

Synthesis and crystal structure of 2-(1,3-dithietan-2-ylidene)cyclohexane-1,3-dione

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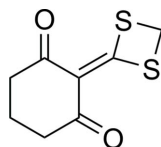
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The title compound, C₈H₈O₂S₂, contains a cyclohexane-1,3-dione ring, which has a twist-boat conformation. The C₂S₂ ring is close to planar (r.m.s. deviation = 0.023 Å) and the dihedral angle between the mean planes of the cyclohexane and 1,3-dithietane rings is 9.1 (3)°. Short intramolecular S...O contacts occur [2.719 (5) and 2.740 (5) Å]. In the crystal, the molecules are linked by weak C—H...S hydrogen bonds and short [3.165 (5) Å] S...O contacts, forming (010) layers. The prevalence of these interactions is illustrated by an analysis of the three-dimensional Hirshfeld surface and by two-dimensional fingerprint plots.

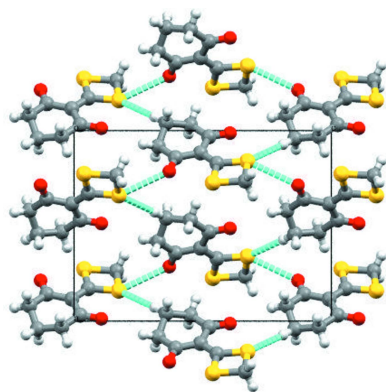
1. Chemical context

Ketene dithioacetals are useful intermediates in organic synthesis and have been used for the preparation of heterocyclic compounds (Kolb, 1990; Ila *et al.*, 2001). The synthesis of trifluoromethyl ketene dithioacetals has applications in the field of pharmaceuticals and agrochemicals (Gouault-Bironneau *et al.*, 2012; Timoshenko & Portella, 2009). The functionalization of ketene dithioacetals provides more powerful tools for the development of new intermediates (Wang *et al.*, 2011; Gao *et al.*, 2010; Hu *et al.*, 2012). The direct formation of a C—C bond has been carried out by reacting a cyano ketene dithioacetal and Morita–Baylis–Hillman (MBH) alcohols resulting from the reaction of acrylonitrile and aryl aldehydes. This reaction led to the corresponding 1,4-pentadiene derivatives (Zhao *et al.*, 2007). Fiala *et al.* (2007) have studied the inhibitive action of some synthetic ketene dithioacetal derivatives towards the corrosion of copper in aerated nitric acid solutions. They concluded that these compounds are good inhibitors of copper corrosion in this medium. In the present study, we report the synthesis, crystal structure and Hirshfeld surface analysis of the new title 1,3-dithian-2-ylidene derivative, C₈H₈O₂S₂, (I).



2. Structural commentary

In the molecular structure of (I), the cyclohexane and dithietane rings are linked by a C=C bond of 1.364 (8) Å (Fig. 1). The cyclohexane-1,3-dione ring adopts a twist-boat



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Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5A\cdots S2^i$	0.97	2.87	3.844 (8)	178

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

conformation, as seen in related compounds (Kuppan Chandrakha *et al.*, 2016; Liu *et al.*, 2011). Atom C5 is displaced by 0.627 (8) Å with respect to the C2/C3/C4/C6/C7 mean plane, similar to the value observed for 2-[chloro(4-methoxyphenyl)methyl]-2-(4-methoxyphenyl)-5,5-dimethylcyclohexane-1,3-dione (Saloua Chelli *et al.*, 2016). The largest endocyclic angle in the cyclohexane ring [$C7-C2-C3 = 123.2 (6)^\circ$] is located opposite the dithietan ring and the largest exo-cyclic angle ($C6-C7-O2$) is $122.3 (5)^\circ$. A difference of 1.3° is observed between the angles located on either side of the $C1=C2$ double bond. In the C_2S_2 ring, the $C1-S1$ and $C1-S2$ bond lengths are indistinguishable at 1.716 (6) Å whereas the $C8-S1$ and $C8-S2$ bond lengths differ slightly [1.819 (7) and 1.801 (7) Å, respectively]. The molecule has local C_s symmetry with a non-crystallographic mirror plane passing through atoms C8, C1, C2 and C5. The dihedral angle between the cyclohexane (all atoms) and dithietane rings is $9.1 (3)^\circ$ and short intramolecular $S1\cdots O2$ [2.719 (5) Å] and $S2\cdots O1$ [2.740 (5) Å] contacts are observed (Fig. 1).

3. Supramolecular features

In the crystal, the molecules stack head-to-tail along the b -axis direction. The molecules are linked by $C5-H5A\cdots S2$ hydrogen bonds (Table 1) and short [3.165 (5) Å compared to a van der Waals separation of 3.32 Å] $S2\cdots O2^{ii}$ [symmetry code: (ii) $\frac{1}{2} - x, y, \frac{1}{2} + z$] contacts, forming (010) layers (Fig. 2).

4. Hirshfeld surface analysis

The nature of the intermolecular interactions in (I) has been computed by *CrystalExplorer17.5* (Turner *et al.*, 2017), using Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) and two-dimensional fingerprint plots (McKinnon *et al.*, 2007). The d_{norm} plot (Fig. 3) shows red spots corresponding to

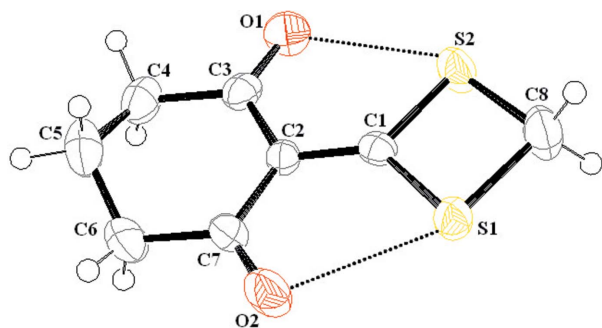


Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. The short intramolecular $S\cdots O$ contacts are shown as dashed lines.

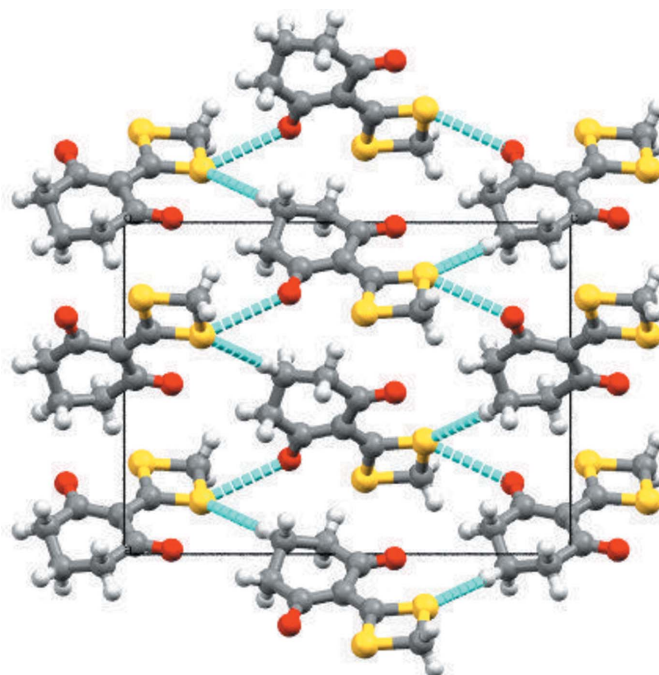


Figure 2

Structure of (I) viewed along the [010] direction, showing the infinite layers propagating parallel to the ac plane. The $C-H\cdots S$ and short $S\cdots O$ contacts are shown as blue dashed lines.

the $C5-H5A\cdots S2$ hydrogen bond and short $S2\cdots O2$ contact. A list of the relative percentage contributions of the close contacts to the HS of (I) are given in Table 2 and the overall two-dimensional fingerprint plot is shown in Fig. 4a. A contribution of 30.7% was found for the $H\cdots O/O\cdots H$ interactions, representing the largest contribution; these contacts are represented by the spikes in the top left ($d_e > d_i$, $H\cdots O$, 14.3%) and bottom right ($d_e < d_i$, $O\cdots H$, 16.5%) of Fig. 4b. Interactions of the type $H\cdots H$ appear in the middle of the scattered points in the fingerprint plots with a pair of spikes at $d_e + d_i = 2.5$ Å and comprise 25.9% of the entire surface (Fig. 4c); the van der Waals radius for this interaction is 2.4 Å, which means it is a weak interaction. The $S\cdots H/H\cdots S$ contacts (Fig. 4d), which account for 23.8% of the Hirshfeld surface, are displayed on the fingerprint plot as a pair of long

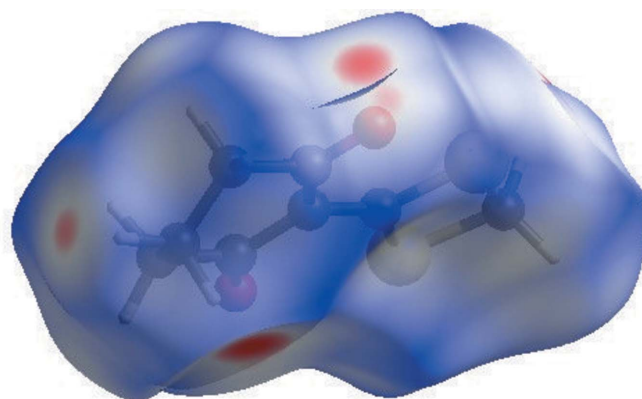


Figure 3

Hirshfeld surface for (I) scaled from -0.16 (red) a.u. to 1.09 (blue) a.u.

Table 2

Relative percentage contributions of the close contacts to the Hirshfeld surface of the title compound.

Contact type	Percentage contribution
O...H/H...O	30.7
H...H	25.9
S...H/H...S	23.8
C...H/H...C	11.6
S...C/S...C	4.0
S...O/O...S	3.3
C...O/O...C	0.7

spikes at $d_e + d_i = 2.7 \text{ \AA}$. This distance differs by $0.3 \text{ \AA}$ from the sum of the van der Waals radii, which means it is the strongest interaction present. The S...C/C...S (4.0%, Fig. 4f) and S...O/O...S (3.3%, Fig. 4g) contacts are seen as pairs of spikes at $d_e + d_i = 3.2$ and $3.05 \text{ \AA}$, respectively. These distances are shorter than the sums of the van der Waals radii of 3.5 and $3.32 \text{ \AA}$, respectively. The C...O/O...C interactions make a contribution of 0.7% to the Hirshfeld surface (Fig. 4h), their interatomic distances ($d_e + d_i = 3.3 \text{ \AA}$) being larger than the sum of the van der Waals radius ($3.22 \text{ \AA}$), so this interaction is very weak in this structure. The fingerprint plot corresponding to C...H/H...C contacts (Fig. 4e) shows a fin-like distribution of points with the edges at $d_e + d_i = 2.8 \text{ \AA}$.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update March 2022; Groom *et al.*, 2016) for the 1,3-dithietane fragment yielded three relevant hits. These

are dispiro[1,3-dithietane-2,2':4,2''-diadamantane] (CSD refcode AFECAP; Linden *et al.*, 2002), *trans*-2,4-bis(isopropyl)-2,4-bis[(2-methyl-1-thioxo)propylsulfanyl]-1,3-dithietane (HUZHOZ; Mahjoub *et al.*, 2003) and 2-(nitromethylene)-1,3-dithietane (WOCQEK; Shanmuga Sundara Raj *et al.*, 2000); in these compounds the dithietane ring is planar. In (I), the angles C1—S1—C8 and S1—C8—S2 are $82.7(3)$ and $93.6(3)^\circ$, respectively, similar to the values observed for the aforementioned compounds, *viz.* 85.76 and 94.24° , 85.40 and 94.60° , 82.8 and 94.00° for AFECAP, HUZHOZ and WOCQEK, respectively. A search for the cyclohexane-1,3-dione fragment revealed over 30 hits. The most relevant structures are 2-(phenylaminomethylidene)cyclohexane-1,3-dione (ISUQAO; Kettmann *et al.*, 2004), (*E*)-5,5-dimethyl-2-[3-(4-nitrophenyl)allylidene]cyclohexane-1,3-dione (VUGVUQ; Jae Kyun Lee *et al.*, 2015), 2-[chloro(4-methoxyphenyl)methyl]-2-(4-methoxyphenyl)-5,5-dimethylcyclohexane-1,3-dione (TACZIJ; Saloua Chelli *et al.*, 2016) and 2-[(1*S**,2*S**)-2-[(*E*)-(2,4-dihydroxybenzylidene)amino]cyclohexyl]isoindoline-1,3-dione (EVABIN; Liu *et al.*, 2011). The cyclohexane ring adopts a chair conformation in all five of these compounds, as in the title compound.

6. Synthesis and crystallization

Potassium carbonate (0.3 mol, 42 g) in DMF (50 ml) was well stirred at room temperature. To this mixture, cyclohexane-1,3-dione (0.1 mol) was added and the resultant solution stirred at room temperature for 20 min. Carbon disulfide (0.15 mol, 9.0 ml) was then added in one lot. The reaction mixture was stirred and kept for 10 min at room temperature. Diiodomethane (0.12 mol) was added dropwise over 20 min and the reaction mixture stirred for 7 h at room temperature. Ice-water (500 ml) was added to the reaction mass, the solid was filtered and washed with water, dried and recrystallized from ethanol solution to give (I) in the form of colourless plates. Yield 81%; m.p. 487 K ; UV (H_2O) λ_{max} , 335 nm (ϵ 18760); IR (KBr, cm^{-1}): 1640 (C=O), ^1H NMR (CDCl_3) δ (ppm): 4.35 (s, 2H, $\text{CH}_2\text{—S}$), 2.52 (t, $J = 6.5 \text{ Hz}$, 4H, $\text{CH}_2\text{—CH}_2\text{—CH}_2$), 1.97 (q, $J = 6.5 \text{ Hz}$, 2H, $\text{CH}_2\text{—CH}_2\text{—CH}_2$); ^{13}C NMR (CDCl_3) δ (ppm): 197.28 (CO), 189.73 (C=C—S), 119.93 (C=C—S), 37.31 ($\text{CH}_2\text{—CH}_2\text{—CH}_2$), 33.39 ($\text{CH}_2\text{—S}$), 18.62 ($\text{CH}_2\text{—CH}_2\text{—CH}_2$).

7. Refinement

Crystal data, data collection and structure refinement details for the title compound are summarized in Table 3. H atoms were positioned geometrically with C—H = $0.97 \text{ \AA}$ and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

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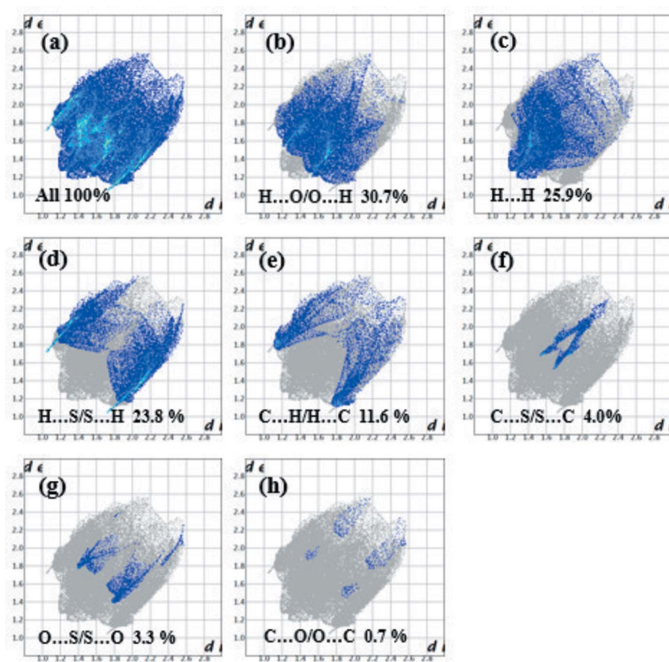


Figure 4

Two-dimensional fingerprint plots for (I): (a) overall, and delineated into contributions from different contacts: (b) H...O/O...H, (c) H...H, (d) H...S/S...H, (e) C...H/H...C, (f) C...S/S...C, (g) O...S/S...O and (h) C...O/O...C.

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₈ H ₈ O ₂ S ₂
<i>M_r</i>	200.28
Crystal system, space group	Orthorhombic, <i>Pca</i> 2 ₁
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.7521 (14), 5.5245 (9), 14.480 (2)
<i>V</i> (Å ³)	860.1 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.57
Crystal size (mm)	0.13 × 0.06 × 0.01
Data collection	
Diffractionmeter	Bruker APEXII
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.960, 0.994
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	3646, 1881, 1230
<i>R</i> _{int}	0.044
(sin θ/λ) _{max} (Å ^{−1})	0.649
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.051, 0.094, 1.00
No. of reflections	1881
No. of parameters	109
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.34, −0.30
Absolute structure	Flack <i>x</i> determined using 396 quotients [(<i>I</i> ⁺) − (<i>I</i> [−])]/[(<i>I</i> ⁺) + (<i>I</i> [−])] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.04 (8)

Computer programs: *APEX2* and (Bruker, 2014), *SHELXT* (Sheldrick, 2015b), *SHELXL2014/7* (Sheldrick, 2015a) and *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012).

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Computing details

Data collection: *SAINT* (Bruker, 2014); cell refinement: *APEX2* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015b); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015a); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

2-(1,3-Dithietan-2-ylidene)cyclohexane-1,3-dione

Crystal data

$C_8H_8O_2S_2$
 $M_r = 200.28$
 Orthorhombic, *Pca*2₁
 Hall symbol: P 2c -2ac
 $a = 10.7521$ (14) Å
 $b = 5.5245$ (9) Å
 $c = 14.480$ (2) Å
 $V = 860.1$ (2) Å³
 $Z = 4$

$F(000) = 416$
 $D_x = 1.547$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 772 reflections
 $\theta = 3.7\text{--}23.4^\circ$
 $\mu = 0.57$ mm⁻¹
 $T = 296$ K
 Plate, colorless
 $0.13 \times 0.06 \times 0.01$ mm

Data collection

Bruker APEXII
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 CCD rotation images, thick slices scans
 Absorption correction: multi-scan
 (SADABS; Krause *et al.*, 2015)
 $T_{\min} = 0.960$, $T_{\max} = 0.994$

3646 measured reflections
 1881 independent reflections
 1230 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -9 \rightarrow 13$
 $k = -4 \rightarrow 7$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.094$
 $S = 1.00$
 1881 reflections
 109 parameters
 1 restraint

0 constraints
 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

$$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack x determined using
396 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.04 (8)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.27332 (13)	0.3620 (3)	0.53923 (11)	0.0371 (5)
S2	0.16018 (17)	0.5982 (3)	0.67352 (10)	0.0430 (5)
O1	0.0128 (4)	0.9617 (7)	0.6058 (4)	0.0457 (16)
O2	0.2139 (4)	0.5407 (8)	0.3699 (3)	0.0520 (19)
C1	0.1711 (5)	0.5968 (10)	0.5553 (4)	0.0273 (19)
C2	0.1164 (5)	0.7427 (12)	0.4911 (4)	0.0260 (17)
C3	0.0319 (5)	0.9299 (10)	0.5239 (5)	0.034 (2)
C4	−0.0307 (6)	1.0849 (12)	0.4519 (5)	0.045 (2)
C5	−0.0404 (7)	0.9587 (14)	0.3579 (6)	0.060 (3)
C6	0.0814 (7)	0.8675 (13)	0.3269 (4)	0.058 (3)
C7	0.1416 (6)	0.7004 (12)	0.3941 (4)	0.034 (2)
C8	0.2644 (7)	0.3440 (12)	0.6645 (5)	0.050 (3)
H4A	−0.11352	1.12679	0.47307	0.0542*
H4B	0.01593	1.23405	0.44470	0.0542*
H5A	−0.07254	1.07203	0.31262	0.0722*
H5B	−0.09848	0.82483	0.36241	0.0722*
H6A	0.07063	0.78338	0.26865	0.0697*
H6B	0.13618	1.00398	0.31609	0.0697*
H8A	0.34374	0.37194	0.69448	0.0598*
H8B	0.22773	0.19389	0.68617	0.0598*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0410 (8)	0.0394 (9)	0.0308 (8)	0.0115 (8)	0.0003 (9)	0.0007 (9)
S2	0.0561 (11)	0.0509 (10)	0.0219 (7)	0.0117 (9)	0.0005 (8)	−0.0001 (10)
O1	0.052 (3)	0.045 (3)	0.040 (2)	0.011 (2)	0.006 (3)	−0.010 (3)
O2	0.070 (4)	0.058 (3)	0.028 (3)	0.020 (3)	0.008 (3)	−0.001 (2)
C1	0.026 (3)	0.028 (4)	0.028 (3)	−0.006 (2)	0.002 (3)	0.000 (3)
C2	0.027 (3)	0.026 (3)	0.025 (3)	0.002 (3)	−0.001 (3)	0.000 (3)
C3	0.026 (3)	0.032 (4)	0.044 (4)	−0.003 (3)	0.001 (3)	0.004 (3)
C4	0.039 (4)	0.038 (4)	0.059 (4)	0.003 (3)	−0.007 (4)	0.009 (4)
C5	0.064 (6)	0.069 (6)	0.048 (4)	0.013 (4)	−0.014 (4)	0.016 (5)
C6	0.061 (5)	0.072 (5)	0.041 (4)	0.020 (4)	0.010 (4)	0.024 (4)

C7	0.035 (4)	0.039 (4)	0.028 (3)	−0.002 (3)	0.003 (3)	0.005 (3)
C8	0.064 (5)	0.052 (5)	0.034 (4)	0.014 (3)	−0.006 (4)	0.006 (4)

Geometric parameters (Å, °)

S1—C1	1.716 (6)	C5—C6	1.473 (11)
S1—C8	1.819 (7)	C6—C7	1.489 (9)
S2—C1	1.716 (6)	C4—H4A	0.9700
S2—C8	1.801 (7)	C4—H4B	0.9700
O1—C3	1.216 (9)	C5—H5A	0.9700
O2—C7	1.227 (8)	C5—H5B	0.9700
C1—C2	1.364 (8)	C6—H6A	0.9700
C2—C3	1.456 (8)	C6—H6B	0.9700
C2—C7	1.449 (8)	C8—H8A	0.9700
C3—C4	1.508 (9)	C8—H8B	0.9700
C4—C5	1.533 (11)		
C1—S1—C8	82.7 (3)	C3—C4—H4B	109.00
C1—S2—C8	83.2 (3)	C5—C4—H4A	109.00
S1—C1—S2	100.5 (3)	C5—C4—H4B	109.00
S1—C1—C2	129.1 (5)	H4A—C4—H4B	108.00
S2—C1—C2	130.4 (5)	C4—C5—H5A	109.00
C1—C2—C3	117.8 (5)	C4—C5—H5B	109.00
C1—C2—C7	119.0 (6)	C6—C5—H5A	109.00
C3—C2—C7	123.2 (6)	C6—C5—H5B	109.00
O1—C3—C2	121.7 (6)	H5A—C5—H5B	108.00
O1—C3—C4	121.1 (5)	C5—C6—H6A	109.00
C2—C3—C4	117.2 (6)	C5—C6—H6B	109.00
C3—C4—C5	112.7 (6)	C7—C6—H6A	109.00
C4—C5—C6	111.5 (6)	C7—C6—H6B	109.00
C5—C6—C7	113.5 (6)	H6A—C6—H6B	108.00
O2—C7—C2	120.7 (6)	S1—C8—H8A	113.00
O2—C7—C6	122.3 (5)	S1—C8—H8B	113.00
C2—C7—C6	116.9 (6)	S2—C8—H8A	113.00
S1—C8—S2	93.6 (3)	S2—C8—H8B	113.00
C3—C4—H4A	109.00	H8A—C8—H8B	110.00
C8—S1—C1—S2	1.5 (3)	C1—C2—C3—C4	−178.3 (5)
C8—S1—C1—C2	−179.6 (6)	C1—C2—C7—C6	−178.9 (6)
C1—S1—C8—S2	−1.4 (3)	C3—C2—C7—O2	179.8 (6)
C8—S2—C1—S1	−1.5 (3)	C1—C2—C7—O2	−2.2 (9)
C8—S2—C1—C2	179.6 (6)	C1—C2—C3—O1	2.2 (8)
C1—S2—C8—S1	1.4 (3)	C3—C2—C7—C6	3.1 (9)
S2—C1—C2—C3	−1.6 (9)	C2—C3—C4—C5	24.6 (8)
S1—C1—C2—C3	179.8 (4)	O1—C3—C4—C5	−155.8 (6)
S1—C1—C2—C7	1.6 (9)	C3—C4—C5—C6	−52.6 (8)
S2—C1—C2—C7	−179.7 (5)	C4—C5—C6—C7	56.3 (8)
C7—C2—C3—O1	−179.8 (6)	C5—C6—C7—C2	−31.5 (9)

C7—C2—C3—C4	−0.2 (8)	C5—C6—C7—O2	151.8 (6)
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Hydrogen-bond geometry (Å, °)

<i>D</i> —H⋯ <i>A</i>	<i>D</i> —H	H⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> —H⋯ <i>A</i>
C5—H5 <i>A</i> ⋯S2 ⁱ	0.97	2.87	3.844 (8)	178

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