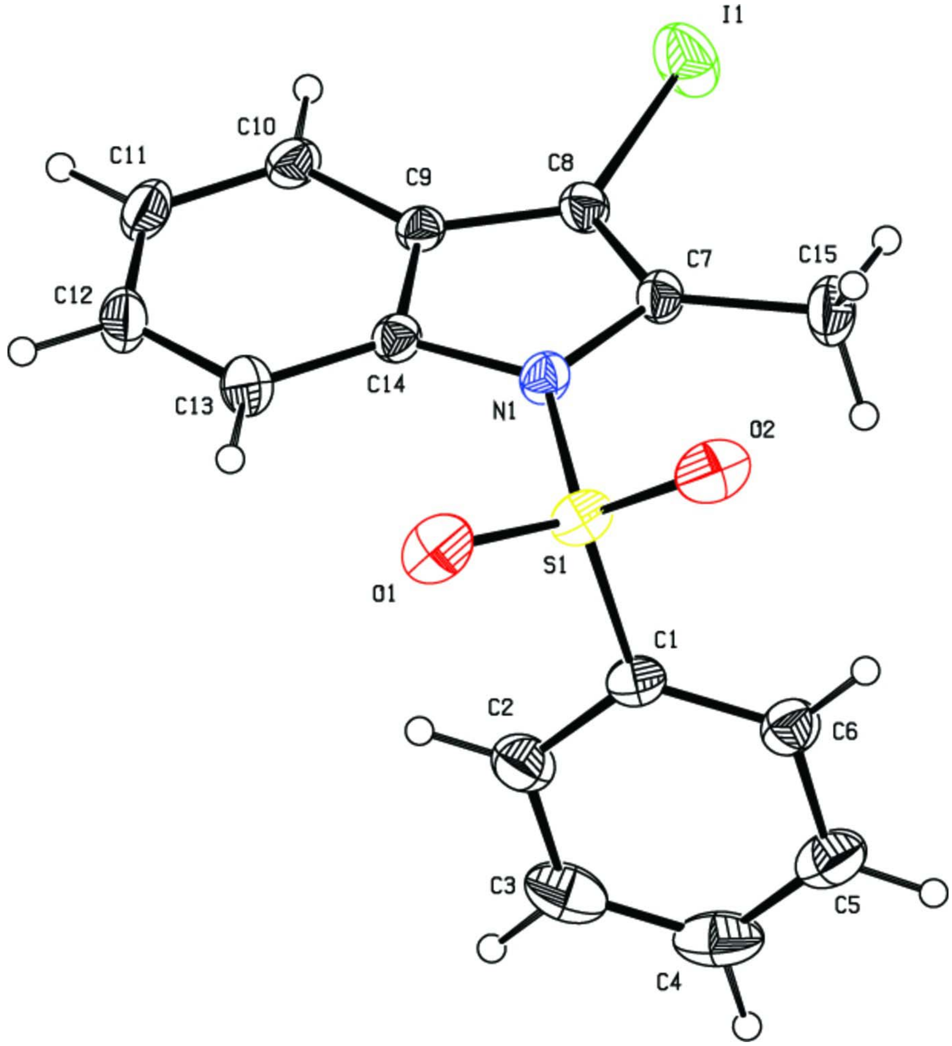

Figure 1

The molecular structure of the title compound with 30% probability displacement ellipsoids for non-H atoms.

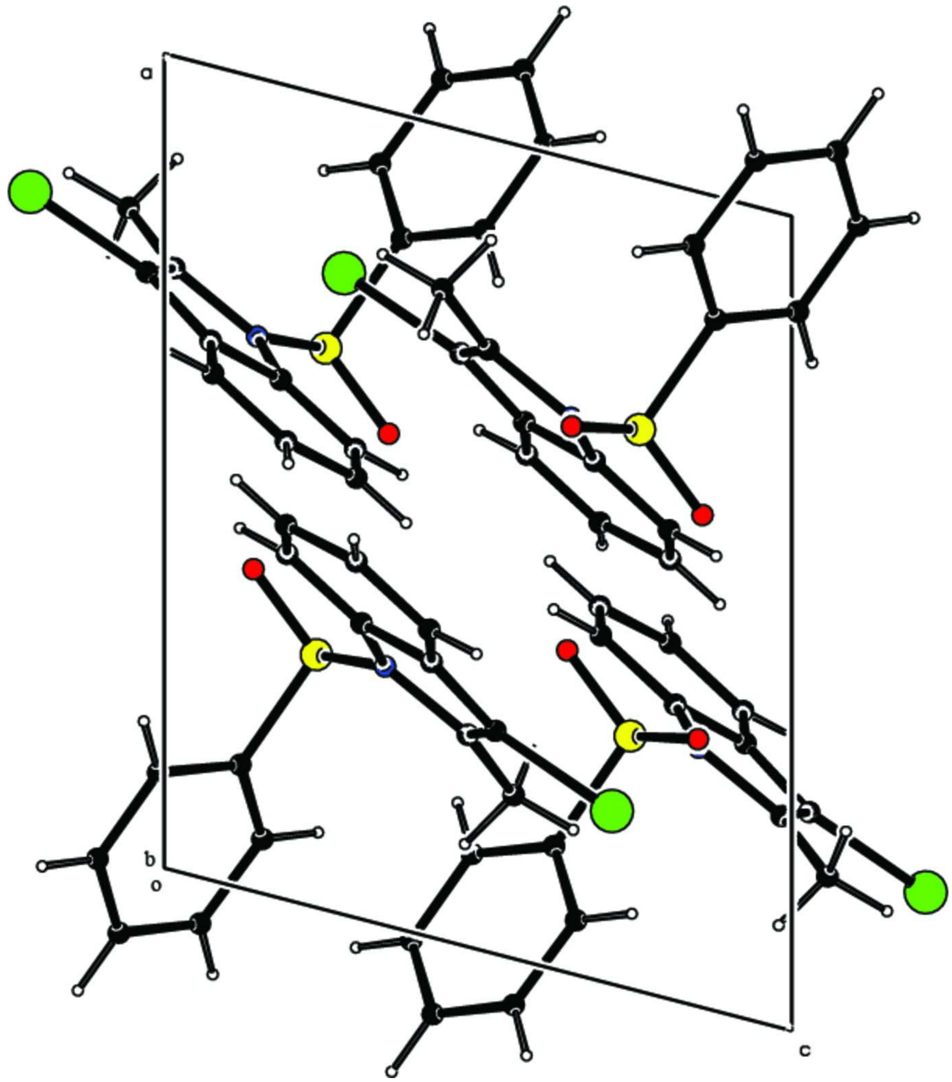

Figure 2

Crystal packing viewed along the *b* axis.

3-Iodo-2-methyl-1-phenylsulfonyl-1*H*-indole

Crystal data

$C_{15}H_{12}INO_2S$
$M_r = 397.22$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.7068$ (3) Å
$b = 16.2670$ (4) Å
$c = 8.5147$ (2) Å
$\beta = 104.540$ (1)°
$V = 1435.49$ (6) Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.838$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8510 reflections
$\theta = 2.5$–30.4°
$\mu = 2.38$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.536, T_{max} = 0.648
21249 measured reflections
5276 independent reflections
3696 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 32.8°, θ_{min} = 2.5°
$h = -15 \rightarrow 16$
$k = -23 \rightarrow 24$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.144
S = 1.06
5276 reflections
182 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2 + 0.987P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −1.56 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.8489 (3)	0.14775 (16)	0.8788 (3)	0.0350 (5)
C2	0.8848 (4)	0.0951 (2)	1.0097 (4)	0.0495 (7)
H2	0.8265	0.0574	1.0324	0.059*
C3	1.0098 (4)	0.0998 (3)	1.1063 (5)	0.0638 (10)
H3	1.0365	0.0646	1.1944	0.077*
C4	1.0940 (4)	0.1562 (3)	1.0722 (5)	0.0643 (11)
H4	1.1778	0.1587	1.1375	0.077*
C5	1.0569 (3)	0.2092 (3)	0.9431 (5)	0.0556 (9)
H5	1.1149	0.2478	0.9227	0.067*
C6	0.9331 (3)	0.20492 (19)	0.8436 (4)	0.0433 (6)
H6	0.9073	0.2398	0.7549	0.052*
C7	0.7397 (3)	0.04833 (16)	0.5161 (3)	0.0329 (5)
C8	0.7262 (3)	−0.03190 (16)	0.4724 (3)	0.0336 (5)
C9	0.6619 (2)	−0.07527 (14)	0.5739 (3)	0.0297 (4)
C10	0.6230 (3)	−0.15718 (17)	0.5777 (4)	0.0387 (6)
H10	0.6379	−0.1950	0.5025	0.046*
C11	0.5626 (3)	−0.1805 (2)	0.6940 (4)	0.0478 (7)
H11	0.5362	−0.2348	0.6978	0.057*
C12	0.5402 (3)	−0.1249 (2)	0.8061 (4)	0.0486 (7)
H12	0.5005	−0.1429	0.8852	0.058*
C13	0.5753 (3)	−0.0428 (2)	0.8043 (4)	0.0435 (6)
H13	0.5585	−0.0055	0.8792	0.052*
C14	0.6367 (2)	−0.01869 (15)	0.6857 (3)	0.0309 (5)
C15	0.7993 (4)	0.1168 (2)	0.4432 (5)	0.0509 (7)
H15A	0.8230	0.0972	0.3483	0.076*

H15B	0.8748	0.1362	0.5208	0.076*
H15C	0.7383	0.1609	0.4137	0.076*
N1	0.6822 (2)	0.05838 (13)	0.6481 (3)	0.0335 (4)
O1	0.6046 (2)	0.13114 (15)	0.8577 (4)	0.0552 (6)
O2	0.6719 (2)	0.21172 (13)	0.6496 (3)	0.0533 (6)
S1	0.68958 (6)	0.14402 (4)	0.75748 (10)	0.03797 (16)
I1	0.78752 (3)	−0.084909 (16)	0.28650 (3)	0.06383 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0355 (12)	0.0307 (11)	0.0379 (13)	0.0043 (9)	0.0078 (10)	−0.0078 (10)
C2	0.0583 (19)	0.0487 (17)	0.0391 (15)	0.0014 (14)	0.0076 (14)	0.0020 (12)
C3	0.071 (3)	0.070 (2)	0.0421 (18)	0.020 (2)	−0.0008 (17)	0.0018 (17)
C4	0.0421 (17)	0.087 (3)	0.056 (2)	0.0121 (17)	−0.0013 (15)	−0.025 (2)
C5	0.0409 (16)	0.065 (2)	0.061 (2)	−0.0088 (14)	0.0131 (14)	−0.0205 (18)
C6	0.0436 (15)	0.0406 (14)	0.0458 (15)	−0.0039 (11)	0.0117 (12)	−0.0062 (12)
C7	0.0368 (12)	0.0290 (11)	0.0337 (12)	−0.0026 (9)	0.0107 (9)	0.0026 (9)
C8	0.0411 (13)	0.0293 (11)	0.0303 (11)	−0.0013 (9)	0.0088 (9)	0.0012 (8)
C9	0.0297 (11)	0.0280 (11)	0.0287 (11)	−0.0016 (8)	0.0025 (8)	0.0014 (8)
C10	0.0444 (14)	0.0295 (12)	0.0376 (13)	−0.0067 (10)	0.0021 (11)	−0.0005 (10)
C11	0.0440 (15)	0.0395 (15)	0.0552 (17)	−0.0157 (12)	0.0036 (13)	0.0100 (13)
C12	0.0407 (15)	0.0578 (19)	0.0489 (17)	−0.0109 (13)	0.0143 (12)	0.0130 (15)
C13	0.0415 (14)	0.0501 (16)	0.0427 (15)	−0.0046 (12)	0.0178 (12)	0.0006 (12)
C14	0.0272 (10)	0.0321 (11)	0.0326 (11)	−0.0008 (8)	0.0058 (9)	0.0005 (9)
C15	0.064 (2)	0.0396 (15)	0.0548 (18)	−0.0110 (14)	0.0261 (15)	0.0073 (14)
N1	0.0389 (11)	0.0255 (9)	0.0373 (11)	−0.0027 (8)	0.0120 (9)	−0.0033 (8)
O1	0.0433 (11)	0.0543 (13)	0.0750 (17)	0.0013 (10)	0.0278 (11)	−0.0227 (12)
O2	0.0528 (13)	0.0308 (10)	0.0659 (15)	0.0113 (9)	−0.0047 (11)	0.0013 (10)
S1	0.0335 (3)	0.0299 (3)	0.0491 (4)	0.0048 (2)	0.0078 (3)	−0.0079 (3)
I1	0.0954 (2)	0.05448 (17)	0.05233 (17)	0.00090 (11)	0.03859 (15)	−0.00527 (9)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C9—C14	1.399 (4)
C1—C2	1.381 (4)	C9—C10	1.399 (3)
C1—S1	1.759 (3)	C10—C11	1.365 (5)
C2—C3	1.386 (6)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.379 (5)
C3—C4	1.367 (7)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.387 (5)
C4—C5	1.375 (6)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.392 (4)
C5—C6	1.384 (5)	C13—H13	0.9300
C5—H5	0.9300	C14—N1	1.411 (3)
C6—H6	0.9300	C15—H15A	0.9600
C7—C8	1.355 (4)	C15—H15B	0.9600
C7—N1	1.420 (3)	C15—H15C	0.9600

C7—C15	1.493 (4)	N1—S1	1.667 (2)
C8—C9	1.421 (4)	O1—S1	1.411 (3)
C8—I1	2.050 (3)	O2—S1	1.416 (3)

C6—C1—C2	121.9 (3)	C9—C10—H10	120.7
C6—C1—S1	119.1 (2)	C10—C11—C12	121.0 (3)
C2—C1—S1	119.0 (2)	C10—C11—H11	119.5
C1—C2—C3	118.5 (4)	C12—C11—H11	119.5
C1—C2—H2	120.8	C11—C12—C13	122.0 (3)
C3—C2—H2	120.8	C11—C12—H12	119.0
C4—C3—C2	120.0 (4)	C13—C12—H12	119.0
C4—C3—H3	120.0	C12—C13—C14	117.2 (3)
C2—C3—H3	120.0	C12—C13—H13	121.4
C3—C4—C5	121.1 (3)	C14—C13—H13	121.4
C3—C4—H4	119.4	C13—C14—C9	121.0 (2)
C5—C4—H4	119.4	C13—C14—N1	132.0 (3)
C4—C5—C6	119.9 (4)	C9—C14—N1	107.0 (2)
C4—C5—H5	120.0	C7—C15—H15A	109.5
C6—C5—H5	120.0	C7—C15—H15B	109.5
C1—C6—C5	118.6 (3)	H15A—C15—H15B	109.5
C1—C6—H6	120.7	C7—C15—H15C	109.5
C5—C6—H6	120.7	H15A—C15—H15C	109.5
C8—C7—N1	106.9 (2)	H15B—C15—H15C	109.5
C8—C7—C15	129.1 (3)	C14—N1—C7	108.7 (2)
N1—C7—C15	123.9 (3)	C14—N1—S1	125.89 (19)
C7—C8—C9	110.2 (2)	C7—N1—S1	124.72 (18)
C7—C8—I1	125.8 (2)	O1—S1—O2	120.43 (16)
C9—C8—I1	124.00 (18)	O1—S1—N1	105.47 (13)
C14—C9—C10	120.1 (2)	O2—S1—N1	107.93 (14)
C14—C9—C8	107.1 (2)	O1—S1—C1	109.09 (15)
C10—C9—C8	132.8 (3)	O2—S1—C1	107.83 (14)
C11—C10—C9	118.7 (3)	N1—S1—C1	105.06 (12)
C11—C10—H10	120.7		

C6—C1—C2—C3	−0.7 (5)	C8—C9—C14—C13	−179.2 (3)
S1—C1—C2—C3	−178.7 (3)	C10—C9—C14—N1	−177.8 (2)
C1—C2—C3—C4	0.7 (6)	C8—C9—C14—N1	1.6 (3)
C2—C3—C4—C5	0.3 (6)	C13—C14—N1—C7	179.0 (3)
C3—C4—C5—C6	−1.1 (6)	C9—C14—N1—C7	−2.0 (3)
C2—C1—C6—C5	−0.1 (5)	C13—C14—N1—S1	8.1 (4)
S1—C1—C6—C5	177.9 (2)	C9—C14—N1—S1	−172.91 (19)
C4—C5—C6—C1	1.0 (5)	C8—C7—N1—C14	1.6 (3)
N1—C7—C8—C9	−0.5 (3)	C15—C7—N1—C14	−179.7 (3)
C15—C7—C8—C9	−179.2 (3)	C8—C7—N1—S1	172.6 (2)
N1—C7—C8—I1	179.13 (18)	C15—C7—N1—S1	−8.7 (4)
C15—C7—C8—I1	0.5 (5)	C14—N1—S1—O1	−19.0 (3)
C7—C8—C9—C14	−0.7 (3)	C7—N1—S1—O1	171.5 (2)
I1—C8—C9—C14	179.62 (18)	C14—N1—S1—O2	−149.0 (2)

C7—C8—C9—C10	178.6 (3)	C7—N1—S1—O2	41.5 (3)
I1—C8—C9—C10	−1.1 (4)	C14—N1—S1—C1	96.2 (2)
C14—C9—C10—C11	−1.3 (4)	C7—N1—S1—C1	−73.3 (2)
C8—C9—C10—C11	179.5 (3)	C6—C1—S1—O1	−139.6 (2)
C9—C10—C11—C12	0.0 (5)	C2—C1—S1—O1	38.4 (3)
C10—C11—C12—C13	1.3 (5)	C6—C1—S1—O2	−7.2 (3)
C11—C12—C13—C14	−1.1 (5)	C2—C1—S1—O2	170.8 (3)
C12—C13—C14—C9	−0.2 (4)	C6—C1—S1—N1	107.7 (2)
C12—C13—C14—N1	178.7 (3)	C2—C1—S1—N1	−74.2 (3)
C10—C9—C14—C13	1.4 (4)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O1	0.93	2.29	2.871 (4)	120
C4—H4···*Cg*3^{i}	0.93	2.65	3.517 (5)	156

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.