

Structural parameters of dimethyl sulfoxide, DMSO, at 100 K, based on a redetermination by use of high-quality single-crystal X-ray data

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The title compound, C_2H_6OS , is a high melting, polar and aprotic solvent widely used in organic and inorganic chemistry. It serves as a H-atom acceptor in hydrogen bonding and is used as an ambidentate ligand in coordination chemistry. The evaluation of the influence of intermolecular interactions on the internal structural parameters of the chemically bonded DMSO molecules affords precise structural data of the free molecule as a point of reference. So far, valid data have been obtained only by use of neutron powder diffraction [Ibberson (2005). *Acta Cryst.* **C61**, o571–o573]. In the present redetermination, structural data have been obtained from a single-crystal X-ray diffraction experiment at 100 K, revealing a better comparison with DMSO molecules in other crystal structures. In the solid state, the pyramidal molecule exhibits a nearly perfect C_s symmetry [including H atoms, which are eclipsed with respect to the $C \cdots C$ axis], with a $C-S-C$ bond angle of $97.73(7)^\circ$ and an $S-O$ bond length of $1.5040(10)$ Å, corresponding very well with an $S=O$ double bond, and with almost equal $S-C$ bond lengths [mean value = $1.783(4)$ Å] and $O-S-C$ bond angles [mean value = $106.57(4)^\circ$]. The crystal packing is influenced by $C-H \cdots O$ interactions (2.42 – 2.47 Å) between all three H atoms of only one methyl group with the O atoms of three neighbouring DMSO molecules. The interactions of the O atom with H atoms (or Lewis acids, or hydrogen-donor groups) of adjacent molecules in relation to the orientation of the complete DMSO molecule are described in terms of the angle ω and the distance d_{norm} ; ω is the angle between the pseudo-mirror plane of the molecule and the plane defined through the $S=O$ bond and the interacting atom, and d_{norm} is the distance of the interacting atom from the plane perpendicular to the $S=O$ bond.

1. Chemical context

Dimethyl sulfoxide (DMSO), $(CH_3)_2SO$, is a colourless polar aprotic solvent with high melting (291 K) and boiling points (462 K), miscible with a wide range of organic solvents and water. It is commonly used in organic and inorganic chemistry because of its capability to dissolve numerous polar or nonpolar compounds. In addition to its solvation properties, the molecule may act as a H-atom acceptor in hydrogen bonding, as well as an ambidentate Lewis base in coordination compounds. In the latter case, DMSO reactivity follows the HSAB principle (Pearson, 1963) which means that in combination with 'hard' acids like tin(IV), DMSO coordinates *via* the 'hard' O atom [e.g. $iPrSnCl_3(DMSO-O)_2$; Kastner & Reuter, 1999] and in combination with 'soft' acids like platinum(II) *via* the 'soft' S atom [e.g. $cis-PtCl_2(DMSO-S)_2$; Melanson & Rochon, 1975], while with acids at the 'hard-soft' borderline like ruthenium(II), both coordination modes can be realized [$cis-RuCl_2(DMSO-O)_1(DMSO-S)_3$; Tarighi &

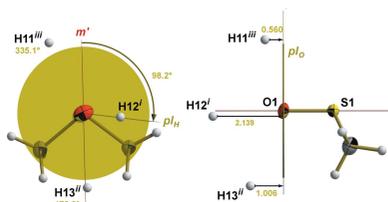
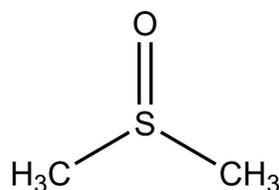


Table 1

Experimental details of previous crystal structure determinations of DMSO and their comparison with the present study.

	Thomas <i>et al.</i> (1966)	Ibberson (2005)	This work
Space group, <i>Z</i>	$P2_1/c$, 4	$P2_1/c$, 4	$P2_1/c$, 4
<i>a</i> (Å)	5.303 (5)	5.2390 (1)	5.2243 (3)
<i>b</i> (Å)	6.829 (3)	6.7581 (1)	6.7414 (4)
<i>c</i> (Å)	11.693 (3)	11.2696 (1)	11.2772 (6)
β (°)	94.5 (3)	94.8053 (3)	94.820 (2)
<i>V</i> (Å ³)	422.2	397.60 (1)	395.77 (4)
<i>T</i> (K)	278	100	100
Sample	single-crystal	powder	single-crystal
Radiation	Mo $K\alpha$	neutron	Mo $K\alpha$
Technique	precession photographs	HRPD	CDC
<i>R</i> value	7.4%	3.77%	2.4%
Number of reflections	777	not given	938
Number of parameters	not given	93	41
H(D) atoms	constrained	refined	constrained
<i>d</i> (S1–O1) (Å)	1.531 (5)	1.496 (2)	1.5040 (10)
<i>d</i> (S1–C1) (Å)	1.775 (8)	1.838 (3)	1.7801 (14)
<i>d</i> (S1–C2) (Å)	1.821 (11)	1.788 (3)	1.7861 (15)
O1–S1–C1 (°)	106.7 (4)	105.2 (2)	106.54 (6)
O1–S1–C2 (°)	106.8 (4)	108.3 (2)	106.60 (7)
C1–S1–C2 (°)	97.4 (4)	96.4 (1)	97.73 (7)

Abbasi, 2007]. DMSO is also used in pharmacology in transdermal drug delivery applications and in veterinary medicine.



Both hydrogen-bond formation and formation of coordination bonds will change the structural parameters of the DMSO molecule, as was shown by Calligaris (2004) for DMSO and other sulfoxides. For the evaluation of the influence of these additional intermolecular bonds on the internal structural parameters of the coordinating or hydrogen-bonded DMSO ligands, precise data on bond lengths and angles within the free molecule are required as a point of reference. The available data, however, in the case of single-crystal X-ray structure determinations, are from the late 1960s (Viswamitra & Kannan, 1966; Thomas *et al.*, 1966) when precession and Weissenberg photographs were state of the art. Therefore,

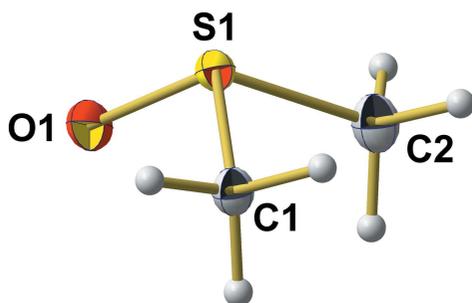


Figure 1

The molecular structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids for the non-H atoms at the 50% probability level.

these data are of less accuracy compared with modern X-ray data obtained with CCD area detectors. More recently, Ibberson (2005) published results on neutron powder diffraction studies of fully deuterated dimethyl sulfoxide at 2 and 100 K. Although, the data obtained are of higher precision than those of the forgoing single-crystal X-ray measurements, they suffer from the limitations of powder diffraction techniques.

In the current study, the results of a redetermination of the crystal structure of DMSO based on single-crystal X-ray data at 100 K are presented. The results are comparatively discussed with the previous structure determinations.

2. Structural commentary

Unit-cell parameters of the current 100 K single-crystal X-ray measurement (SCXD) are consistent with those of the neutron

powder diffraction (NPD) data of Ibberson (2005), but structural parameters of the DMSO molecule differ considerably between the two refinements (Table 1). In the pyramidal molecule of crystallographic point group symmetry C_1 (Fig. 1, atom positions and atom labelling according to NPD), the S atom lies 0.6994 (9) Å above the triangular base formed by the O and C atoms. The S–O bond length of 1.5040 (10) Å is slightly longer than the value [1.496 (2) Å] determined by Ibberson at 100 K, but corresponds very well with a S=O double bond in sulfoxides [1.497 (13) Å; Allen *et al.*, 1987].

Other differences between the single-crystal X-ray and neutron powder diffraction data, however, are strongly expressed with respect to S–C bond lengths and even more with respect to O–S–C bond angles (Table 1). In the case of the neutron data, the difference between both S–C bonds is 0.05 Å [S–C1 = 1.838 (3) Å and S–C2 = 1.788 (3) Å], while in the case of the X-ray data, the difference between both bonds is reduced by a factor of about 10 to 0.006 Å [S–C1 = 1.7801 (14) Å and S–C2 = 1.7861 (15) Å]. Moreover, the bond to atom C1 is shorter than the bond to C2, in contrast to the bond-length distribution observed by Ibberson. This is of

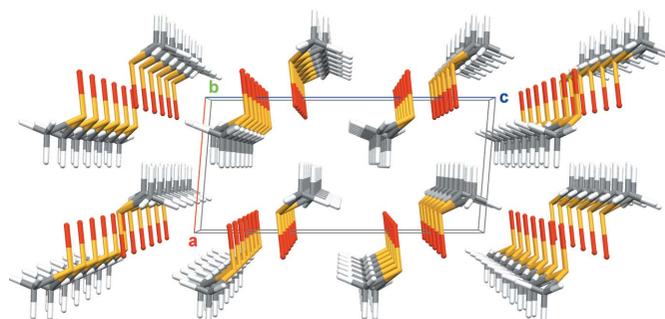


Figure 2

Crystal packing showing the tube-like arrangement of the molecules along the *b* axis.

Table 2
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>
C1–H11···O1 ⁱ	0.98	2.42	3.3318 (18)	155
C1–H12···O1 ⁱⁱ	0.98	2.42	3.3184 (17)	152
C1–H13···O1 ⁱⁱⁱ	0.98	2.47	3.4450 (19)	173
C2–H22···O1 ⁱⁱ	0.98	2.61	3.4618 (18)	146

special interest in view of the C–H···O interactions discussed below. With respect to the C–S–O bond angles, structural differences between the NPD and SCXD model are enormous: the difference between both bond angles of 3.09° [O–S–C1 = 105.21 (16)° and O–S–C2 = 108.30 (15)°] found by Ibberson at 100 K can be compared with a difference of only 0.06° [O–S–C1 = 106.54 (6)° and O–S–C2 = 106.60 (7)°] in the case of the present work. All in all, the ideal *C_s* point group symmetry of the gaseous and liquid DMSO molecule is much better approached in the crystalline state, even at 100 K, than originally assumed from neutron powder data.

Although this symmetry consideration is not affected by the bond angle between the S atom and the methyl groups, it is important – on the background of coordination that seems to have a great influence on this bond angle – to emphasize that in the SCXD model [C–S–C = 97.73 (3)°], this angle is about 1.4° larger than in the NPD model [C–S–C = 96.37 (12)° at 100 K]. With respect to the hydrogen/deuterium positions, no differences occur, as both methyl groups show an eclipsed orientation with respect to C···C, thus fulfilling the nearly ideal *C_s* symmetry, too.

For the sake of completeness, structural data of the previous single-crystal X-ray structure determination by Thomas *et al.* (1966) are also compiled in Table 1.

3. Supramolecular features

C–H···O contacts are the most prominent intermolecular interactions responsible for the three-dimensional arrangement of the DMSO molecules in the solid state (Fig. 2). In order to compare our results with the results of the neutron powder diffraction experiment, one must take into account the different validity and refinement strategies for the H/D atoms in both methods. Under consideration of the van der Waals radii of H (1.10 Å) and O (1.52 Å) supplied by Mantina *et al.* (2009), relevant H···O distances should be shorter than 2.62 Å. From the H atoms attached to C2, only one (H22) shows an interatomic distance below this threshold. With an H22···O1ⁱⁱ (for symmetry code, see Table 2) distance of 2.61 Å, a binding C–H···O interaction other than a van der Waals interaction can be excluded. Just the opposite is observed in case of the H atoms attached to C1: all three H atoms show an intermolecular contact to one O atom of three different DMSO molecules in the range 2.42–2.47 Å (Table 2). In this case, these contacts fall below the van der Waals distance by 7.6–5.7% (0.20–0.15 Å) which justifies the assumption of binding C–H···O interactions. The corresponding intermolecular donor–acceptor distances are in the

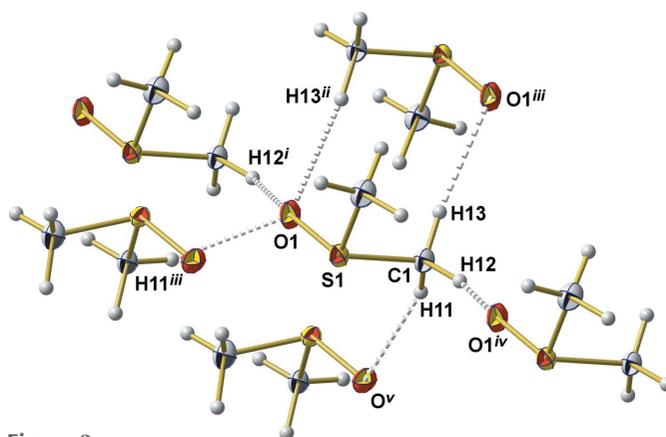


Figure 3
C–H···O contacts (grey broken sticks) between the DMSO molecule and its neighbours. [Symmetry codes used to generate equivalent atoms: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $-1 + x, y, z$; (iii) $-x, -y, -z$; (iv) $1 + x, y, z$; (v) $-x, -\frac{1}{2} + y, \frac{1}{2} - z$.]

range 3.318 (2)–3.445 (2) Å, while the C–H···O angles are in the range 152.0–173.0° (Table 2). In summary, each DMSO molecule participates in six C–H···O contacts to five neighbouring molecules (Fig. 3). The extent of the van der Waals and hydrogen-bonding interactions on the overlapping of the molecules is visualized in Fig. 4. Obviously, there is no weakening influence of these interactions on the S–C bond length. Quite the opposite, the S1–C1 bond is somewhat shorter than the S1–C2 bond (see above).

With respect to the O atom as an acceptor atom, bond angles (S=O···H) of the van der Waals contacts come to 114.0° for H13² (² = $-1 + x, y, z$), 152.1° for H12¹ (¹ = $-x, 0.5 + y, 0.5 - z$), and 103.4° for H11³ (³ = $-x, -y, -z$). The geometrical aspects of these van der Waals interactions (or of coordinatively or hydrogen-bonded DMSO molecules) are described only incompletely with the foregoing used distances and angles as they disregard the orientation of the complete DMSO molecule in relation to the interactions described. In order to unambiguously account for this specific relationship, indexation by two additional values, ω and d_{norm} , using two planes as a reference (Fig. 5) is suggested. The first plane is identical, with the pseudo-mirror plane *m'* defined by O1, S1 and the mid-point between both C atoms. The second plane, *pl_O*, is perpendicular to the S=O bond and located in O1.

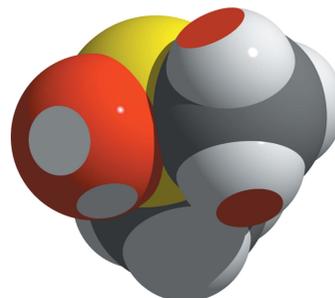
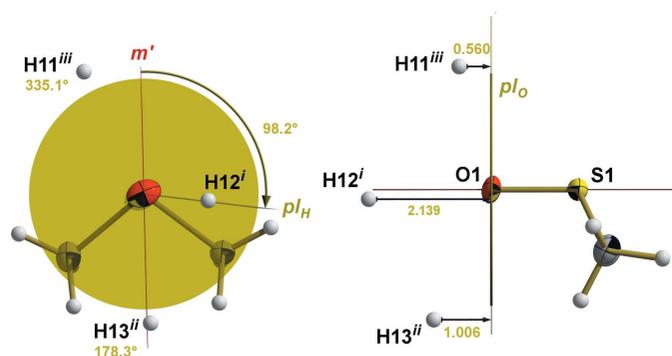


Figure 4
Space-filling model of the DMSO molecule showing four of the six C–H···O contacts. Spheres overlap has been visualized by removing the resulting caps.


Figure 5

Geometrical boundary conditions for the determination of ω (left) and d_{norm} (right, distances in Å) by use of the pseudo-mirror plane m' (definition: O1, S1, mid-point between C1 and C2), the plane pl_H (definition: the interacting atom, S=O bond), and the plane pl_O (definition: O1, S=O bond = normal vector). [Symmetry codes used to generate equivalent atoms: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $-1 + x, y, z$; (iii) $-x, -y, -z$.]

While d_{norm} represents the distance between the interacting atom (*via* a van der Waals interaction, a hydrogen bond or a coordinative bond) and pl_O , the angle ω marks the angle between m' and the plane pl_H defined by O1, S1 and the interacting atom. Values of ω can stretch from 0 to 360° when looking down the O=S bond as in a Newman projection. In the case of the van der Waals interactions discussed here, the corresponding ω/d_{norm} values are: $H12^1 = 98.2^\circ/2.139 \text{ \AA}$, $H13^2 = 178.3^\circ/1.006 \text{ \AA}$ and $H11^3 = 335.1^\circ/0.560 \text{ \AA}$.

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₂ H ₆ OS
M_r	78.13
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	5.2243 (3), 6.7414 (4), 11.2772 (6)
β (°)	94.820 (2)
V (Å ³)	395.77 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.60
Crystal size (mm)	0.21 × 0.17 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2009)
$T_{\text{min}}, T_{\text{max}}$	0.883, 0.913
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5476, 938, 801
R_{int}	0.030
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.024, 0.062, 1.13
No. of reflections	938
No. of parameters	41
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.26, -0.25

Computer programs: APEX2 (Bruker, 2009), SAINT (Bruker, 2009), SHELX597 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), DIAMOND (Brandenburg, 2006), Mercury (Macrae *et al.* (2008) and SHELXTL (Sheldrick, 2008).

4. Synthesis and crystallization

Single crystals were grown from a commercial available sample (Sigma–Aldrich) within a 0.3 mm thick Lindemann capillary using the Kryoflex low-temperature device of the diffractometer.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All six H atoms were found in a difference-Fourier map. They could be refined without any restraints in meaningful positions [C–H range = 0.91 (2)–0.97 (2) Å; H–C–H range = 107.6 (11)–112.2 (15)°] with individual isotropic displacement parameters [range = 0.018 (4)–0.036 (5) Å²]. In order to obtain a structure model comparable to typical refinement techniques of DMSO molecules in the structures of coordination compounds or with hydrogen bonds, conventional constraints [AFIX 137, C–H = 0.99 Å, H–C–H = 109.6° in SHELXL (Sheldrick, 2015)] with two common isotropic displacement parameters, one for each methyl group, have been applied. In summary, these restraints only slightly affected the final results: the final R value increased from 2.37 to 2.42%, while the bond lengths and bond angles remained unchanged. All data have been approved by a second independently grown crystal.

Acknowledgements

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Structural parameters of dimethyl sulfoxide, DMSO, at 100 K, based on a redetermination by use of high-quality single-crystal X-ray data

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2006) and *Mercury* (Macrae *et al.* (2008)); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Dimethyl sulfoxide

Crystal data

C_2H_6OS	$F(000) = 168$
$M_r = 78.13$	$D_x = 1.311 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 5.2243 (3) \text{ \AA}$	Cell parameters from 3349 reflections
$b = 6.7414 (4) \text{ \AA}$	$\theta = 3.5\text{--}28.0^\circ$
$c = 11.2772 (6) \text{ \AA}$	$\mu = 0.60 \text{ mm}^{-1}$
$\beta = 94.820 (2)^\circ$	$T = 100 \text{ K}$
$V = 395.77 (4) \text{ \AA}^3$	Bloc, colourless
$Z = 4$	$0.21 \times 0.17 \times 0.16 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	938 independent reflections
φ and ω scans	801 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$R_{\text{int}} = 0.030$
$T_{\text{min}} = 0.883$, $T_{\text{max}} = 0.913$	$\theta_{\text{max}} = 28.0^\circ$, $\theta_{\text{min}} = 3.5^\circ$
5476 measured reflections	$h = -6 \rightarrow 6$
	$k = -8 \rightarrow 8$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 0.1531P]$
$wR(F^2) = 0.062$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} < 0.001$
938 reflections	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
41 parameters	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
0 restraints	

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.18232 (6)	0.14961 (5)	0.19283 (3)	0.01776 (12)
O1	-0.10440 (18)	0.13580 (16)	0.16758 (10)	0.0245 (3)
C1	0.3139 (3)	-0.0633 (2)	0.12708 (13)	0.0187 (3)
H11	0.2663	-0.1825	0.1698	0.027 (3)*
H12	0.5015	-0.0518	0.1317	0.027 (3)*
H13	0.2465	-0.0729	0.0435	0.027 (3)*
C2	0.2905 (3)	0.3307 (2)	0.09280 (15)	0.0247 (3)
H21	0.2217	0.2994	0.0114	0.033 (3)*
H22	0.4786	0.3299	0.0972	0.033 (3)*
H23	0.2305	0.4623	0.1149	0.033 (3)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01277 (18)	0.02359 (19)	0.0170 (2)	-0.00180 (13)	0.00161 (12)	-0.00362 (15)
O1	0.0115 (5)	0.0353 (6)	0.0269 (6)	-0.0008 (4)	0.0030 (4)	-0.0069 (5)
C1	0.0159 (6)	0.0194 (7)	0.0209 (8)	0.0003 (5)	0.0030 (6)	0.0000 (6)
C2	0.0236 (7)	0.0198 (7)	0.0312 (9)	-0.0001 (6)	0.0042 (6)	0.0018 (6)

Geometric parameters (\AA , $^\circ$)

S1—O1	1.5040 (10)	C1—H13	0.9800
S1—C1	1.7801 (14)	C2—H21	0.9800
S1—C2	1.7861 (15)	C2—H22	0.9800
C1—H11	0.9800	C2—H23	0.9800
C1—H12	0.9800		
O1—S1—C1	106.54 (6)	H12—C1—H13	109.5
O1—S1—C2	106.60 (7)	S1—C2—H21	109.5
C1—S1—C2	97.73 (7)	S1—C2—H22	109.5
S1—C1—H11	109.5	H21—C2—H22	109.5
S1—C1—H12	109.5	S1—C2—H23	109.5
H11—C1—H12	109.5	H21—C2—H23	109.5
S1—C1—H13	109.5	H22—C2—H23	109.5
H11—C1—H13	109.5		

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

<i>D—H\cdotsA</i>	<i>D—H</i>	<i>H\cdotsA</i>	<i>D\cdotsA</i>	<i>D—H\cdotsA</i>
C1—H11 \cdots O1 ⁱ	0.98	2.42	3.3318 (18)	155

C1—H12···O1 ⁱⁱ	0.98	2.42	3.3184 (17)	152
C1—H13···O1 ⁱⁱⁱ	0.98	2.47	3.4450 (19)	173
C2—H22···O1 ⁱⁱ	0.98	2.61	3.4618 (18)	146

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