C—H···O contacts in the crystal structure of 1,3-dithiane 1,1,3,3-tetraoxide

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The crystal structure of 1,3-dithiane 1,1,3,3-tetraoxide, $C_4H_8O_4S_2$, has been determined to examine the intermolecular C—H···O hydrogen bonds in a small molecule with highly polarized hydrogen atoms. The crystals are monoclinic, space group Pn, with $a = 4.9472 (5)$, $b = 9.9021 (10)$, $c = 7.1002 (7)$ Å and $\beta = 91.464 (3)°$ with $Z = 2$. The molecules form two stacks parallel to the a axis with the molecules being one a translation distance from each other. This stacking involves axial hydrogen atoms on one molecule and the axial oxygen atoms on the adjacent molecule in the stack. None of these C—H···O contacts is particularly short (all are > 2.4 Å). The many C—H···O contacts between the two stacks involve at least one equatorial hydrogen or oxygen atom. Again, no unusually short contacts are found. The whole crystal structure basically consists of a complex network of C—H···O contacts with no single, linear C—H···O contacts, only contacts that involve two (bifurcated), and mostly three or four neighbors.

1. Chemical context

This is the second in a series looking at the C—H···O contacts in cyclic organic structures containing multiple sulfone groups [see Harlow *et al.* (2019) for the first structure in the series: 1,4-dithiane 1,1,4,4-tetraoxide]. Any methylene group adjacent to a sulfone has polarized hydrogen atoms. Methylene groups bonded to two sulfones are polarized to such an extent that they may form a C—H···X (X = N, O) hydrogen bond (Harlow *et al.*, 1984) as illustrated.
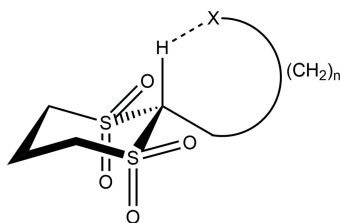
The structure of the unsubstituted 1,3-disulfone, however, has not been previously reported and was of interest particularly because of its high melting point (583 K) and decomposition temperatures (*ca* 623 K), which are suggestive of potentially strong C—H···O contacts. The ^{1}H NMR spectrum of the compound dissolved in DMSO shows a singlet, 2H, at δ = 5.238 ppm (highly polarized hydrogen atoms on C2 between the two SO_2 groups); a triplet, 4H, at 3.370 ppm (moderately polarized hydrogen atoms on C4 and C6 with one adjacent SO_2 group); and a pentet, 2H, at 2.260 ppm (relatively unpolarized hydrogen atoms on C5). See Li & Sammes (1983)
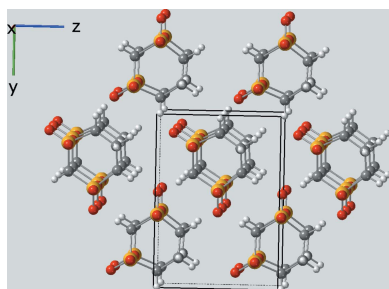
for further details of ^{1}H NMR spectra and hydrogen-atom polarity in disulfones.
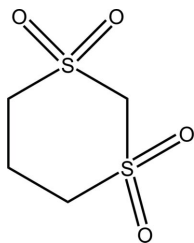
2. Structural commentary

Fig. 1 is an ORTEP drawing of the 1,3-dithiane 1,1,3,3-tetra-oxide molecule with atom labels using the suffix 'a' for axial and 'e' for equatorial atoms. The bond distances and angles are very similar to those reported for the 1,4-disulfone taking into consideration the small amount of distortion related to the different positions of the two sulfonyl groups, *i.e.* 1,3- *vs* 1,4-sites in the ring.

The hydrogen atoms were fully refined with isotropic displacement parameters as there seemed to be a correlation between the 'strength' of the C—H polarization and the displacement parameters of the hydrogen atoms: more polarization seems to yield a smaller radius. Any further comments on this correlation from a structural standpoint would require a diffraction study using neutrons instead of X-rays to better define both the positions and the displacement parameters of the hydrogen atoms.

3. Supramolecular features

Obviously, it is the packing of the molecules that is especially fascinating given that the molecules stack parallel to the *a* axis
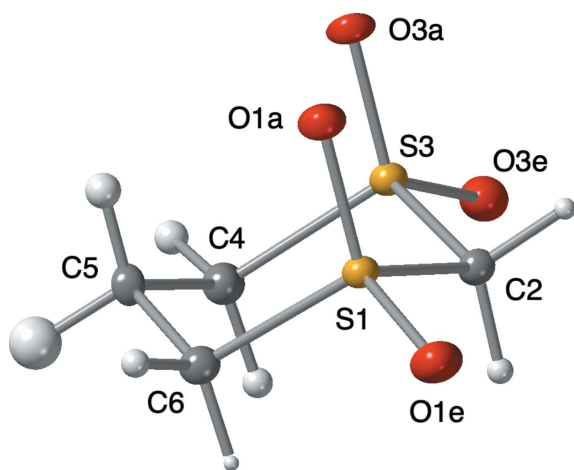

Figure 2
Packing diagram showing the stacking of the molecules parallel to the *a* axis.

at a distance of one translation on *a*, *i.e.* the length of the *a* axis, *ca* 4.9472 (5) Å at 120 K. A general packing diagram is shown in Fig. 2. The *n*-glide, the only symmetry operator in space group *Pn*, curiously preserves the polarity of the stacks and creates a polar crystal with, for example, all of the axial oxygen atoms in the stacks pointing in the same *a*-axis direction (up in Fig. 3) and most of the axial hydrogen atoms pointing down. The stacking is directly stabilized by C—H⋯O contacts between neighboring molecules in the stack and only involves the axial oxygen and hydrogen atoms (see Fig. 4 for the details). In Table 1, these axial C—H⋯O contacts are designated with symmetry 'i'.

In addition, there are multiple O⋯H contacts between the stacks, all of which involve at least one equatorial atom. Some

Figure 1
Labeled *ORTEP* drawing (50% probability) of the 1,3-dithiane 1,1,3,3-tetraoxide molecule. The lower case suffixes 'a' and 'e' are used to distinguish whether the atoms are in the axial or equatorial position on the ring.
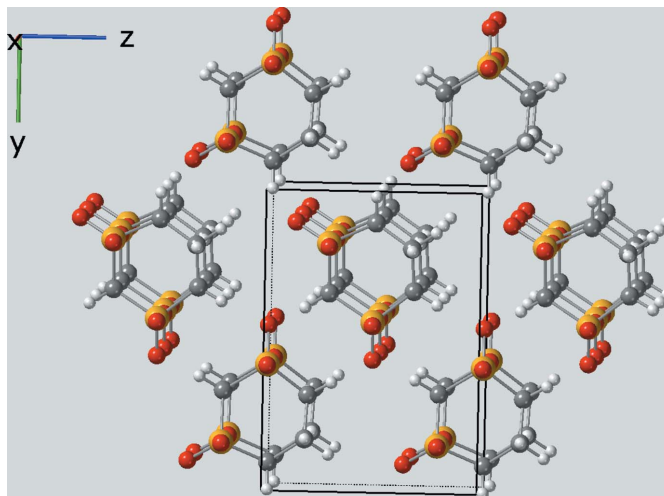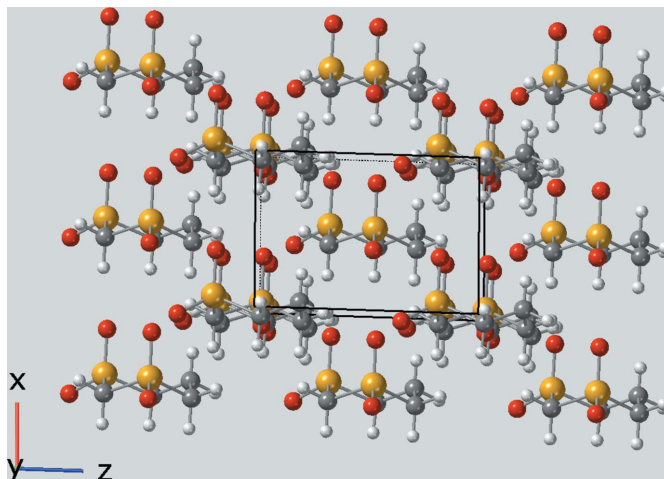

Figure 3
Packing diagram rotated to a view approximately parallel to the *b* axis to show that the stacks created by the *n*-glide are displaced by $x + \frac{1}{2}$. The figure also shows that both stacks are crystallographically polar with, for example, all the axial oxygen atoms pointing upward and most of the axial hydrogen atoms pointing downward except those on C5.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2a$\cdots$O1a^{i}	0.98 (4)	2.47 (4)	3.315 (4)	143 (3)
C2—H2a$\cdots$O3a^{i}	0.98 (4)	2.76 (4)	3.520 (5)	134 (3)
C2—H2a$\cdots$O3e^{ii}	0.98 (4)	2.91 (4)	3.556 (4)	124 (3)
C2—H2e$\cdots$O3a^{ii}	0.97 (4)	2.49 (4)	3.201 (4)	130 (3)
C2—H2e$\cdots$O3e^{iii}	0.97 (4)	2.49 (4)	3.370 (4)	151 (3)
C4—H4a$\cdots$O3a^{i}	0.99 (4)	2.46 (4)	3.329 (4)	147 (3)
C4—H4e$\cdots$O3a^{iv}	0.94 (4)	2.70 (4)	3.462 (4)	138 (3)
C4—H4e$\cdots$O3e^{v}	0.94 (4)	2.63 (4)	3.454 (4)	146 (3)
C5—H5e$\cdots$O1a^{vi}	1.00 (5)	2.91 (5)	3.598 (5)	127 (3)
C5—H5e$\cdots$O1e^{vii}	1.00 (5)	2.50 (5)	3.395 (4)	150 (4)
C6—H6a$\cdots$O1a^{i}	0.95 (4)	2.45 (4)	3.287 (4)	147 (3)
C6—H6a$\cdots$O1e^{vi}	0.95 (4)	2.65 (4)	3.269 (5)	124 (3)
C6—H6e$\cdots$O1a^{vi}	0.95 (4)	2.81 (4)	3.344 (5)	116 (3)
C6—H6e$\cdots$O1e^{viii}	0.95 (4)	2.44 (4)	3.186 (5)	135 (3)

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

of these also serve to bridge adjacent molecules within a stack further cementing the molecules in the stack. Examination of the O$\cdots$H contacts in Table 1 quickly shows that there are no short H$\cdots$O contacts (disappointing) but simply a plethora of contacts that hold the molecules in this crystal structure
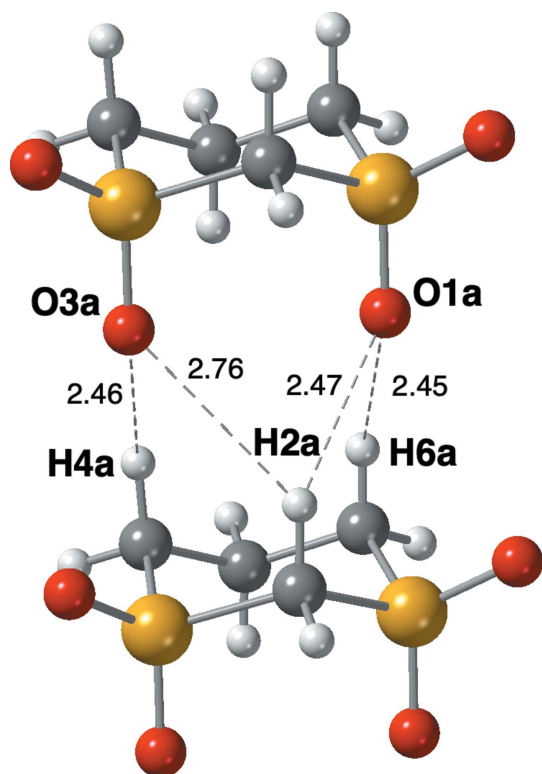

Figure 4
Two adjacent molecules of a stack with the O$\cdots$H contacts detailed. The discrepancy in the H2a$\cdots$O bonds is caused by the molecules in the stacks being slightly tilted as evidenced by S1 and S3 not having the same x coordinate: 0.568 *vs* 0.546 (even though the molecules are related by a translation along a). This leads to a difference in the S1$\cdots$S3^{i} and S3$\cdots$S1^{i} distances, for example, of 5.646 *vs* 5.898 Å. The longer S$\cdots$S distance is associated with the longer H2a$\cdots$O distance.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_8O_4S_2$
M_r	184.22
Crystal system, space group	Monoclinic, Pn
Temperature (K)	120
a, b, c (Å)	4.9472 (5), 9.9021 (10), 7.1002 (7)
β (°)	91.464 (3)
V (Å^3)	347.71 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.72
Crystal size (mm)	0.54 × 0.11 × 0.05
Data collection	
Diffractometer	Bruker PHOTON-II
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.579, 0.746
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	6109, 1513, 1473
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.640
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.055, 1.15
No. of reflections	1513
No. of parameters	123
No. of restraints	2
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.28, −0.40
Absolute structure	Flack x determined using 682 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter	0.07 (4)

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *olex2.solve* (Dolomanov *et al.*, 2009), *SHELXL2018/3* (Sheldrick, 2015), *CrystalMaker* (Palmer, 2014), and *publCIF* (Westrip, 2010).

together. When the environment of each oxygen atom is surveyed in detail, it is found that they all interact with four hydrogen atoms, which generally form a distorted quadrilateral with O$\cdots$H contact distances that vary from 2.44 to 3.09 Å. This is very similar to what was found for the 1,4-disulfone structure where example figures can be found (Harlow *et al.*, 2019). The main difference is that the O$\cdots$H distances in the 1,4-disulfone structure were relatively uniform and, in this structure, they are not.

One mystery that remains is why a small molecule with mirror symmetry crystallizes in a non-centrosymmetric, polar space group?

4. Database survey

A Cambridge Crystallographic Database survey of the 1,3-disulfone moiety reveals 22 structures with that motif (CSD version 5.41 + three updates; Groom *et al.*, 2016). Four of the structures were authored by Harlow and Sammes and served as an impetus for the present study. A paper entitled in part 'Study of the Interaction of Silver(I) with β-Disulfone in Aqueous Alkaline Media' was of particular interest because it suggested that metal salts could be made with our title compound, *i.e.* one of the hydrogen atoms on C2 was acidic

enough to be easily removed (DeMember *et al.*, 1983) in a solution of KOH.

5. Synthesis and crystallization

To a stirred solution of 1,3-dithiane (1.05 g, 5.70 mmol, Alfa-Aeser) in glacial acetic acid (25 mL) was added a solution of 30% H_2O_2 (10 mL) in glacial acetic acid (25 mL) and the mixture was heated to 323 K overnight. The white precipitate was separated on a Buchner funnel and washed with water (3 × 25 mL) and dried in air. Colorless, rod-like crystals of the compound were harvested from an evaporated KOH (0.5 M) solution of the the 1,3-disulfone. ^{1}H NMR (400 MHz, DMSO-d_6), δ: 5.238 (*singlet*, 2H, H2*a*/e), 3.370 (*triplet*, 4H, $^3J_{H,H}$ = 5 Hz, H4*a*/e, H6*a*/e), 2.260 (*pentet*, 2H, $^3J_{H,H}$ = 6 Hz, H5*a*/e); ^{13}C NMR (100.13 MHz, DMSO-d_6), δ: 70.12 (C2), 50.09 (C4/C6), 17.60 (C4). HRMS (negative ion mode, $[C_4H_7O_4S_2]^-$) *m/z* found: 182.9803; calculated: 182.9786.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Non-hydrogen atoms were refined with anisotropic displacement parameters and all hydrogen atoms were located from a difference-Fourier map and refined freely.

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C—H⋯O contacts in the crystal structure of 1,3-dithiane 1,1,3,3-tetraoxide

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Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: *olex2.solve* (Dolomanov *et al.*, 2009); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (Palmer, 2014); software used to prepare material for publication: *publCIF* (Westrip, 2010).

1,3-Dithiane 1,1,3,3-tetraoxide

Crystal data

$C_4H_8O_4S_2$	$F(000) = 192$
$M_r = 184.22$	$D_x = 1.760$ Mg m^{-3}
Monoclinic, Pn	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.9472$ (5) Å	Cell parameters from 5408 reflections
$b = 9.9021$ (10) Å	$\theta = 3.5$–27.1°
$c = 7.1002$ (7) Å	$\mu = 0.72$ mm^{-1}
$\beta = 91.464$ (3)°	$T = 120$ K
$V = 347.71$ (6) Å^3	Rod, colorless
$Z = 2$	$0.54 \times 0.11 \times 0.05$ mm

Data collection

Bruker PHOTON-II diffractometer	$T_{min} = 0.579$, $T_{max} = 0.746$
Radiation source: fine-focus sealed tube	6109 measured reflections
Bruker TRIUMPH curved-graphite monochromator	1513 independent reflections
	1473 reflections with $I > 2\sigma(I)$
Detector resolution: 7.41 pixels mm^{-1}	$R_{int} = 0.039$
combination of ω and φ–scans	$\theta_{max} = 27.1°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$h = -6 \rightarrow 6$
	$k = -12 \rightarrow 12$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.027$	$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 0.148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.055$	
$S = 1.15$	$(\Delta/\sigma)_{max} < 0.001$
1513 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
123 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
2 restraints	Absolute structure: Flack x determined using 682 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Primary atom site location: iterative	
Secondary atom site location: difference Fourier map	Absolute structure parameter: 0.07 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.56801 (14)	0.16084 (8)	0.31351 (11)	0.01036 (19)
S3	0.54595 (15)	0.42138 (8)	0.52142 (12)	0.01083 (19)
O1a	0.8592 (5)	0.1643 (3)	0.3226 (4)	0.0167 (5)
O1e	0.4403 (5)	0.0944 (3)	0.1549 (4)	0.0173 (6)
O3a	0.8376 (5)	0.4249 (3)	0.5291 (4)	0.0162 (5)
O3e	0.4048 (5)	0.5484 (2)	0.5189 (4)	0.0170 (6)
C2	0.4419 (7)	0.3292 (4)	0.3144 (5)	0.0125 (7)
C4	0.4299 (7)	0.3185 (4)	0.7058 (5)	0.0155 (7)
C5	0.5438 (8)	0.1749 (4)	0.6975 (5)	0.0166 (8)
C6	0.4464 (8)	0.0935 (4)	0.5261 (5)	0.0155 (8)
H2a	0.244 (8)	0.323 (3)	0.309 (6)	0.006 (9)*
H2e	0.515 (8)	0.376 (4)	0.206 (6)	0.004 (9)*
H4a	0.231 (8)	0.326 (4)	0.697 (5)	0.007 (9)*
H4e	0.489 (7)	0.362 (4)	0.817 (6)	0.011 (10)*
H5a	0.724 (9)	0.179 (4)	0.706 (6)	0.011 (10)*
H5e	0.475 (9)	0.123 (5)	0.807 (7)	0.025 (12)*
H6a	0.255 (7)	0.094 (4)	0.513 (6)	0.002 (8)*
H6e	0.523 (8)	0.005 (4)	0.529 (6)	0.007 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0083 (4)	0.0114 (4)	0.0114 (4)	0.0005 (4)	0.0006 (3)	−0.0008 (3)
S3	0.0098 (4)	0.0107 (4)	0.0120 (4)	−0.0004 (3)	−0.0004 (3)	−0.0015 (3)
O1a	0.0091 (12)	0.0200 (13)	0.0209 (14)	0.0015 (10)	0.0017 (10)	−0.0001 (11)
O1e	0.0161 (13)	0.0203 (13)	0.0153 (13)	−0.0022 (11)	−0.0004 (10)	−0.0076 (10)
O3a	0.0085 (12)	0.0191 (13)	0.0210 (13)	−0.0026 (10)	−0.0019 (10)	−0.0017 (11)
O3e	0.0167 (14)	0.0120 (13)	0.0224 (14)	0.0027 (10)	0.0024 (11)	−0.0019 (10)
C2	0.0120 (18)	0.0124 (17)	0.0130 (17)	−0.0006 (13)	−0.0015 (14)	0.0003 (13)
C4	0.0146 (18)	0.0211 (19)	0.0108 (16)	0.0000 (15)	0.0023 (14)	−0.0010 (14)
C5	0.0138 (19)	0.022 (2)	0.0136 (19)	0.0005 (15)	0.0007 (15)	0.0071 (14)
C6	0.0119 (16)	0.0177 (19)	0.0170 (18)	0.0002 (14)	−0.0002 (14)	0.0021 (14)

Geometric parameters (Å, º)

S1—O1e	1.437 (3)	C2—H2e	0.97 (4)
S1—O1a	1.441 (3)	C4—C5	1.531 (5)
S1—C6	1.769 (4)	C4—H4a	0.99 (4)
S1—C2	1.780 (4)	C4—H4e	0.94 (4)

S3—O3e	1.439 (3)	C5—C6	1.528 (5)
S3—O3a	1.443 (3)	C5—H5a	0.89 (4)
S3—C4	1.767 (4)	C5—H5e	1.00 (5)
S3—C2	1.795 (4)	C6—H6a	0.95 (4)
C2—H2a	0.98 (4)	C6—H6e	0.95 (4)
O1e—S1—O1a	117.72 (16)	C5—C4—S3	112.3 (3)
O1e—S1—C6	110.10 (17)	C5—C4—H4a	116 (2)
O1a—S1—C6	109.38 (17)	S3—C4—H4a	105 (2)
O1e—S1—C2	106.54 (16)	C5—C4—H4e	111 (2)
O1a—S1—C2	109.14 (16)	S3—C4—H4e	105 (3)
C6—S1—C2	102.89 (17)	H4a—C4—H4e	108 (3)
O3e—S3—O3a	117.64 (15)	C6—C5—C4	114.3 (3)
O3e—S3—C4	110.27 (17)	C6—C5—H5a	112 (3)
O3a—S3—C4	109.24 (17)	C4—C5—H5a	109 (3)
O3e—S3—C2	107.81 (16)	C6—C5—H5e	104 (3)
O3a—S3—C2	107.99 (16)	C4—C5—H5e	108 (3)
C4—S3—C2	102.81 (18)	H5a—C5—H5e	109 (4)
S1—C2—S3	112.73 (19)	C5—C6—S1	111.9 (3)
S1—C2—H2a	107 (2)	C5—C6—H6a	112 (2)
S3—C2—H2a	109 (2)	S1—C6—H6a	106 (2)
S1—C2—H2e	108 (2)	C5—C6—H6e	111 (3)
S3—C2—H2e	107 (2)	S1—C6—H6e	103 (2)
H2a—C2—H2e	113 (3)	H6a—C6—H6e	114 (3)
O1e—S1—C2—S3	172.32 (18)	O3a—S3—C4—C5	−57.4 (3)
O1a—S1—C2—S3	−59.6 (2)	C2—S3—C4—C5	57.1 (3)
C6—S1—C2—S3	56.5 (2)	S3—C4—C5—C6	−66.1 (4)
O3e—S3—C2—S1	−172.54 (18)	C4—C5—C6—S1	66.5 (4)
O3a—S3—C2—S1	59.4 (2)	O1e—S1—C6—C5	−171.4 (3)
C4—S3—C2—S1	−56.0 (2)	O1a—S1—C6—C5	57.8 (3)
O3e—S3—C4—C5	171.8 (3)	C2—S1—C6—C5	−58.2 (3)

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2a⋯O1a[i]	0.98 (4)	2.47 (4)	3.315 (4)	143 (3)
C2—H2a⋯O3a[i]	0.98 (4)	2.76 (4)	3.520 (5)	134 (3)
C2—H2a⋯O3e[ii]	0.98 (4)	2.91 (4)	3.556 (4)	124 (3)
C2—H2e⋯O3a[ii]	0.97 (4)	2.49 (4)	3.201 (4)	130 (3)
C2—H2e⋯O3e[iii]	0.97 (4)	2.49 (4)	3.370 (4)	151 (3)
C4—H4a⋯O3a[i]	0.99 (4)	2.46 (4)	3.329 (4)	147 (3)
C4—H4e⋯O3a[iv]	0.94 (4)	2.70 (4)	3.462 (4)	138 (3)
C4—H4e⋯O3e[v]	0.94 (4)	2.63 (4)	3.454 (5)	146 (3)
C5—H5e⋯O1a[vi]	1.00 (5)	2.91 (5)	3.598 (5)	127 (3)
C5—H5e⋯O1e[vii]	1.00 (5)	2.50 (5)	3.395 (4)	150 (4)
C6—H6a⋯O1a[i]	0.95 (4)	2.45 (4)	3.287 (4)	147 (3)
C6—H6a⋯O1e[vi]	0.95 (4)	2.65 (4)	3.269 (5)	124 (3)

C6—H6*e*···O1*a*[vi]	0.95 (4)	2.81 (4)	3.344 (5)	116 (3)
C6—H6*e*···O1*e*[viii]	0.95 (4)	2.44 (4)	3.186 (5)	135 (3)

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