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Methyl (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)glyoxylate

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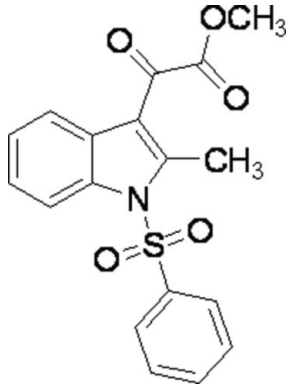
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.132; data-to-parameter ratio = 24.4.

In the title compound, $C_{18}H_{15}NO_5S$, the phenyl ring makes a dihedral angle of 85.33 (5)° with the indole ring system. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular C—H···O and C—H···π interactions.

Related literature

For related literature, see: Amal Raj *et al.* (2003); Jiang *et al.* (2004); Palani *et al.* (2006); Senthil Kumar *et al.* (2006). A similar phenylsulfonylindole compound with a nitro group has been reported (Kishbaugh *et al.*, 2006).



Experimental

Crystal data

$C_{18}H_{15}NO_5S$
M_r = 357.37
Monoclinic, $P2_1/n$
a = 9.7005 (3) Å
b = 12.9924 (4) Å
c = 13.4224 (3) Å
β = 96.189 (1)°
V = 1681.80 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 295 (2) K
0.20 × 0.16 × 0.16 mm

Data collection

Bruker Kappa APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.882, T_{max} = 0.966
23482 measured reflections
5550 independent reflections
4082 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.132
S = 1.04
5550 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 and *Cg*3 are the centroids of the C1–C6 and N1/C7–C14 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O3^{i}	0.93	2.46	3.219 (2)	139
C15—H15A···O4^{ii}	0.96	2.60	3.533 (2)	164
C6—H6···O1	0.93	2.54	2.908 (2)	104
C8—H8···O1	0.93	2.54	3.024 (2)	113
C11—H11···O3	0.93	2.51	3.021 (2)	115
C15—H15B···O2	0.96	2.42	2.793 (2)	103
C4—H4···*Cg*3^{iii}	0.93	2.80	3.495 (2)	132
C5—H5···*Cg*1^{iii}	0.93	2.88	3.526 (3)	128

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: IS2199).

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supplementary materials

Acta Cryst. (2007). E**63**, o3673 [**doi:10.1107/S1600536807036987**]

Methyl (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)glyoxylate

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Comment

The derivatives of pyrrolidine have been found to exhibit antifungal and antimicrobial activities (Amal Raj *et al.*, 2003) and inhibit human immunodeficiency virus type-I (HIV-I) (Jiang *et al.*, 2004).

The geometric parameters in the title compound, (I), agree with the reported values of similar structures (Palani *et al.*, 2006; Senthil Kumar *et al.*, 2006). The phenyl ring makes a dihedral angle of 85.33 (5)° with the indole ring system (Fig. 1). The five-membered N1/C7/C12/C13/C14 and six-membered C7—C12 rings in the indole group are planar, with a dihedral angle of 1.19 (5)° between these rings. The sum of the bond angles around N1 (359.9°) indicates that N1 is sp^2-hybridized. The torsion angles O2—S1—N1—C14 and O1—S1—N1—C7 [−2.26 (14)° and 44.21 (12)°, respectively] indicate the *syn* conformation of the sulfonyl moiety.

The details of the hydrogen bonding are given in Table 1. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing of (I) (Fig. 2) is stabilized by weak intermolecular C—H···O interactions and C—H···π interactions involving the C1—C6 (centroid *Cg*1) and N1/C7—C14 (centroid *Cg*3) rings.

Experimental

To a solution of methyl 2-(2-methyl-1*H*-indole-3-yl)-2-oxo acetate (10 g, 43.0 mmol) in dry dichloromethane (80 ml) under nitrogen, triethylamine (8.3 ml, 59.9 mmol) followed by dimethyl amino pyridine (0.56 g, 4.6 mmol) were added slowly and stirred at 273 K for 30 min. To this benzenesulfonyl chloride (8.3 ml, 64.9 mmol), dry dichloromethane (10 ml) was slowly added at 273 K for 30 min. Then the reaction mixture was stirred at room temperature, poured over crushed ice and then extracted with dichloromethane (3 × 20 ml) and dried with sodium sulfate. The solvent was removed under vacuum. Then the crude product was recrystallized from methanol. Single crystals suitable for X-ray analysis were grown by slow evaporation of a methanol solution at room temperature.

Refinement

H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined using riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

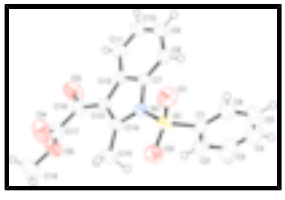

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

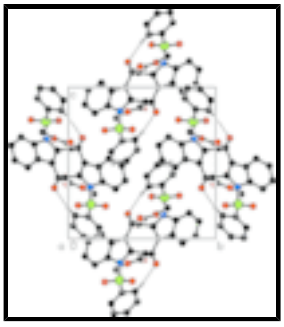

Fig. 2. A packing scheme of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Methyl (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)glyoxylate

Crystal data

$C_{18}H_{15}NO_5S$	F_{000} = 744
M_r = 357.37	D_x = 1.411 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8031 reflections
a = 9.7005 (3) Å	θ = 2.2–31.5º
b = 12.9924 (4) Å	μ = 0.22 mm^{-1}
c = 13.4224 (3) Å	T = 295 (2) K
β = 96.189 (1)º	Block, colourless
V = 1681.80 (8) Å^3	0.20 × 0.16 × 0.16 mm
Z = 4	

Data collection

Bruker Kappa APEX II diffractometer	5550 independent reflections
Radiation source: fine-focus sealed tube	4082 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 295(2) K	θ_{max} = 31.5º
ω and φ scans	θ_{min} = 2.2º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −14→14
T_{min} = 0.882, T_{max} = 0.966	k = −19→18
23482 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.3886P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
5550 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
227 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22348 (3)	0.15223 (3)	0.22741 (2)	0.03990 (10)
O1	0.27574 (12)	0.25315 (10)	0.21547 (9)	0.0561 (3)
O2	0.31128 (12)	0.06594 (11)	0.22066 (8)	0.0573 (3)
O3	0.07775 (17)	0.09577 (12)	0.66431 (10)	0.0759 (4)
O4	0.38110 (14)	0.01270 (13)	0.63615 (13)	0.0854 (5)
O5	0.21156 (14)	−0.09720 (10)	0.66195 (11)	0.0674 (4)
N1	0.16706 (12)	0.14918 (8)	0.34140 (8)	0.0370 (2)
C1	0.07180 (15)	0.13594 (11)	0.14580 (10)	0.0418 (3)
C6	0.0345 (2)	0.20882 (15)	0.07398 (16)	0.0675 (5)
H6	0.0864	0.2686	0.0701	0.081*
C5	−0.0825 (3)	0.1911 (2)	0.00724 (19)	0.0883 (7)
H5	−0.1091	0.2392	−0.0424	0.106*
C4	−0.1588 (2)	0.1040 (2)	0.01384 (19)	0.0791 (6)
H4	−0.2368	0.0930	−0.0315	0.095*
C3	−0.1220 (2)	0.03292 (19)	0.08598 (17)	0.0730 (6)
H3	−0.1757	−0.0259	0.0904	0.088*
C2	−0.00486 (19)	0.04757 (15)	0.15289 (13)	0.0579 (4)
H2	0.0216	−0.0014	0.2018	0.069*
C7	0.08779 (13)	0.23051 (10)	0.37651 (9)	0.0357 (3)
C8	0.03879 (17)	0.32027 (12)	0.32950 (11)	0.0460 (3)
H8	0.0549	0.3353	0.2640	0.055*
C9	−0.03507 (18)	0.38639 (13)	0.38433 (13)	0.0531 (4)
H9	−0.0692	0.4475	0.3552	0.064*
C10	−0.05955 (18)	0.36374 (13)	0.48191 (13)	0.0540 (4)
H10	−0.1101	0.4098	0.5166	0.065*
C11	−0.01053 (15)	0.27462 (12)	0.52831 (11)	0.0455 (3)
H11	−0.0275	0.2599	0.5937	0.055*
C12	0.06533 (13)	0.20672 (10)	0.47474 (10)	0.0357 (3)
C13	0.13518 (13)	0.11059 (10)	0.49999 (10)	0.0365 (3)
C14	0.19335 (13)	0.07571 (10)	0.41739 (10)	0.0363 (3)
C15	0.26489 (19)	−0.02360 (12)	0.40328 (13)	0.0532 (4)
H15A	0.3627	−0.0117	0.4041	0.080*
H15B	0.2295	−0.0533	0.3402	0.080*
H15C	0.2487	−0.0699	0.4565	0.080*
C16	0.14712 (16)	0.06658 (12)	0.59968 (11)	0.0452 (3)
C17	0.26169 (17)	−0.00983 (13)	0.63236 (11)	0.0493 (3)
C18	0.3109 (3)	−0.1732 (2)	0.7043 (2)	0.1025 (9)
H18A	0.2623	−0.2333	0.7232	0.154*
H18B	0.3641	−0.1449	0.7623	0.154*

H18C	0.3718	−0.1916	0.6554	0.154*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03642 (17)	0.0496 (2)	0.03534 (16)	−0.00086 (13)	0.01146 (12)	−0.00074 (13)
O1	0.0557 (6)	0.0625 (7)	0.0528 (6)	−0.0192 (5)	0.0178 (5)	0.0020 (5)
O2	0.0503 (6)	0.0744 (8)	0.0496 (6)	0.0197 (5)	0.0165 (5)	−0.0029 (5)
O3	0.0956 (10)	0.0845 (10)	0.0541 (7)	0.0276 (8)	0.0372 (7)	0.0252 (7)
O4	0.0485 (7)	0.0996 (12)	0.1047 (12)	−0.0061 (7)	−0.0072 (7)	0.0266 (9)
O5	0.0687 (8)	0.0525 (7)	0.0791 (9)	0.0015 (6)	−0.0009 (7)	0.0213 (6)
N1	0.0418 (6)	0.0379 (5)	0.0323 (5)	0.0055 (4)	0.0089 (4)	0.0006 (4)
C1	0.0414 (7)	0.0487 (7)	0.0360 (6)	0.0014 (6)	0.0077 (5)	−0.0040 (5)
C6	0.0771 (13)	0.0509 (9)	0.0697 (12)	0.0030 (9)	−0.0141 (10)	0.0070 (8)
C5	0.0920 (16)	0.0773 (14)	0.0865 (16)	0.0199 (13)	−0.0320 (13)	0.0062 (12)
C4	0.0535 (10)	0.0934 (16)	0.0852 (15)	0.0111 (11)	−0.0156 (10)	−0.0224 (13)
C3	0.0543 (10)	0.0954 (15)	0.0699 (12)	−0.0223 (10)	0.0094 (9)	−0.0153 (11)
C2	0.0584 (9)	0.0706 (11)	0.0453 (8)	−0.0178 (8)	0.0088 (7)	0.0030 (7)
C7	0.0355 (6)	0.0367 (6)	0.0355 (6)	0.0020 (5)	0.0062 (5)	−0.0005 (5)
C8	0.0529 (8)	0.0445 (7)	0.0411 (7)	0.0079 (6)	0.0073 (6)	0.0063 (6)
C9	0.0588 (9)	0.0451 (8)	0.0556 (9)	0.0163 (7)	0.0071 (7)	0.0045 (7)
C10	0.0546 (9)	0.0527 (9)	0.0565 (9)	0.0165 (7)	0.0137 (7)	−0.0065 (7)
C11	0.0449 (7)	0.0527 (8)	0.0408 (7)	0.0056 (6)	0.0131 (6)	−0.0030 (6)
C12	0.0340 (6)	0.0386 (6)	0.0351 (6)	−0.0002 (5)	0.0066 (5)	0.0001 (5)
C13	0.0364 (6)	0.0364 (6)	0.0373 (6)	−0.0019 (5)	0.0066 (5)	0.0028 (5)
C14	0.0359 (6)	0.0347 (6)	0.0385 (6)	−0.0001 (5)	0.0052 (5)	0.0010 (5)
C15	0.0637 (10)	0.0426 (8)	0.0547 (9)	0.0151 (7)	0.0125 (7)	0.0026 (6)
C16	0.0475 (7)	0.0473 (7)	0.0417 (7)	−0.0019 (6)	0.0092 (6)	0.0086 (6)
C17	0.0504 (8)	0.0546 (8)	0.0419 (7)	−0.0008 (7)	0.0000 (6)	0.0078 (6)
C18	0.118 (2)	0.0718 (14)	0.114 (2)	0.0262 (14)	−0.0091 (17)	0.0351 (14)

Geometric parameters (Å, °)

S1—O2	1.4167 (12)	C7—C8	1.3855 (19)
S1—O1	1.4211 (12)	C7—C12	1.3940 (17)
S1—N1	1.6800 (11)	C8—C9	1.381 (2)
S1—C1	1.7498 (15)	C8—H8	0.9300
O3—C16	1.2146 (19)	C9—C10	1.388 (2)
O4—C17	1.190 (2)	C9—H9	0.9300
O5—C17	1.313 (2)	C10—C11	1.375 (2)
O5—C18	1.452 (3)	C10—H10	0.9300
N1—C14	1.4001 (17)	C11—C12	1.3968 (18)
N1—C7	1.4171 (16)	C11—H11	0.9300
C1—C6	1.372 (2)	C12—C13	1.4437 (18)
C1—C2	1.377 (2)	C13—C14	1.3740 (18)
C6—C5	1.387 (3)	C13—C16	1.4482 (19)
C6—H6	0.9300	C14—C15	1.4868 (19)
C5—C4	1.361 (4)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600

C4—C3	1.357 (3)	C15—H15C	0.9600
C4—H4	0.9300	C16—C17	1.519 (2)
C3—C2	1.383 (3)	C18—H18A	0.9600
C3—H3	0.9300	C18—H18B	0.9600
C2—H2	0.9300	C18—H18C	0.9600
O2—S1—O1	119.91 (8)	C8—C9—H9	119.2
O2—S1—N1	107.26 (6)	C10—C9—H9	119.2
O1—S1—N1	106.24 (6)	C11—C10—C9	121.33 (14)
O2—S1—C1	109.57 (7)	C11—C10—H10	119.3
O1—S1—C1	109.09 (7)	C9—C10—H10	119.3
N1—S1—C1	103.46 (6)	C10—C11—C12	118.31 (13)
C17—O5—C18	117.05 (18)	C10—C11—H11	120.8
C14—N1—C7	109.20 (10)	C12—C11—H11	120.8
C14—N1—S1	128.90 (9)	C7—C12—C11	119.45 (12)
C7—N1—S1	121.80 (9)	C7—C12—C13	107.25 (11)
C6—C1—C2	121.38 (16)	C11—C12—C13	133.27 (12)
C6—C1—S1	119.78 (13)	C14—C13—C12	108.61 (11)
C2—C1—S1	118.79 (12)	C14—C13—C16	128.05 (13)
C1—C6—C5	118.3 (2)	C12—C13—C16	123.18 (12)
C1—C6—H6	120.8	C13—C14—N1	107.73 (11)
C5—C6—H6	120.8	C13—C14—C15	128.83 (12)
C4—C5—C6	120.6 (2)	N1—C14—C15	123.34 (12)
C4—C5—H5	119.7	C14—C15—H15A	109.5
C6—C5—H5	119.7	C14—C15—H15B	109.5
C3—C4—C5	120.62 (19)	H15A—C15—H15B	109.5
C3—C4—H4	119.7	C14—C15—H15C	109.5
C5—C4—H4	119.7	H15A—C15—H15C	109.5
C4—C3—C2	120.3 (2)	H15B—C15—H15C	109.5
C4—C3—H3	119.9	O3—C16—C13	122.78 (14)
C2—C3—H3	119.9	O3—C16—C17	116.24 (14)
C1—C2—C3	118.81 (18)	C13—C16—C17	120.53 (13)
C1—C2—H2	120.6	O4—C17—O5	126.15 (16)
C3—C2—H2	120.6	O4—C17—C16	121.99 (16)
C8—C7—C12	122.44 (12)	O5—C17—C16	111.65 (14)
C8—C7—N1	130.39 (12)	O5—C18—H18A	109.5
C12—C7—N1	107.16 (11)	O5—C18—H18B	109.5
C9—C8—C7	116.94 (14)	H18A—C18—H18B	109.5
C9—C8—H8	121.5	O5—C18—H18C	109.5
C7—C8—H8	121.5	H18A—C18—H18C	109.5
C8—C9—C10	121.51 (14)	H18B—C18—H18C	109.5
O2—S1—N1—C14	−2.26 (14)	C8—C7—C12—C11	0.7 (2)
O1—S1—N1—C14	−131.63 (12)	N1—C7—C12—C11	179.80 (12)
C1—S1—N1—C14	113.53 (13)	C8—C7—C12—C13	−177.69 (13)
O2—S1—N1—C7	173.58 (11)	N1—C7—C12—C13	1.38 (14)
O1—S1—N1—C7	44.21 (12)	C10—C11—C12—C7	−0.6 (2)
C1—S1—N1—C7	−70.63 (12)	C10—C11—C12—C13	177.32 (15)
O2—S1—C1—C6	−123.37 (15)	C7—C12—C13—C14	−2.33 (15)
O1—S1—C1—C6	9.72 (16)	C11—C12—C13—C14	179.56 (15)

N1—S1—C1—C6	122.50 (15)	C7—C12—C13—C16	173.39 (13)
O2—S1—C1—C2	54.13 (14)	C11—C12—C13—C16	−4.7 (2)
O1—S1—C1—C2	−172.79 (12)	C12—C13—C14—N1	2.31 (15)
N1—S1—C1—C2	−60.00 (13)	C16—C13—C14—N1	−173.13 (13)
C2—C1—C6—C5	−0.6 (3)	C12—C13—C14—C15	−174.14 (14)
S1—C1—C6—C5	176.80 (18)	C16—C13—C14—C15	10.4 (2)
C1—C6—C5—C4	0.6 (4)	C7—N1—C14—C13	−1.47 (15)
C6—C5—C4—C3	0.2 (4)	S1—N1—C14—C13	174.79 (10)
C5—C4—C3—C2	−1.0 (4)	C7—N1—C14—C15	175.23 (13)
C6—C1—C2—C3	−0.2 (3)	S1—N1—C14—C15	−8.5 (2)
S1—C1—C2—C3	−177.64 (14)	C14—C13—C16—O3	−170.51 (16)
C4—C3—C2—C1	1.0 (3)	C12—C13—C16—O3	14.6 (2)
C14—N1—C7—C8	178.98 (15)	C14—C13—C16—C17	17.5 (2)
S1—N1—C7—C8	2.4 (2)	C12—C13—C16—C17	−157.34 (14)
C14—N1—C7—C12	0.00 (15)	C18—O5—C17—O4	0.7 (3)
S1—N1—C7—C12	−176.57 (9)	C18—O5—C17—C16	−174.17 (19)
C12—C7—C8—C9	−0.3 (2)	O3—C16—C17—O4	−110.8 (2)
N1—C7—C8—C9	−179.13 (15)	C13—C16—C17—O4	61.7 (2)
C7—C8—C9—C10	−0.3 (3)	O3—C16—C17—O5	64.3 (2)
C8—C9—C10—C11	0.4 (3)	C13—C16—C17—O5	−123.17 (16)
C9—C10—C11—C12	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3^{i}	0.93	2.46	3.219 (2)	139
C15—H15A···O4^{ii}	0.96	2.60	3.533 (2)	164
C6—H6···O1	0.93	2.54	2.908 (2)	104
C8—H8···O1	0.93	2.54	3.024 (2)	113
C11—H11···O3	0.93	2.51	3.021 (2)	115
C15—H15B···O2	0.96	2.42	2.793 (2)	103
C4—H4···Cg3^{iii}	0.93	2.80	3.495 (2)	132
C5—H5···Cg1^{iii}	0.93	2.88	3.526 (3)	128

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

Fig. 1

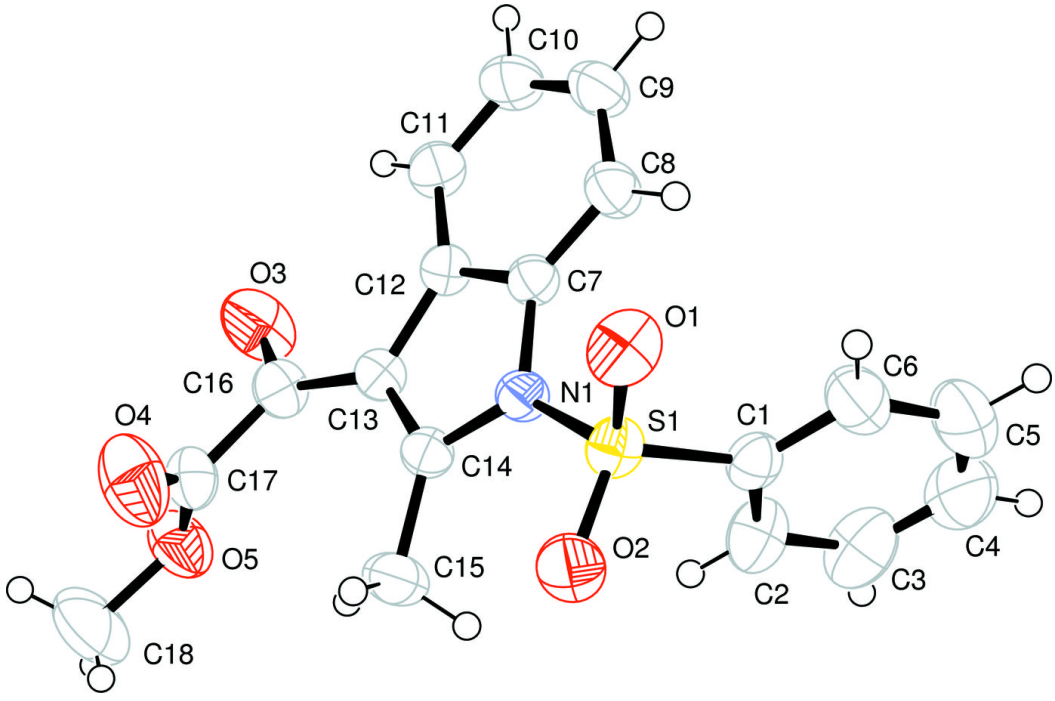
C10
C9
C11
C8
O3
C12
C7
O1
C16
N1
C6
O4
C13
S1
C1
C5
C17
C14
O2
C4
O5
C15
C2
C3
C18

Fig. 2