

1-(Phenylsulfonyl)benzo[1,2:2',3']-thieno[5',4'-b]carbazole

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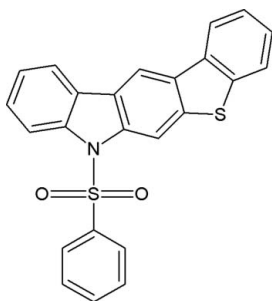
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.057; wR factor = 0.192; data-to-parameter ratio = 24.5.

In the title compound, $\text{C}_{24}\text{H}_{15}\text{NO}_2\text{S}_2$, the ring system composed of the five fused rings is almost planar (r.m.s. deviation for all non-H atoms = 0.056 Å). The dihedral angle between the fused ring system and the phenyl ring is 83.4 (9)°. The crystal packing is stabilized by C—H... π and π — π interactions between parallel ring systems [centroid—centroid distances = 3.526 (3), 3.877 (3) and 3.712 (3) Å].

Related literature

For related structures, see: Murugavel *et al.* (2009); Chakkaravarthi *et al.* (2008); Ravishankar *et al.* (2005).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{15}\text{NO}_2\text{S}_2$
 $M_r = 413.49$

Triclinic, $P\bar{1}$
 $a = 7.463$ (5) Å

$b = 10.462$ (5) Å
 $c = 12.335$ (5) Å
 $\alpha = 80.438$ (5)°
 $\beta = 89.433$ (5)°
 $\gamma = 81.876$ (5)°
 $V = 940.1$ (9) Å³

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.31$ mm⁻¹
 $T = 293$ K
 $0.25 \times 0.22 \times 0.19$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.981$, $T_{\max} = 0.985$

24843 measured reflections
6428 independent reflections
4863 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.192$
 $S = 1.01$
6428 reflections
262 parameters

3 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.98$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.62$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg6 is the centroid of the C19–C24 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15...Cg6 ⁱ	0.93	2.78	3.685 (4)	166

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

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: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

ST and ASP thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5204).

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supplementary materials

Acta Cryst. (2010). E66, o954 [doi:10.1107/S1600536810010044]

1-(Phenylsulfonyl)benzo[1,2:2',3']thieno[5',4'-b]carbazole

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Comment

Carbazole and its derivatives have become quite attractive compounds owing to their applications in pharmacy and molecular electronics.

In order to obtain detailed information on molecular conformations in the solid state, an X-ray study of the title compound was carried out.

The ring system composed of the five rings is almost planar (r.m.s. deviation for all non-H atoms 0.056 Å). The crystal packing is stabilized by C–H...O and C–H... π (Table. 1) hydrogen bonds. In addition, there are π – π interactions between the extended ring system with a mean distance between the ring planes of 3.7 Å.

Experimental

To a solution of diethyl-2-((2-(bromomethyl)-1-(phenylsulfonyl)-1*H*-indol-3-yl) methylene)malonate (0.3 g 0.57 mmol) in dry 1,2-DCE (10 ml), InBr₃ (0.02 g 0.06 mmol) and benzo[b]thiophene (0.09 g, 0.67 mmol) were added. The reaction mixture was stirred at room temperature for 4 h and then refluxed for 1 h under N₂ atmosphere. It was then poured over ice-water (30 ml) containing 1 ml of Conc.HCl, extracted with chloroform (2 X 10 ml) and dried (Na₂SO₄). The removal of solvent followed by flash column chromatographic purification (silica gel, 230-420 mesh, n-hexane/ethyl acetate 99:1) afforded the product as a colorless solid. The product was recrystallization from CDCl₃

Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C–H distances fixed in the range 0.93–0.97 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H 1.2 $U_{\text{eq}}(\text{C})$ for other H atoms.

Figures

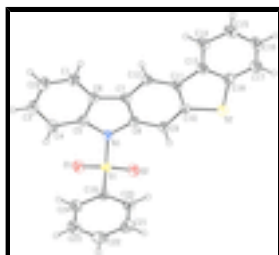


Fig. 1. The structure of showing the atom-numbering scheme and intramolecular hydrogen bond. Displacement ellipsoids are drawn at the 30% probability level.

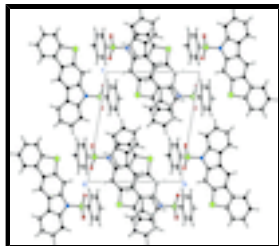


Fig. 2. The molecular packing viewed down the a axis.

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Crystal data

$C_{24}H_{15}NO_2S_2$

$M_r = 413.49$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.463 (5) \text{ \AA}$

$b = 10.462 (5) \text{ \AA}$

$c = 12.335 (5) \text{ \AA}$

$\alpha = 80.438 (5)^\circ$

$\beta = 89.433 (5)^\circ$

$\gamma = 81.876 (5)^\circ$

$V = 940.1 (9) \text{ \AA}^3$

$Z = 2$

$F(000) = 428$

$D_x = 1.461 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 6428 reflections

$\theta = 1.7\text{--}32.2^\circ$

$\mu = 0.31 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, white crystalline

$0.25 \times 0.22 \times 0.19 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

ω and φ scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.981$, $T_{\max} = 0.985$

24843 measured reflections

6428 independent reflections

4863 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 32.2^\circ$, $\theta_{\min} = 1.7^\circ$

$h = -11 \rightarrow 11$

$k = -15 \rightarrow 15$

$l = -18 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.192$

$S = 1.01$

6428 reflections

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

$w = 1/[\sigma^2(F_o^2) + (0.1079P)^2 + 0.4678P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

262 parameters

$$\Delta\rho_{\max} = 0.98 \text{ e } \text{\AA}^{-3}$$

3 restraints

$$\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8004 (3)	0.5479 (2)	0.66419 (19)	0.0477 (5)
H1	0.8537	0.4628	0.6910	0.057*
C2	0.7893 (3)	0.5939 (3)	0.5527 (2)	0.0538 (5)
H2	0.8355	0.5391	0.5038	0.065*
C3	0.7106 (3)	0.7203 (3)	0.51279 (18)	0.0517 (5)
H3	0.7050	0.7491	0.4372	0.062*
C4	0.6398 (3)	0.8051 (2)	0.58229 (17)	0.0456 (4)
H4	0.5878	0.8904	0.5550	0.055*
C5	0.6495 (3)	0.75792 (19)	0.69390 (15)	0.0367 (4)
C6	0.7303 (3)	0.63112 (18)	0.73581 (16)	0.0368 (4)
C7	0.7156 (2)	0.61248 (17)	0.85389 (15)	0.0347 (3)
C8	0.6261 (2)	0.72886 (17)	0.88294 (15)	0.0344 (3)
C9	0.5880 (3)	0.74249 (19)	0.99044 (16)	0.0394 (4)
H9	0.5291	0.8202	1.0089	0.047*
C10	0.6430 (3)	0.63321 (19)	1.06946 (15)	0.0380 (4)
C11	0.7341 (2)	0.51533 (18)	1.04347 (15)	0.0360 (4)
C12	0.7710 (3)	0.50503 (19)	0.93443 (16)	0.0388 (4)
H12	0.8314	0.4279	0.9158	0.047*
C13	0.7743 (3)	0.4149 (2)	1.13958 (16)	0.0402 (4)
C14	0.8661 (3)	0.2850 (2)	1.1441 (2)	0.0502 (5)
H14	0.9123	0.2541	1.0815	0.060*
C15	0.8825 (4)	0.2076 (2)	1.2471 (2)	0.0564 (5)
H15	0.9393	0.1215	1.2554	0.068*
C16	0.8114 (3)	0.2611 (3)	1.34032 (18)	0.0531 (5)
H16	0.8280	0.2079	1.4088	0.064*
C17	0.7254 (4)	0.3785 (3)	1.3365 (2)	0.0593 (6)
H17	0.6768	0.4077	1.3992	0.071*
C18	0.7093 (3)	0.4578 (2)	1.23556 (18)	0.0482 (5)
C19	0.6988 (3)	1.05404 (18)	0.76966 (16)	0.0378 (4)
C20	0.7881 (3)	1.0581 (2)	0.86625 (19)	0.0478 (5)

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H20	0.7459	1.0208	0.9336	0.057*
C21	0.9420 (3)	1.1189 (3)	0.8608 (2)	0.0579 (6)
H21	1.0036	1.1228	0.9250	0.070*
C22	1.0040 (4)	1.1735 (3)	0.7611 (3)	0.0606 (6)
H22	1.1082	1.2133	0.7581	0.073*
C23	0.9128 (4)	1.1697 (3)	0.6658 (2)	0.0648 (7)
H23	0.9549	1.2078	0.5987	0.078*
C24	0.7592 (3)	1.1098 (2)	0.6689 (2)	0.0517 (5)
H24	0.6974	1.1070	0.6044	0.062*
N1	0.5814 (2)	0.81927 (16)	0.78385 (13)	0.0385 (3)
O1	0.4119 (2)	1.01545 (15)	0.67159 (13)	0.0470 (3)
O2	0.4131 (2)	0.99247 (15)	0.87383 (13)	0.0461 (3)
S1	0.50484 (6)	0.97634 (4)	0.77433 (4)	0.03684 (13)
S2	0.60075 (9)	0.62317 (6)	1.20851 (5)	0.05295 (17)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0510 (11)	0.0457 (11)	0.0460 (11)	0.0000 (9)	0.0036 (9)	-0.0127 (9)
C2	0.0555 (13)	0.0620 (14)	0.0468 (12)	-0.0036 (10)	0.0082 (10)	-0.0223 (10)
C3	0.0546 (12)	0.0650 (14)	0.0358 (10)	-0.0087 (10)	0.0050 (9)	-0.0093 (9)
C4	0.0495 (11)	0.0495 (11)	0.0351 (9)	-0.0042 (9)	-0.0001 (8)	-0.0014 (8)
C5	0.0378 (9)	0.0393 (9)	0.0331 (8)	-0.0059 (7)	0.0009 (7)	-0.0055 (7)
C6	0.0359 (8)	0.0373 (9)	0.0375 (9)	-0.0053 (7)	0.0006 (7)	-0.0064 (7)
C7	0.0342 (8)	0.0341 (8)	0.0356 (8)	-0.0046 (6)	0.0002 (6)	-0.0053 (6)
C8	0.0366 (8)	0.0312 (8)	0.0346 (8)	-0.0055 (6)	0.0005 (6)	-0.0026 (6)
C9	0.0485 (10)	0.0346 (8)	0.0348 (9)	-0.0041 (7)	0.0029 (7)	-0.0070 (7)
C10	0.0439 (10)	0.0366 (9)	0.0348 (8)	-0.0096 (7)	0.0007 (7)	-0.0067 (7)
C11	0.0358 (8)	0.0364 (8)	0.0351 (8)	-0.0065 (7)	-0.0028 (7)	-0.0027 (6)
C12	0.0414 (9)	0.0351 (8)	0.0389 (9)	-0.0019 (7)	0.0001 (7)	-0.0065 (7)
C13	0.0391 (9)	0.0427 (8)	0.0385 (9)	-0.0114 (7)	-0.0037 (7)	-0.0006 (7)
C14	0.0469 (11)	0.0470 (9)	0.0523 (12)	-0.0071 (8)	-0.0063 (9)	0.0053 (9)
C15	0.0573 (13)	0.0452 (11)	0.0607 (12)	-0.0046 (10)	-0.0072 (10)	0.0071 (9)
C16	0.0505 (12)	0.0673 (12)	0.0383 (9)	-0.0205 (9)	-0.0106 (8)	0.0116 (8)
C17	0.0689 (15)	0.0661 (12)	0.0443 (11)	-0.0252 (10)	-0.0056 (11)	-0.0001 (10)
C18	0.0519 (12)	0.0587 (13)	0.0379 (10)	-0.0244 (10)	-0.0010 (8)	-0.0053 (9)
C19	0.0377 (9)	0.0340 (8)	0.0402 (9)	-0.0014 (7)	0.0009 (7)	-0.0051 (7)
C20	0.0466 (11)	0.0518 (12)	0.0438 (11)	-0.0014 (9)	-0.0003 (8)	-0.0093 (9)
C21	0.0500 (13)	0.0619 (14)	0.0647 (15)	-0.0057 (10)	-0.0092 (11)	-0.0199 (12)
C22	0.0475 (12)	0.0555 (14)	0.0813 (18)	-0.0152 (10)	0.0011 (12)	-0.0116 (12)
C23	0.0622 (15)	0.0656 (16)	0.0658 (16)	-0.0245 (13)	0.0082 (12)	0.0045 (12)
C24	0.0561 (13)	0.0546 (12)	0.0434 (11)	-0.0166 (10)	0.0006 (9)	0.0021 (9)
N1	0.0475 (9)	0.0335 (7)	0.0325 (7)	-0.0013 (6)	0.0013 (6)	-0.0033 (6)
O1	0.0434 (8)	0.0467 (8)	0.0464 (8)	0.0002 (6)	-0.0085 (6)	0.0007 (6)
O2	0.0452 (8)	0.0437 (8)	0.0460 (8)	0.0023 (6)	0.0109 (6)	-0.0060 (6)
S1	0.0362 (2)	0.0344 (2)	0.0371 (2)	-0.00038 (16)	0.00092 (17)	-0.00168 (16)
S2	0.0709 (4)	0.0497 (3)	0.0405 (3)	-0.0133 (3)	0.0044 (2)	-0.0102 (2)

Geometric parameters (Å, °)

C1—C2	1.379 (3)	C14—C15	1.386 (3)
C1—C6	1.389 (3)	C14—H14	0.9300
C1—H1	0.9300	C15—C16	1.426 (4)
C2—C3	1.381 (4)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.297 (4)
C3—C4	1.383 (3)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.372 (3)
C4—C5	1.382 (3)	C17—H17	0.9300
C4—H4	0.9300	C18—S2	1.783 (3)
C5—C6	1.394 (3)	C19—C20	1.381 (3)
C5—N1	1.427 (2)	C19—C24	1.382 (3)
C6—C7	1.442 (3)	C19—S1	1.753 (2)
C7—C12	1.388 (3)	C20—C21	1.385 (4)
C7—C8	1.403 (3)	C20—H20	0.9300
C8—C9	1.380 (3)	C21—C22	1.371 (4)
C8—N1	1.426 (2)	C21—H21	0.9300
C9—C10	1.389 (3)	C22—C23	1.373 (4)
C9—H9	0.9300	C22—H22	0.9300
C10—C11	1.406 (3)	C23—C24	1.380 (4)
C10—S2	1.729 (2)	C23—H23	0.9300
C11—C12	1.389 (3)	C24—H24	0.9300
C11—C13	1.450 (3)	N1—S1	1.6469 (18)
C12—H12	0.9300	O1—S1	1.4212 (16)
C13—C18	1.393 (3)	O2—S1	1.4223 (16)
C13—C14	1.425 (3)		
C2—C1—C6	118.7 (2)	C13—C14—H14	122.0
C2—C1—H1	120.6	C14—C15—C16	119.5 (2)
C6—C1—H1	120.6	C14—C15—H15	120.3
C1—C2—C3	120.7 (2)	C16—C15—H15	120.3
C1—C2—H2	119.6	C17—C16—C15	124.7 (2)
C3—C2—H2	119.6	C17—C16—H16	117.6
C2—C3—C4	121.7 (2)	C15—C16—H16	117.6
C2—C3—H3	119.1	C16—C17—C18	116.9 (3)
C4—C3—H3	119.1	C16—C17—H17	121.5
C5—C4—C3	117.2 (2)	C18—C17—H17	121.5
C5—C4—H4	121.4	C17—C18—C13	122.7 (3)
C3—C4—H4	121.4	C17—C18—S2	125.7 (2)
C4—C5—C6	121.90 (19)	C13—C18—S2	111.53 (16)
C4—C5—N1	129.92 (19)	C20—C19—C24	121.4 (2)
C6—C5—N1	108.16 (16)	C20—C19—S1	119.55 (16)
C1—C6—C5	119.68 (19)	C24—C19—S1	119.07 (17)
C1—C6—C7	132.31 (19)	C19—C20—C21	118.7 (2)
C5—C6—C7	107.97 (16)	C19—C20—H20	120.7
C12—C7—C8	120.30 (17)	C21—C20—H20	120.7
C12—C7—C6	131.54 (17)	C22—C21—C20	120.4 (2)
C8—C7—C6	108.15 (16)	C22—C21—H21	119.8

supplementary materials

C9—C8—C7	122.62 (17)	C20—C21—H21	119.8
C9—C8—N1	129.72 (17)	C21—C22—C23	120.3 (2)
C7—C8—N1	107.63 (16)	C21—C22—H22	119.9
C8—C9—C10	116.03 (18)	C23—C22—H22	119.9
C8—C9—H9	122.0	C22—C23—C24	120.5 (3)
C10—C9—H9	122.0	C22—C23—H23	119.7
C9—C10—C11	122.92 (18)	C24—C23—H23	119.7
C9—C10—S2	124.73 (16)	C23—C24—C19	118.7 (2)
C11—C10—S2	112.31 (14)	C23—C24—H24	120.6
C12—C11—C10	119.59 (17)	C19—C24—H24	120.6
C12—C11—C13	127.69 (18)	C8—N1—C5	108.07 (15)
C10—C11—C13	112.69 (18)	C8—N1—S1	126.27 (13)
C7—C12—C11	118.53 (17)	C5—N1—S1	124.47 (13)
C7—C12—H12	120.7	O1—S1—O2	120.28 (10)
C11—C12—H12	120.7	O1—S1—N1	106.82 (9)
C18—C13—C14	120.1 (2)	O2—S1—N1	106.80 (9)
C18—C13—C11	112.01 (19)	O1—S1—C19	108.43 (10)
C14—C13—C11	127.9 (2)	O2—S1—C19	108.38 (10)
C15—C14—C13	116.0 (2)	N1—S1—C19	105.12 (10)
C15—C14—H14	122.0	C10—S2—C18	91.45 (10)
C6—C1—C2—C3	0.1 (4)	C15—C16—C17—C18	-2.9 (4)
C1—C2—C3—C4	-0.1 (4)	C16—C17—C18—C13	2.7 (4)
C2—C3—C4—C5	-0.6 (4)	C16—C17—C18—S2	-179.09 (18)
C3—C4—C5—C6	1.3 (3)	C14—C13—C18—C17	-1.7 (3)
C3—C4—C5—N1	-176.6 (2)	C11—C13—C18—C17	177.6 (2)
C2—C1—C6—C5	0.5 (3)	C14—C13—C18—S2	179.82 (16)
C2—C1—C6—C7	177.8 (2)	C11—C13—C18—S2	-0.8 (2)
C4—C5—C6—C1	-1.3 (3)	C24—C19—C20—C21	-0.4 (3)
N1—C5—C6—C1	177.01 (18)	S1—C19—C20—C21	179.44 (18)
C4—C5—C6—C7	-179.18 (18)	C19—C20—C21—C22	-0.2 (4)
N1—C5—C6—C7	-0.9 (2)	C20—C21—C22—C23	0.7 (4)
C1—C6—C7—C12	1.5 (4)	C21—C22—C23—C24	-0.7 (5)
C5—C6—C7—C12	179.1 (2)	C22—C23—C24—C19	0.1 (4)
C1—C6—C7—C8	-177.7 (2)	C20—C19—C24—C23	0.4 (4)
C5—C6—C7—C8	-0.2 (2)	S1—C19—C24—C23	-179.4 (2)
C12—C7—C8—C9	-0.4 (3)	C9—C8—N1—C5	-179.31 (19)
C6—C7—C8—C9	178.97 (17)	C7—C8—N1—C5	-1.7 (2)
C12—C7—C8—N1	-178.20 (17)	C9—C8—N1—S1	12.8 (3)
C6—C7—C8—N1	1.1 (2)	C7—C8—N1—S1	-169.59 (14)
C7—C8—C9—C10	-0.3 (3)	C4—C5—N1—C8	179.7 (2)
N1—C8—C9—C10	176.99 (18)	C6—C5—N1—C8	1.6 (2)
C8—C9—C10—C11	0.8 (3)	C4—C5—N1—S1	-12.1 (3)
C8—C9—C10—S2	-176.55 (14)	C6—C5—N1—S1	169.78 (14)
C9—C10—C11—C12	-0.6 (3)	C8—N1—S1—O1	-156.86 (17)
S2—C10—C11—C12	177.07 (15)	C5—N1—S1—O1	37.10 (18)
C9—C10—C11—C13	-178.95 (18)	C8—N1—S1—O2	-27.0 (2)
S2—C10—C11—C13	-1.3 (2)	C5—N1—S1—O2	167.01 (16)
C8—C7—C12—C11	0.6 (3)	C8—N1—S1—C19	88.06 (18)
C6—C7—C12—C11	-178.54 (19)	C5—N1—S1—C19	-77.97 (17)

C10—C11—C12—C7	-0.2 (3)	C20—C19—S1—O1	164.32 (16)
C13—C11—C12—C7	177.95 (18)	C24—C19—S1—O1	-15.8 (2)
C12—C11—C13—C18	-176.85 (19)	C20—C19—S1—O2	32.19 (19)
C10—C11—C13—C18	1.4 (2)	C24—C19—S1—O2	-147.95 (18)
C12—C11—C13—C14	2.4 (3)	C20—C19—S1—N1	-81.72 (18)
C10—C11—C13—C14	-179.34 (19)	C24—C19—S1—N1	98.14 (19)
C18—C13—C14—C15	0.8 (3)	C9—C10—S2—C18	178.30 (19)
C11—C13—C14—C15	-178.4 (2)	C11—C10—S2—C18	0.71 (15)
C13—C14—C15—C16	-1.0 (3)	C17—C18—S2—C10	-178.3 (2)
C14—C15—C16—C17	2.2 (4)	C13—C18—S2—C10	0.08 (16)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg6 is the centroid of the C19–C24 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15 \cdots Cg6 ⁱ	0.93	2.78	3.685 (4)	166

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

Fig. 1

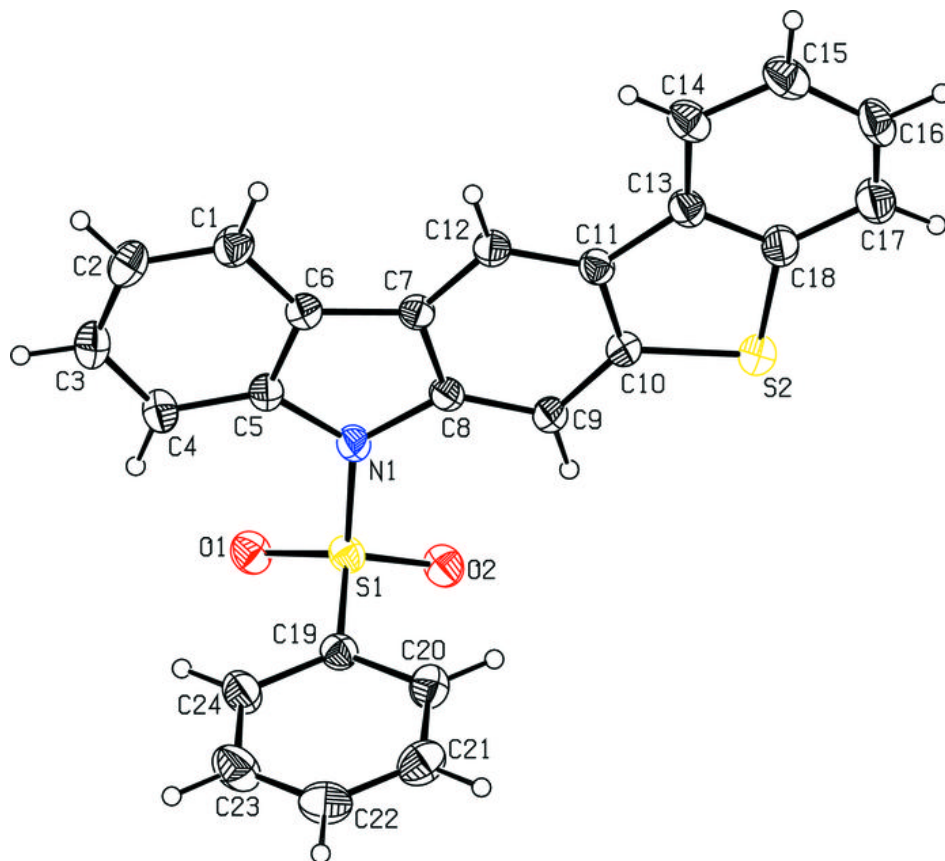


Fig. 2

