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(*S*)-1,1-Dimethyl-*N*-[(*S*)-1-phenyl-3-(phenylsulfonyl)but-3-enyl]ethane-2-sulfinamide

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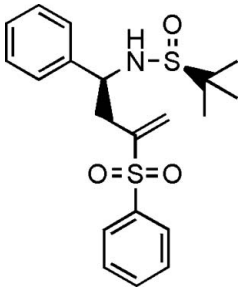
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.007 Å; R factor = 0.064; wR factor = 0.160; data-to-parameter ratio = 18.3.

The title compound, $C_{20}H_{25}NO_3S_2$, was obtained by the reaction of (*S*)-2-methyl-*N*-[(*S*)-1-phenyl-3-(phenylthio)but-3-enyl]propane-2-sulfinamide with 3-chloroperoxybenzoic acid (mCPBA) in dichloromethane solution. The absolute configuration was assigned by reference to the unchanging chiral centre in the synthetic procedure. The dihedral angle between the two benzene rings is 73.3 (2)°. The molecular conformation is likely influenced in part by intramolecular C—H···O hydrogen bonds, while the crystal packing is stabilized by intermolecular N—H···O hydrogen bonds and C—H···π interactions.

Related literature

For biological and pharmaceutical activities of sulfone derivatives, see: Reddy & Padmaja (1994); Tokio *et al.* (1993); Yasuo *et al.* (1993); Vedula *et al.* (2003). Many derivatives of these compounds have been prepared by: Carr *et al.* (1983); Xu *et al.* (2003). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{25}NO_3S_2$
M_r = 391.53
Orthorhombic, $P2_12_12_1$
a = 10.6163 (13) Å
b = 10.9054 (13) Å
c = 17.542 (2) Å
V = 2030.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 297 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
12058 measured reflections
4417 independent reflections
2616 reflections with $I > 2\sigma(I)$
R_{int} = 0.128

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.160
S = 0.94
4417 reflections
241 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Absolute structure: Flack (1983), with 1895 Friedel pairs
Flack parameter: 0.15 (13)

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

Cg is the centroid of the ring C11–C16.

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18*C*···O3	0.96	2.45	2.946 (6)	112
C10—H10···O2	0.98	2.38	3.131 (5)	133
N1—H1···O1^{i}	0.84 (2)	2.50 (2)	3.338 (4)	175 (4)
C18—H18*A*···*Cg*^{ii}	0.96	2.75 (1)	3.700	172

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (ii) $-x+\frac{3}{2}, -y+2, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2512).

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supplementary materials

Acta Cryst. (2007). E**63**, o4221 [**doi:10.1107/S160053680704737X**]

(*S*)-1,1-Dimethyl-*N*-[(*S*)-1-phenyl-3-(phenylsulfonyl)but-3-enyl]ethane-2-sulfinamide

D. Zhan, Z.-A. Xiao, H.-J. Liu and X.-P. Shi

Comment

Sulphone derivatives are important compounds with versatile biological and pharmacological activities (Reddy & Padmaja, 1994; Tokio *et al.*, 1993; Yasuo *et al.*, 1993; Vedula *et al.*, 2003). In this paper, we report the crystal structure of the title compound (I) (Fig. 1).

In (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The molecules are stabilized by intra and intermolecular hydrogen bonds (Table 1). Further stability is provided by C–H···π hydrogen bonds stacking interactions [C18–H18A···Cg^{ii} = 2.75 (1) Å; symmetry code: (ii) 3/2 − *x*, 2 − *y*, 1/2 + *z*]. *Cg* is the centroid defined by ring atoms C11–C16.

Experimental

To a precooled solution of anhydrous (*S*)-2-methyl-*N*-((*S*)-1-phenyl-3-(phenylthio) but-3-enyl)propane-2-sulfinamide (196 mg, 0.5 mmol) in anhydrous CH_2Cl_2 (5 ml) at 273 K, was added dropwise a solution of mCPBA (238 mg, 1.1 mmol) in CH_2Cl_2 (5 ml). After stirring for 2 h, the reaction solution was washed with saturated aqueous $NaHCO_3$ (5 ml), brine (5 ml), dried over anhydrous $MgSO_4$. After this solution was concentrated, the residue was purified by flash column chromatography to give the titled compound as a white solid with 51% yield. Colourless crystals suitable for X-ray structure analysis were grown from a mixture of dichloromethane and petroleum ether (*v*/*v*, 1:8).

Refinement

All H atoms bonded to carbon atoms were located at the geometrical positions with C—H = 0.93 Å (aromatic and CH_2═), 0.97 Å (methylene), 0.98 Å (methine) and U_{iso}(H) = 1.5U_{eq}(methyl C) and 1.2U_{eq}(other C atoms). H atom boned to N atom was located on the difference fourier map with constraint of N—H = 0.86 (2) Å and U_{iso}(H) = 1.2U_{eq}(N).

Figures

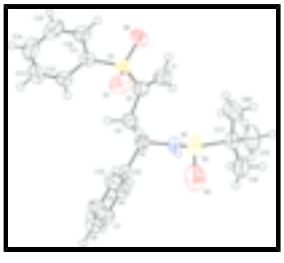

Fig. 1. The molecular structure showing 50% probability displacement ellipsoids and the atom-numbering scheme.

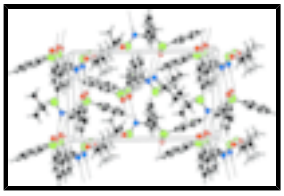

Fig. 2. The crystal packing with hydrogen bonds drawn as dashed lines.

(*S*)-1,1-Dimethyl-*N*-[(*S*)-1-phenyl-3-(phenylsulfonyl)but-3-enyl]ethane-2- sulfinamide

Crystal data

$C_{20}H_{25}NO_3S_2$	F_{000} = 832
M_r = 391.53	D_x = 1.281 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2471 reflections
a = 10.6163 (13) Å	θ = 2.2–24.7º
b = 10.9054 (13) Å	μ = 0.28 mm^{-1}
c = 17.542 (2) Å	T = 297 (2) K
V = 2030.9 (4) Å^3	Block, colourless
Z = 4	0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer	2616 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.128
Monochromator: graphite	θ_{max} = 27.0º
T = 297(2) K	θ_{min} = 2.2º
φ and ω scans	h = −13→12
Absorption correction: none	k = −13→13
12058 measured reflections	l = −20→22
4417 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.064	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.160	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.94	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
4417 reflections	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
241 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 1895 Friedel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0.15 (13)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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_{iso}*/U_{eq}
C1	0.9030 (4)	0.6805 (3)	0.7868 (2)	0.0437 (9)
C2	0.8699 (4)	0.5702 (4)	0.7540 (3)	0.0586 (12)
H2	0.8782	0.4976	0.7814	0.070*
C3	0.8245 (5)	0.5681 (5)	0.6809 (3)	0.0758 (15)
H3	0.8017	0.4938	0.6589	0.091*
C4	0.8125 (5)	0.6738 (7)	0.6398 (3)	0.0829 (16)
H4	0.7807	0.6716	0.5905	0.099*
C5	0.8472 (6)	0.7822 (5)	0.6716 (3)	0.0810 (17)
H5	0.8394	0.8540	0.6433	0.097*
C6	0.8932 (5)	0.7877 (4)	0.7439 (3)	0.0604 (13)
H6	0.9180	0.8625	0.7645	0.072*
C7	0.8233 (4)	0.7089 (3)	0.9361 (2)	0.0462 (10)
C8	0.7855 (5)	0.6186 (4)	0.9794 (3)	0.0631 (13)
H8A	0.7142	0.6279	1.0097	0.076*
H8B	0.8297	0.5450	0.9798	0.076*
C9	0.7585 (4)	0.8328 (3)	0.9309 (2)	0.0474 (10)
H9A	0.6722	0.8248	0.9485	0.057*
H9B	0.7563	0.8589	0.8780	0.057*
C10	0.8261 (4)	0.9309 (3)	0.9788 (2)	0.0422 (9)
H10	0.9155	0.9279	0.9651	0.051*
C11	0.7782 (4)	1.0606 (3)	0.9587 (2)	0.0437 (9)
C12	0.8640 (4)	1.1477 (4)	0.9383 (3)	0.0566 (12)
H12	0.9493	1.1285	0.9372	0.068*
C13	0.8241 (5)	1.2649 (4)	0.9192 (3)	0.0687 (14)
H13	0.8831	1.3241	0.9058	0.082*
C14	0.7019 (6)	1.2932 (4)	0.9199 (3)	0.0654 (13)
H14	0.6767	1.3719	0.9064	0.078*
C15	0.6126 (5)	1.2080 (4)	0.9404 (3)	0.0634 (13)
H15	0.5274	1.2280	0.9409	0.076*
C16	0.6531 (4)	1.0904 (4)	0.9605 (2)	0.0551 (11)

H16	0.5943	1.0318	0.9753	0.066*
N1	0.8170 (3)	0.9009 (3)	1.05940 (18)	0.0425 (8)
H1	0.741 (2)	0.904 (3)	1.071 (2)	0.051*
O1	1.0118 (3)	0.5697 (3)	0.8986 (2)	0.0749 (10)
O2	1.0366 (3)	0.7933 (3)	0.8876 (2)	0.0715 (9)
O3	0.9446 (4)	1.0631 (3)	1.1351 (2)	0.1109 (15)
S1	0.94171 (11)	0.93283 (11)	1.11069 (7)	0.0615 (3)
S2	0.95831 (10)	0.68636 (9)	0.87966 (6)	0.0514 (3)
C17	0.9056 (4)	0.8466 (4)	1.1971 (2)	0.0801 (11)
C18	0.7938 (5)	0.9044 (5)	1.2358 (3)	0.0844 (17)
H18A	0.7877	0.8744	1.2871	0.127*
H18B	0.7184	0.8838	1.2084	0.127*
H18C	0.8039	0.9918	1.2366	0.127*
C20	1.0229 (5)	0.8582 (5)	1.2455 (3)	0.0893 (18)
H20A	1.0362	0.9428	1.2583	0.134*
H20B	1.0942	0.8280	1.2175	0.134*
H20C	1.0127	0.8111	1.2913	0.134*
C19	0.8826 (7)	0.7138 (4)	1.1777 (4)	0.107 (2)
H19A	0.8730	0.6674	1.2238	0.161*
H19B	0.9528	0.6825	1.1492	0.161*
H19C	0.8073	0.7069	1.1477	0.161*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.043 (2)	0.033 (2)	0.055 (3)	0.0036 (18)	0.0026 (18)	−0.0003 (19)
C2	0.071 (3)	0.047 (3)	0.058 (3)	0.001 (2)	0.006 (2)	−0.001 (2)
C3	0.089 (4)	0.077 (4)	0.062 (3)	−0.016 (3)	0.013 (3)	−0.024 (3)
C4	0.089 (4)	0.113 (5)	0.047 (3)	0.002 (4)	0.014 (3)	0.007 (3)
C5	0.108 (5)	0.082 (4)	0.054 (3)	0.019 (4)	0.012 (3)	0.023 (3)
C6	0.083 (4)	0.042 (2)	0.055 (3)	0.008 (2)	0.009 (3)	0.004 (2)
C7	0.052 (3)	0.041 (2)	0.046 (2)	−0.0037 (19)	−0.001 (2)	−0.0018 (18)
C8	0.081 (3)	0.051 (3)	0.057 (3)	−0.006 (2)	0.006 (3)	−0.004 (2)
C9	0.047 (2)	0.050 (2)	0.045 (2)	0.0050 (19)	−0.0056 (19)	−0.0012 (19)
C10	0.040 (2)	0.045 (2)	0.041 (2)	0.0017 (19)	0.0014 (18)	0.0030 (19)
C11	0.054 (3)	0.040 (2)	0.036 (2)	0.008 (2)	−0.0014 (19)	0.0009 (17)
C12	0.058 (3)	0.050 (3)	0.062 (3)	0.004 (2)	0.002 (2)	0.005 (2)
C13	0.082 (4)	0.043 (3)	0.082 (4)	−0.006 (2)	−0.010 (3)	0.007 (2)
C14	0.097 (4)	0.044 (3)	0.056 (3)	0.011 (3)	−0.004 (3)	0.000 (2)
C15	0.066 (3)	0.070 (3)	0.055 (3)	0.025 (3)	0.005 (2)	−0.003 (2)
C16	0.061 (3)	0.053 (3)	0.051 (3)	0.005 (2)	0.007 (2)	0.008 (2)
N1	0.0432 (19)	0.0498 (19)	0.0346 (18)	−0.0031 (16)	−0.0004 (16)	0.0060 (14)
O1	0.080 (2)	0.073 (2)	0.071 (2)	0.0374 (17)	−0.0090 (18)	0.0142 (18)
O2	0.0460 (17)	0.075 (2)	0.093 (3)	−0.0138 (17)	0.002 (2)	−0.0218 (18)
O3	0.181 (4)	0.067 (2)	0.085 (3)	−0.069 (3)	−0.032 (3)	0.0103 (19)
S1	0.0537 (7)	0.0810 (8)	0.0498 (7)	−0.0187 (6)	−0.0049 (6)	0.0108 (6)
S2	0.0456 (6)	0.0504 (6)	0.0584 (7)	0.0097 (5)	−0.0038 (6)	−0.0031 (5)
C17	0.082 (3)	0.094 (3)	0.054 (3)	−0.006 (2)	−0.005 (2)	0.0161 (19)

C18	0.087 (4)	0.117 (4)	0.050 (3)	0.023 (3)	0.008 (3)	0.017 (3)
C20	0.072 (4)	0.132 (5)	0.064 (4)	−0.015 (3)	−0.023 (3)	0.025 (3)
C19	0.182 (7)	0.052 (3)	0.088 (5)	−0.005 (4)	−0.029 (5)	0.013 (3)

Geometric parameters (Å, °)

C1—C2	1.379 (6)	C12—H12	0.9300
C1—C6	1.395 (6)	C13—C14	1.334 (7)
C1—S2	1.732 (4)	C13—H13	0.9300
C2—C3	1.371 (7)	C14—C15	1.376 (7)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.365 (8)	C15—C16	1.397 (6)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.357 (7)	C16—H16	0.9300
C4—H4	0.9300	N1—S1	1.638 (3)
C5—C6	1.361 (7)	N1—H1	0.840 (19)
C5—H5	0.9300	O1—S2	1.433 (3)
C6—H6	0.9300	O2—S2	1.439 (3)
C7—C8	1.307 (6)	O3—S1	1.484 (4)
C7—C9	1.519 (5)	S1—C17	1.824 (4)
C7—S2	1.759 (4)	C17—C18	1.506 (6)
C8—H8A	0.9300	C17—C19	1.508 (6)
C8—H8B	0.9300	C17—C20	1.513 (6)
C9—C10	1.538 (5)	C18—H18A	0.9600
C9—H9A	0.9700	C18—H18B	0.9600
C9—H9B	0.9700	C18—H18C	0.9600
C10—N1	1.455 (5)	C20—H20A	0.9600
C10—C11	1.543 (5)	C20—H20B	0.9600
C10—H10	0.9800	C20—H20C	0.9600
C11—C12	1.364 (5)	C19—H19A	0.9600
C11—C16	1.368 (6)	C19—H19B	0.9600
C12—C13	1.388 (6)	C19—H19C	0.9600
C2—C1—C6	119.1 (4)	C13—C14—C15	121.1 (4)
C2—C1—S2	120.7 (3)	C13—C14—H14	119.4
C6—C1—S2	120.2 (3)	C15—C14—H14	119.4
C3—C2—C1	119.6 (4)	C14—C15—C16	118.2 (4)
C3—C2—H2	120.2	C14—C15—H15	120.9
C1—C2—H2	120.2	C16—C15—H15	120.9
C4—C3—C2	120.9 (5)	C11—C16—C15	120.8 (4)
C4—C3—H3	119.6	C11—C16—H16	119.6
C2—C3—H3	119.6	C15—C16—H16	119.6
C5—C4—C3	119.6 (5)	C10—N1—S1	115.6 (3)
C5—C4—H4	120.2	C10—N1—H1	108 (3)
C3—C4—H4	120.2	S1—N1—H1	129 (3)
C4—C5—C6	121.2 (5)	O3—S1—N1	112.3 (2)
C4—C5—H5	119.4	O3—S1—C17	104.9 (2)
C6—C5—H5	119.4	N1—S1—C17	100.20 (18)
C5—C6—C1	119.6 (4)	O1—S2—O2	117.9 (2)
C5—C6—H6	120.2	O1—S2—C1	108.7 (2)

C1—C6—H6	120.2	O2—S2—C1	108.5 (2)
C8—C7—C9	124.5 (4)	O1—S2—C7	108.5 (2)
C8—C7—S2	118.2 (3)	O2—S2—C7	107.59 (19)
C9—C7—S2	117.4 (3)	C1—S2—C7	104.95 (19)
C7—C8—H8A	120.0	C18—C17—C19	112.1 (5)
C7—C8—H8B	120.0	C18—C17—C20	111.1 (4)
H8A—C8—H8B	120.0	C19—C17—C20	109.9 (4)
C7—C9—C10	112.0 (3)	C18—C17—S1	108.9 (3)
C7—C9—H9A	109.2	C19—C17—S1	110.0 (4)
C10—C9—H9A	109.2	C20—C17—S1	104.5 (3)
C7—C9—H9B	109.2	C17—C18—H18A	109.5
C10—C9—H9B	109.2	C17—C18—H18B	109.5
H9A—C9—H9B	107.9	H18A—C18—H18B	109.5
N1—C10—C9	110.1 (3)	C17—C18—H18C	109.5
N1—C10—C11	114.0 (3)	H18A—C18—H18C	109.5
C9—C10—C11	111.0 (3)	H18B—C18—H18C	109.5
N1—C10—H10	107.1	C17—C20—H20A	109.5
C9—C10—H10	107.1	C17—C20—H20B	109.5
C11—C10—H10	107.1	H20A—C20—H20B	109.5
C12—C11—C16	119.2 (4)	C17—C20—H20C	109.5
C12—C11—C10	118.5 (4)	H20A—C20—H20C	109.5
C16—C11—C10	122.2 (4)	H20B—C20—H20C	109.5
C11—C12—C13	120.1 (4)	C17—C19—H19A	109.5
C11—C12—H12	119.9	C17—C19—H19B	109.5
C13—C12—H12	119.9	H19A—C19—H19B	109.5
C14—C13—C12	120.5 (5)	C17—C19—H19C	109.5
C14—C13—H13	119.8	H19A—C19—H19C	109.5
C12—C13—H13	119.8	H19B—C19—H19C	109.5
C6—C1—C2—C3	−1.9 (6)	C14—C15—C16—C11	−1.0 (7)
S2—C1—C2—C3	179.0 (4)	C9—C10—N1—S1	143.0 (3)
C1—C2—C3—C4	0.4 (8)	C11—C10—N1—S1	−91.5 (4)
C2—C3—C4—C5	0.7 (8)	C10—N1—S1—O3	83.1 (3)
C3—C4—C5—C6	−0.4 (9)	C10—N1—S1—C17	−166.0 (3)
C4—C5—C6—C1	−1.1 (8)	C2—C1—S2—O1	24.7 (4)
C2—C1—C6—C5	2.3 (7)	C6—C1—S2—O1	−154.4 (3)
S2—C1—C6—C5	−178.7 (4)	C2—C1—S2—O2	154.0 (3)
C8—C7—C9—C10	100.5 (5)	C6—C1—S2—O2	−25.0 (4)
S2—C7—C9—C10	−79.7 (4)	C2—C1—S2—C7	−91.2 (4)
C7—C9—C10—N1	−65.8 (4)	C6—C1—S2—C7	89.8 (4)
C7—C9—C10—C11	167.1 (3)	C8—C7—S2—O1	−6.0 (4)
N1—C10—C11—C12	109.1 (4)	C9—C7—S2—O1	174.2 (3)
C9—C10—C11—C12	−125.9 (4)	C8—C7—S2—O2	−134.6 (4)
N1—C10—C11—C16	−71.2 (5)	C9—C7—S2—O2	45.6 (3)
C9—C10—C11—C16	53.8 (5)	C8—C7—S2—C1	110.0 (4)
C16—C11—C12—C13	−0.4 (6)	C9—C7—S2—C1	−69.8 (3)
C10—C11—C12—C13	179.4 (4)	O3—S1—C17—C18	49.1 (4)
C11—C12—C13—C14	−0.6 (8)	N1—S1—C17—C18	−67.4 (4)
C12—C13—C14—C15	0.8 (8)	O3—S1—C17—C19	172.3 (4)
C13—C14—C15—C16	0.0 (7)	N1—S1—C17—C19	55.8 (4)

C12—C11—C16—C15	1.2 (6)	O3—S1—C17—C20	−69.7 (4)
C10—C11—C16—C15	−178.6 (4)	N1—S1—C17—C20	173.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18C···O3	0.96	2.45	2.946 (6)	112
C10—H10···O2	0.98	2.38	3.131 (5)	133
N1—H1···O1^{i}	0.84 (2)	2.50 (2)	3.338 (4)	175 (4)
C18—H18A···Cg^{ii}	0.96	2.75 (1)	3.700	172

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+2; (ii) −*x*+3/2, −*y*+2, *z*+1/2.

Fig. 1

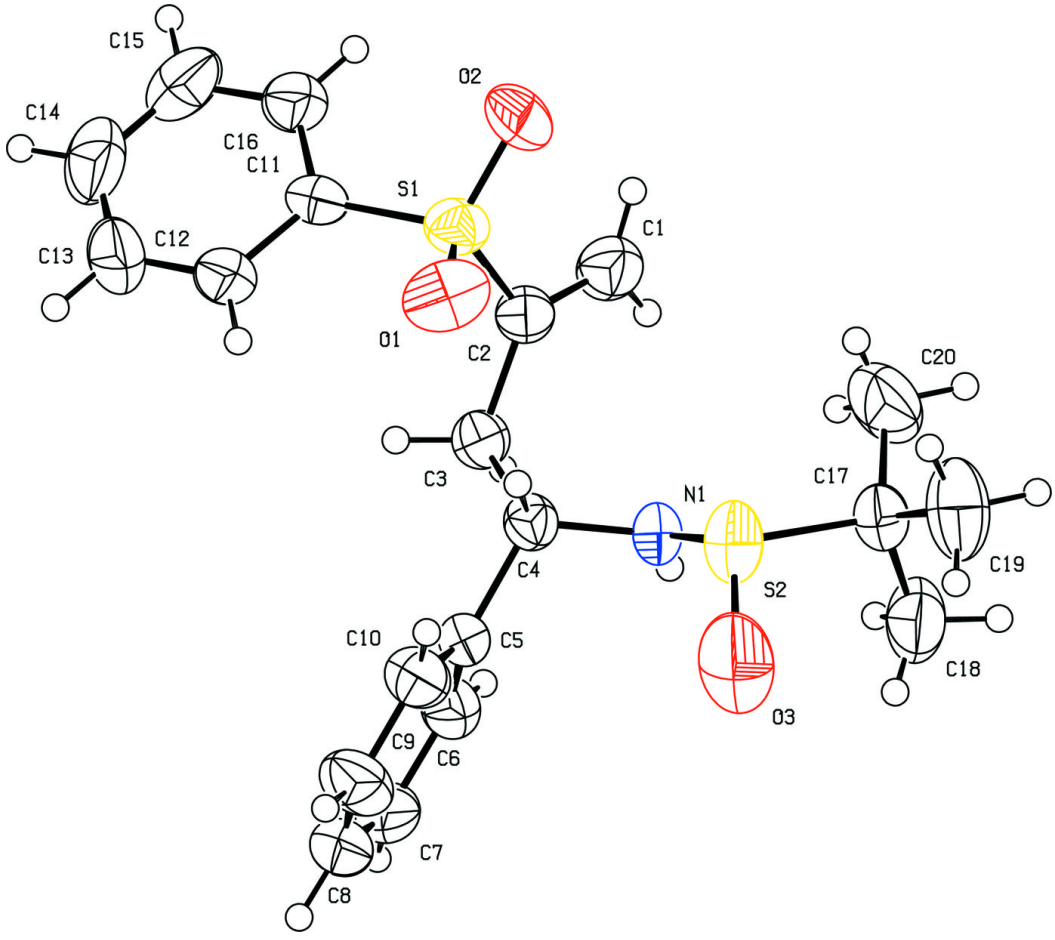
C15
C14
C16
C11
O2
S1
C1
C12
C13
O1
C2
C20
C3
C17
N1
C4
S2
C19
C10
C5
C18
O3
C9
C6
C7
C8

Fig. 2