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(*S*)-*N*-(Phenylsulfanyl-[1,2-$^{13}C_2$]-acetyl)-2,10-camphorsultam

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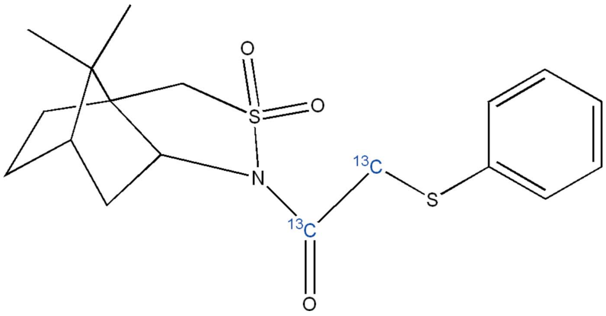
Key indicators: single-crystal X-ray study; *T* = 100 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.022; *wR* factor = 0.057; data-to-parameter ratio = 21.7.

The title compound, $C_{18}H_{23}NO_3S_2$, is used as a starting material for the synthesis of thiooxamates. The NMR spectrum was very complicated to interpret as a result of chirality of the sultam unit and the fact that the two C atoms of an acetyl group are labelled isotope ^{13}C atoms. The camphorsultam group imposes chirality on the (*S*)-phenyl acetyl group when extended at the acidic position by substitution. The molecules in the crystal are arranged in a head-to-tail orientation with a specific packing promoted by the bulky camphorsultam group.

Related literature

Structures similar to the structure of the title compound with bulky substituents at the acidic position have been previously reported (Ma *et al.*, 2005; Zhang *et al.*, 2002).

For related literature, see: Asani *et al.* (2007); Miyabe *et al.* (2000); Stocking *et al.* (2001); Tsai *et al.* (1994).



Experimental

Crystal data

$C_{18}H_{23}NO_3S_2$
M_r = 365.51
Orthorhombic, $P2_12_12_1$
a = 7.7413 (16) Å
b = 14.370 (3) Å
c = 15.951 (3) Å
V = 1774.4 (6) Å^3
Z = 4
Mo *Kα* radiation
μ = 0.32 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.902, T_{max} = 0.969
25461 measured reflections
4705 independent reflections
4640 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.057
S = 1.01
4705 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 2914 Friedel pairs
Flack parameter: −0.01 (4)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2019).

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supplementary materials

Acta Cryst. (2007). E**63**, o3450 [**doi:10.1107/S1600536807031935**]

(*S*)-*N*-(Phenylsulfanyl-[1,2-$^{13}C_2$]-acetyl)-2,10-camphorsultam

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Comment

The camphorsultam is widely used for the synthesis of chiral species that have significant biological and pharmaceutical applications. Most of the studies involving the use of the sultam have been done in the pharmaceutical sector. For instance, glyoxylic oxime ether has been attached to the camphorsultam and D–Valine was obtained after extension and hydrolysis on the sultam (Miyabe *et al.*, 2000). Stocking *et al.* (2001) synthesized L–[5–^{13}C,5–2H_3]–isoleucine through a series of reactions beginning with the addition of a methacrylate to the sultam. Tsai *et al.* (1994) synthesized optically active β–thioesters by treating the sultam with a methacrylate followed by a selective Michael addition of a thiol in a reaction promoted by LiOH. Therefore, title compound (3) (see Scheme 1) could be used to synthesize oxamate as illustrated in our first paper (Asani *et al.*, 2007), which could be reduced at the carbonyl to give the chiral alcohol.

The molecular structure of (3) together with its atomic numbering scheme is shown in Fig.1. The structure of (3) reveals two main planar fragments, namely: S2/C1—C6 (A) with mean deviation 0.0076 (8)Å and O3/N1/C7/C8 (B) with mean deviation 0.0131 (5) Å, while the rest of the molecule is basically non–planar. Dihedral angle between planes A and B is 41.10 (4)°. The C10—N1—S1 bond angle is 112.64 (7)° similar to that found in *N*-((2*S*)-2-(2-chlorophenylsulfanyl)-2-methylpenta-3,4-dienoyl)-2, 10-camphorsultam (111.23°; Ma *et al.*, 2005), *N*-((2*R*)-(phenylthio)-2-allyl- 2-phenylacetyl)-(1*S*)-camphorsultam (109.16°; Zhang *et al.*, 2002), and (1*S*)- *N*-((2*S*)-2-(2-chlorophenylsulfanyl)-2-methylpent-4-enoyl)-2,10-camphorsultam (105.42°; Ma *et al.*, 2005). However the N1—C8—C7 bond angle is 117.56 (9)° smaller than that found in these publications. The differences could be accounted for the presence of two bulky substituents at C7 atom responsible for the increase in the N1—C8—C7 bond angle in these publications. The C1—S2—C7 bond angle (103.26 (5)°) is very similar to that found in *N*-((2*R*)-(phenylthio)-2-allyl-2-phenylacetyl)-(1*S*)-camphorsultam (102.23°; Zhang *et al.*, 2002).

Experimental

The 1H and ^{13}C NMR spectra were recorded on a Bruker AC 300 s pectrometer using TMS as internal reference and $CDCl_3$ as solvent. The melting point was recorded using an Electrothermal Melt-Temp 3.0 single-crystal melting point apparatus.

(1*R*)–(+)–2,10–Camphorsultam (6.5 g, 301 mmol, 1.05 equivalent) was dissolved into anhydrous acetonitrile (66 ml) in a 500 ml round bottom flask set in a heating mantle equipped with a stir bar and a reflux condenser. The reflux condenser was attached to a recirculating chiller set to 268 K. 2–Thiophenyl–acetyl chloride (5.4 g, 28.6 mmol, 1 eq) was added by syringe in a single portion and the reaction mixture was heated to 354 K while stirring (Sheme 1). After 36 h, the reaction mixture was cooled to a room temperature and volatiles were removed by rotary evaporator. The resulting oil was partitioned between dichloromethane (50 ml) and water (50 ml). The layers were separated, the organic layer was filtered through cotton, and the volatiles removed by rotary evaporator followed by hi–vac to yield a tan oil which was recrystallized from an ether/hexanes 1:1 mixture to give colorless crystals of the product suitable for *X*–ray analysis (10.5 g, 99.9%), which had a melting point range of 350–353 K. ^{1}H NMR ($CDCl_3$, 300 MHz): 0.96 (s, 3H), 1.11 (s, 3H), 1.43–1.28 (m, 2H), 2.05–1.85

(m, 5H), 3.48 (dd, 2H, J = 21.70, J = 13.98 Hz), 3.98 (t, 1H, J = 6.44 Hz), 4.11 (dd, 2H, J = 71.52, J = 16.00 Hz), 7.30–7.17 (m, 3H), 7.41 (d, 2H, J = 12.14 Hz). ^{13}C NMR ($CDCl_3$, 75 MHz): 20.0, 20.9, 26.6, 32.9, 38.1, 38.3, 44.8, 48.0, 48.9, 53.0, 65.5, 127.1, 129.2, 130.3, 134.9, and 167.4

Refinement

All H atoms, were geometrically placed (C—H = 0.950 Å to 1.000 Å at 100 K) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C), except H atoms on methyl groups that were geometrically placed (0.990Å at 100 K) and refined as riding with U_{iso}(H) = 1.5U_{eq}(C).

Figures

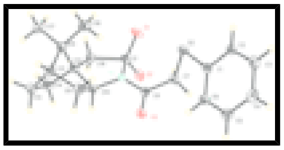

Fig. 1. The molecular structure and atoms numbering scheme of (3). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are drawn as circles of arbitrary radius.

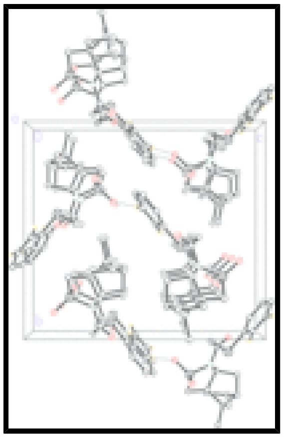

Fig. 2. Projection of the crystal packing of (3) along the *a* axis. Dashed lines indicate hydrogen bonds.

Fig. 3. The reaction scheme for the formation of the title compound.

(*S*)—*N*-(Phenylsulfanyl-[1,2-^{13}C$_2$]-acetyl)-2,10-camphorsultam

Crystal data

$C_{18}H_{23}NO_3S_2$	F_{000} = 776
M_r = 365.51	D_x = 1.368 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 7566 reflections
a = 7.7413 (16) Å	θ = 2.8–30.6°
b = 14.370 (3) Å	μ = 0.32 mm^{-1}
c = 15.951 (3) Å	*T* = 100 (2) K
V = 1774.4 (6) Å^3	Prism, colorless

$Z = 4$	0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	4705 independent reflections
Radiation source: fine–focus sealed tube	4640 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.026$
$T = 100(2)$ K	$\theta_{\text{max}} = 29.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.902$, $T_{\text{max}} = 0.969$	$k = -19 \rightarrow 19$
25461 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.49P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.057$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.33$ e Å^{-3}
4705 reflections	$\Delta\rho_{\text{min}} = -0.22$ e Å^{-3}
217 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2014 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.01 (4)

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 $F^2 > 2\sigma(F^2)$ 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}
S1	0.70241 (3)	0.69923 (2)	0.802224 (15)	0.01766 (6)
S2	0.37395 (3)	0.573846 (19)	0.644032 (18)	0.01936 (6)
O1	0.52928 (11)	0.73373 (7)	0.79357 (6)	0.0278 (2)

O2	0.73402 (11)	0.63203 (7)	0.86715 (5)	0.02579 (18)
O3	0.80681 (11)	0.52480 (6)	0.63157 (6)	0.02489 (17)
N1	0.76889 (11)	0.65471 (6)	0.70898 (6)	0.01592 (17)
C1	0.33729 (14)	0.47935 (7)	0.57418 (7)	0.01673 (19)
C2	0.16813 (14)	0.46941 (8)	0.54480 (7)	0.0187 (2)
H2	0.0806	0.5112	0.5629	0.022*
C3	0.12827 (16)	0.39807 (8)	0.48890 (7)	0.0222 (2)
H3	0.0141	0.3922	0.4677	0.027*
C4	0.25513 (16)	0.33535 (8)	0.46400 (7)	0.0236 (2)
H4	0.2274	0.2861	0.4266	0.028*
C5	0.42257 (16)	0.34511 (8)	0.49408 (8)	0.0228 (2)
H5	0.5088	0.3018	0.4776	0.027*
C6	0.46565 (14)	0.41769 (8)	0.54810 (7)	0.0197 (2)
H6	0.5812	0.4251	0.5670	0.024*
C7	0.54538 (14)	0.53091 (8)	0.71177 (7)	0.0192 (2)
H7A	0.5245	0.5517	0.7701	0.023*
H7B	0.5461	0.4620	0.7111	0.023*
C8	0.71857 (13)	0.56734 (8)	0.68175 (7)	0.01757 (19)
C9	0.95263 (16)	0.71405 (8)	0.58588 (7)	0.0204 (2)
H9A	1.0450	0.6758	0.5602	0.025*
H9B	0.8425	0.7022	0.5562	0.025*
C10	0.93571 (13)	0.69403 (7)	0.68101 (6)	0.01507 (18)
H10	1.0334	0.6539	0.7004	0.018*
C11	0.99964 (16)	0.81870 (8)	0.58442 (7)	0.0211 (2)
H11	0.9883	0.8487	0.5281	0.025*
C12	0.94901 (13)	0.79214 (7)	0.72109 (6)	0.01553 (19)
C13	1.18005 (15)	0.82958 (9)	0.62503 (8)	0.0248 (2)
H13A	1.2285	0.8922	0.6141	0.030*
H13B	1.2613	0.7820	0.6037	0.030*
C14	1.14348 (14)	0.81530 (8)	0.72072 (7)	0.0215 (2)
H14A	1.2127	0.7634	0.7439	0.026*
H14B	1.1679	0.8726	0.7531	0.026*
C15	0.87731 (15)	0.85899 (7)	0.65212 (7)	0.01818 (19)
C16	0.68440 (16)	0.84877 (8)	0.63135 (8)	0.0238 (2)
H16A	0.6157	0.8610	0.6818	0.036*
H16B	0.6616	0.7854	0.6116	0.036*
H16C	0.6529	0.8934	0.5875	0.036*
C17	0.90827 (18)	0.96226 (8)	0.67196 (8)	0.0267 (3)
H17A	1.0326	0.9737	0.6774	0.040*
H17B	0.8504	0.9784	0.7246	0.040*
H17C	0.8616	1.0006	0.6265	0.040*
C18	0.85942 (15)	0.79024 (8)	0.80568 (7)	0.0197 (2)
H18A	0.8027	0.8507	0.8168	0.024*
H18B	0.9443	0.7782	0.8508	0.024*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

S1	0.01329 (11)	0.02605 (13)	0.01363 (11)	0.00041 (10)	0.00175 (9)	−0.00218 (10)
S2	0.01468 (11)	0.01995 (12)	0.02345 (13)	0.00229 (9)	0.00053 (10)	−0.00354 (10)
O1	0.0162 (4)	0.0407 (5)	0.0265 (4)	0.0055 (3)	0.0016 (3)	−0.0081 (4)
O2	0.0247 (4)	0.0360 (5)	0.0167 (4)	−0.0054 (4)	0.0011 (3)	0.0043 (3)
O3	0.0184 (4)	0.0227 (4)	0.0336 (4)	−0.0018 (3)	0.0059 (4)	−0.0075 (3)
N1	0.0132 (4)	0.0203 (4)	0.0143 (4)	−0.0011 (3)	0.0032 (3)	−0.0017 (3)
C1	0.0162 (5)	0.0168 (4)	0.0173 (4)	−0.0008 (4)	0.0012 (4)	0.0014 (4)
C2	0.0146 (5)	0.0198 (5)	0.0219 (5)	−0.0006 (4)	0.0009 (4)	0.0050 (4)
C3	0.0197 (5)	0.0253 (5)	0.0216 (5)	−0.0046 (4)	−0.0027 (4)	0.0050 (4)
C4	0.0302 (6)	0.0210 (5)	0.0197 (5)	−0.0054 (4)	0.0000 (4)	−0.0003 (4)
C5	0.0249 (5)	0.0212 (5)	0.0223 (5)	0.0014 (4)	0.0038 (4)	−0.0013 (4)
C6	0.0155 (5)	0.0217 (5)	0.0218 (5)	0.0008 (4)	0.0017 (4)	0.0000 (4)
C7	0.0150 (5)	0.0231 (5)	0.0194 (5)	−0.0033 (4)	0.0003 (4)	0.0019 (4)
C8	0.0144 (4)	0.0194 (5)	0.0189 (4)	−0.0006 (4)	−0.0003 (4)	0.0012 (4)
C9	0.0235 (5)	0.0215 (5)	0.0162 (5)	−0.0013 (4)	0.0048 (4)	−0.0016 (4)
C10	0.0126 (4)	0.0161 (4)	0.0165 (4)	0.0004 (4)	0.0018 (3)	−0.0003 (4)
C11	0.0255 (5)	0.0202 (5)	0.0175 (5)	−0.0014 (4)	0.0029 (4)	0.0026 (4)
C12	0.0145 (4)	0.0169 (5)	0.0152 (4)	0.0012 (4)	−0.0009 (4)	−0.0009 (4)
C13	0.0206 (5)	0.0250 (5)	0.0289 (6)	−0.0035 (4)	0.0061 (4)	0.0030 (4)
C14	0.0160 (4)	0.0226 (5)	0.0260 (5)	−0.0024 (4)	−0.0019 (4)	0.0009 (4)
C15	0.0206 (5)	0.0169 (4)	0.0171 (4)	0.0023 (4)	−0.0020 (4)	0.0014 (4)
C16	0.0224 (5)	0.0252 (5)	0.0238 (5)	0.0050 (4)	−0.0057 (4)	0.0020 (4)
C17	0.0326 (6)	0.0171 (5)	0.0305 (6)	0.0025 (5)	−0.0029 (5)	0.0011 (4)
C18	0.0205 (5)	0.0230 (5)	0.0155 (4)	−0.0021 (4)	−0.0012 (4)	−0.0036 (4)

Geometric parameters (Å, °)

S1—O1	1.4356 (9)	C9—H9A	0.9900
S1—O2	1.4370 (9)	C9—H9B	0.9900
S1—N1	1.6988 (9)	C10—C12	1.5515 (15)
S1—C18	1.7863 (12)	C10—H10	1.0000
S2—C1	1.7793 (11)	C11—C13	1.5474 (18)
S2—C7	1.8192 (12)	C11—C15	1.5486 (16)
O3—C8	1.2169 (14)	C11—H11	1.0000
N1—C8	1.3844 (14)	C12—C18	1.5174 (14)
N1—C10	1.4785 (13)	C12—C14	1.5418 (15)
C1—C6	1.3948 (15)	C12—C15	1.5625 (15)
C1—C2	1.3981 (15)	C13—C14	1.5659 (17)
C2—C3	1.3933 (16)	C13—H13A	0.9900
C2—H2	0.9500	C13—H13B	0.9900
C3—C4	1.3909 (18)	C14—H14A	0.9900
C3—H3	0.9500	C14—H14B	0.9900
C4—C5	1.3893 (18)	C15—C17	1.5361 (16)
C4—H4	0.9500	C15—C16	1.5367 (17)
C5—C6	1.3934 (16)	C16—H16A	0.9800
C5—H5	0.9500	C16—H16B	0.9800
C6—H6	0.9500	C16—H16C	0.9800
C7—C8	1.5169 (15)	C17—H17A	0.9800
C7—H7A	0.9900	C17—H17B	0.9800

C7—H7B	0.9900	C17—H17C	0.9800
C9—C11	1.5474 (16)	C18—H18A	0.9900
C9—C10	1.5500 (15)	C18—H18B	0.9900

O1—S1—O2	117.40 (6)	C9—C11—C13	107.70 (10)
O1—S1—N1	109.19 (5)	C9—C11—C15	102.07 (9)
O2—S1—N1	109.05 (5)	C13—C11—C15	102.84 (9)
O1—S1—C18	112.67 (6)	C9—C11—H11	114.3
O2—S1—C18	110.72 (5)	C13—C11—H11	114.3
N1—S1—C18	95.54 (5)	C15—C11—H11	114.3
C1—S2—C7	103.27 (5)	C18—C12—C14	116.97 (9)
C8—N1—C10	119.84 (9)	C18—C12—C10	108.64 (9)
C8—N1—S1	122.07 (7)	C14—C12—C10	105.03 (8)
C10—N1—S1	112.64 (7)	C18—C12—C15	118.35 (9)
C6—C1—C2	120.16 (10)	C14—C12—C15	102.21 (9)
C6—C1—S2	123.91 (8)	C10—C12—C15	104.19 (8)
C2—C1—S2	115.93 (8)	C11—C13—C14	103.39 (9)
C3—C2—C1	119.81 (11)	C11—C13—H13A	111.1
C3—C2—H2	120.1	C14—C13—H13A	111.1
C1—C2—H2	120.1	C11—C13—H13B	111.1
C4—C3—C2	120.21 (11)	C14—C13—H13B	111.1
C4—C3—H3	119.9	H13A—C13—H13B	109.0
C2—C3—H3	119.9	C12—C14—C13	102.03 (9)
C5—C4—C3	119.65 (11)	C12—C14—H14A	111.4
C5—C4—H4	120.2	C13—C14—H14A	111.4
C3—C4—H4	120.2	C12—C14—H14B	111.4
C4—C5—C6	120.83 (11)	C13—C14—H14B	111.4
C4—C5—H5	119.6	H14A—C14—H14B	109.2
C6—C5—H5	119.6	C17—C15—C16	106.76 (9)
C5—C6—C1	119.30 (10)	C17—C15—C11	114.17 (10)
C5—C6—H6	120.4	C16—C15—C11	114.09 (10)
C1—C6—H6	120.4	C17—C15—C12	113.17 (9)
C8—C7—S2	109.89 (8)	C16—C15—C12	115.99 (9)
C8—C7—H7A	109.7	C11—C15—C12	92.51 (8)
S2—C7—H7A	109.7	C15—C16—H16A	109.5
C8—C7—H7B	109.7	C15—C16—H16B	109.5
S2—C7—H7B	109.7	H16A—C16—H16B	109.5
H7A—C7—H7B	108.2	C15—C16—H16C	109.5
O3—C8—N1	120.27 (10)	H16A—C16—H16C	109.5
O3—C8—C7	122.03 (10)	H16B—C16—H16C	109.5
N1—C8—C7	117.56 (9)	C15—C17—H17A	109.5
C11—C9—C10	102.42 (9)	C15—C17—H17B	109.5
C11—C9—H9A	111.3	H17A—C17—H17B	109.5
C10—C9—H9A	111.3	C15—C17—H17C	109.5
C11—C9—H9B	111.3	H17A—C17—H17C	109.5
C10—C9—H9B	111.3	H17B—C17—H17C	109.5
H9A—C9—H9B	109.2	C12—C18—S1	107.26 (7)
N1—C10—C9	116.12 (9)	C12—C18—H18A	110.3
N1—C10—C12	106.31 (8)	S1—C18—H18A	110.3
C9—C10—C12	103.24 (9)	C12—C18—H18B	110.3

N1—C10—H10	110.3	S1—C18—H18B	110.3
C9—C10—H10	110.3	H18A—C18—H18B	108.5
C12—C10—H10	110.3		

O1—S1—N1—C8	−78.89 (10)	C9—C10—C12—C18	155.50 (9)
O2—S1—N1—C8	50.58 (10)	N1—C10—C12—C14	158.71 (8)
C18—S1—N1—C8	164.77 (9)	C9—C10—C12—C14	−78.61 (10)
O1—S1—N1—C10	127.28 (8)	N1—C10—C12—C15	−94.21 (9)
O2—S1—N1—C10	−103.25 (8)	C9—C10—C12—C15	28.48 (10)
C18—S1—N1—C10	10.93 (8)	C9—C11—C13—C14	−74.03 (11)
C7—S2—C1—C6	−31.86 (11)	C15—C11—C13—C14	33.30 (11)
C7—S2—C1—C2	148.63 (8)	C18—C12—C14—C13	−169.56 (9)
C6—C1—C2—C3	−0.43 (16)	C10—C12—C14—C13	69.90 (10)
S2—C1—C2—C3	179.10 (8)	C15—C12—C14—C13	−38.63 (10)
C1—C2—C3—C4	1.68 (17)	C11—C13—C14—C12	3.38 (11)
C2—C3—C4—C5	−1.06 (17)	C9—C11—C15—C17	173.72 (9)
C3—C4—C5—C6	−0.82 (18)	C13—C11—C15—C17	62.14 (12)
C4—C5—C6—C1	2.04 (17)	C9—C11—C15—C16	−63.13 (12)
C2—C1—C6—C5	−1.41 (17)	C13—C11—C15—C16	−174.70 (9)
S2—C1—C6—C5	179.10 (9)	C9—C11—C15—C12	56.88 (10)
C1—S2—C7—C8	98.08 (8)	C13—C11—C15—C12	−54.69 (9)
C10—N1—C8—O3	−3.75 (15)	C18—C12—C15—C17	69.65 (13)
S1—N1—C8—O3	−155.76 (9)	C14—C12—C15—C17	−60.44 (12)
C10—N1—C8—C7	−179.42 (9)	C10—C12—C15—C17	−169.62 (9)
S1—N1—C8—C7	28.57 (13)	C18—C12—C15—C16	−54.24 (13)
S2—C7—C8—O3	−90.63 (12)	C14—C12—C15—C16	175.67 (9)
S2—C7—C8—N1	84.95 (10)	C10—C12—C15—C16	66.49 (11)
C8—N1—C10—C9	64.60 (12)	C18—C12—C15—C11	−172.67 (9)
S1—N1—C10—C9	−140.92 (8)	C14—C12—C15—C11	57.24 (10)
C8—N1—C10—C12	178.76 (9)	C10—C12—C15—C11	−51.93 (9)
S1—N1—C10—C12	−26.76 (10)	C14—C12—C18—S1	−143.91 (8)
C11—C9—C10—N1	123.71 (10)	C10—C12—C18—S1	−25.29 (10)
C11—C9—C10—C12	7.81 (11)	C15—C12—C18—S1	93.12 (10)
C10—C9—C11—C13	65.88 (11)	O1—S1—C18—C12	−104.50 (8)
C10—C9—C11—C15	−41.99 (11)	O2—S1—C18—C12	121.76 (8)
N1—C10—C12—C18	32.82 (10)	N1—S1—C18—C12	8.98 (8)

Fig. 1

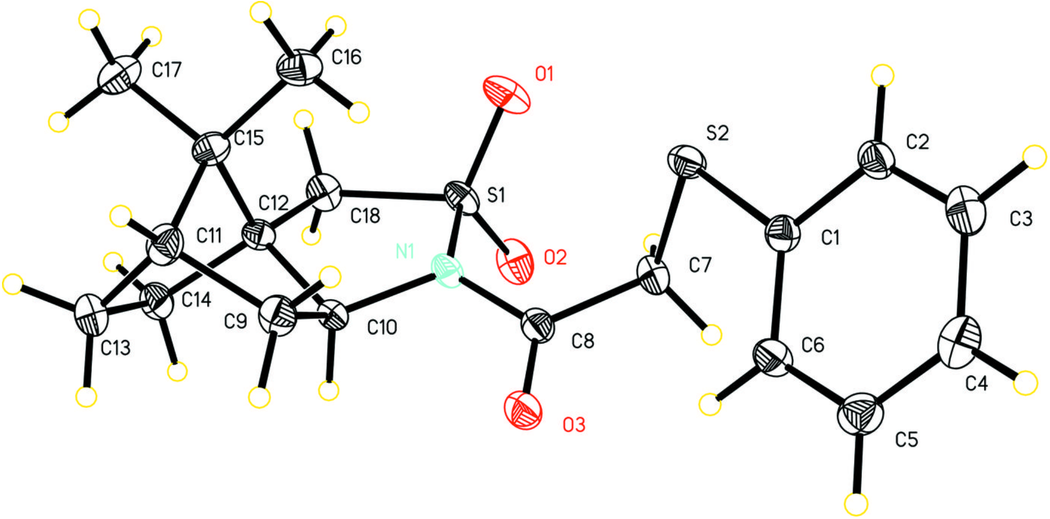
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Fig. 2

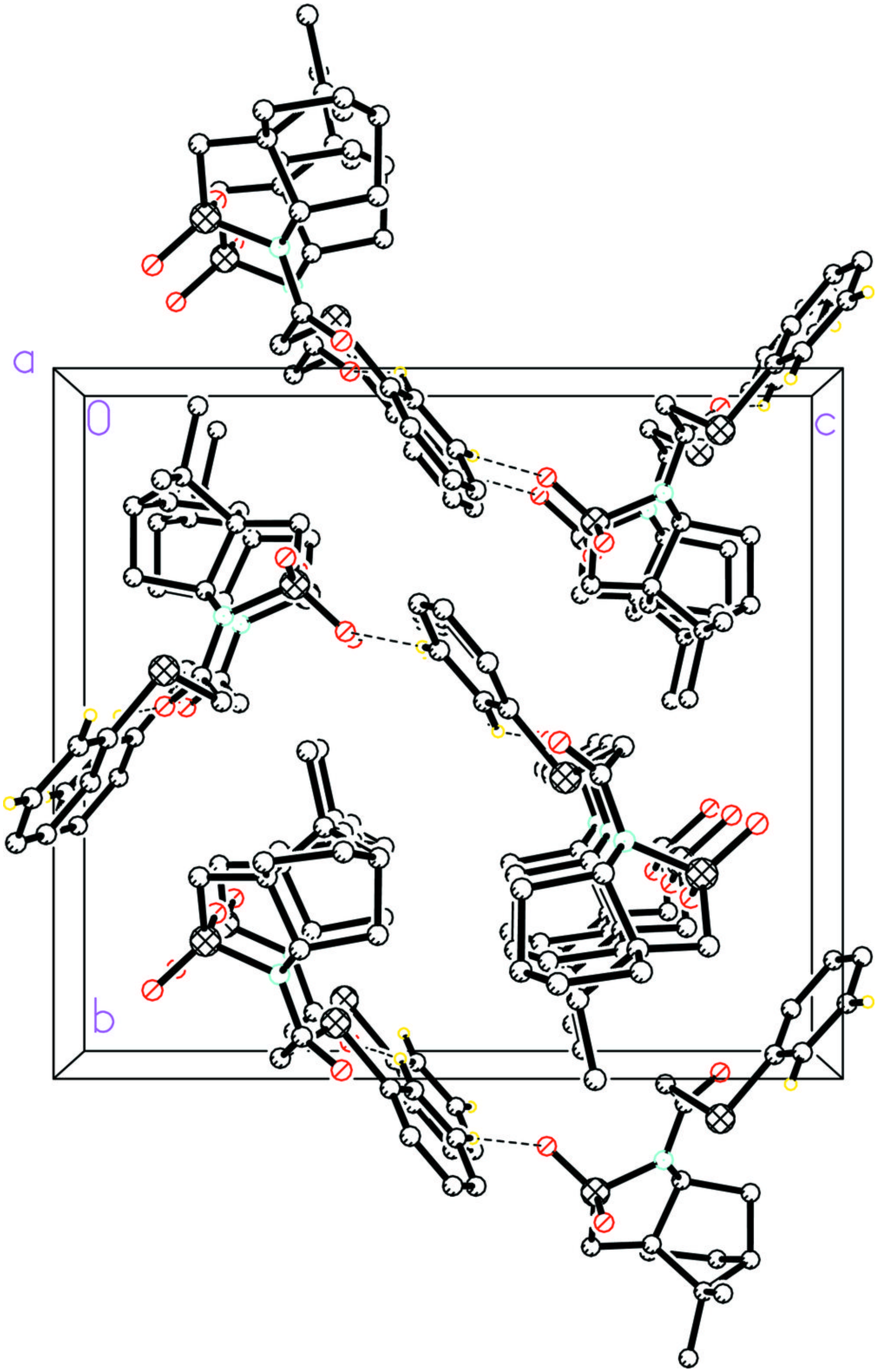

Fig. 3