



Crystal structure of 2-methoxy-2-[(4-methoxyphenyl)sulfanyl]-1-phenyl-ethanone

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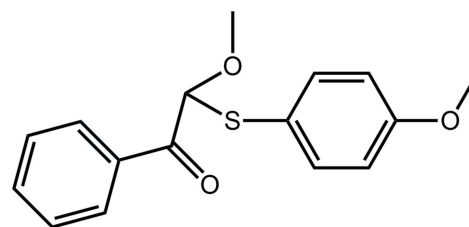
In the title β -thiocarbonyl compound, $C_{16}H_{16}O_3S$, the adjacent methoxy and carbonyl O atoms are synperiplanar [the O—C—C—O torsion angle is $19.8(4)^\circ$] and are separated by $2.582(3)$ Å. The dihedral angle between the rings is $40.11(16)^\circ$, and the methoxy group is coplanar with the benzene ring to which it is connected [the C—C—O—C torsion angle is $179.1(3)^\circ$]. The most notable feature of the crystal packing is the formation of methine and methyl C—H \cdots O(carbonyl) interactions that lead to a supramolecular chain with a zigzag topology along the c axis. Chains pack with no specific intermolecular interactions between them.

Keywords: crystal structure; C—H \cdots O interactions; β -thiocarbonyl; conformation.

CCDC reference: 1416521

1. Related literature

For background to the present structural study, see: Vinhato *et al.* (2013); Zukerman-Schpector *et al.* (2008, 2015); Olivato *et al.* (2013); Distefano *et al.* (1996). For the structure of the methyl derivative, see: Zukerman-Schpector *et al.* (2015). For synthetic procedures, see: Ali & McDermott (2002); Zoretic & Soja (1976).



2. Experimental

2.1. Crystal data

$C_{16}H_{16}O_3S$
 $M_r = 288.35$
Orthorhombic, $Pca2_1$
 $a = 18.769(3)$ Å
 $b = 7.643(1)$ Å
 $c = 10.0578(16)$ Å

$V = 1442.8(4)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.23$ mm⁻¹
 $T = 296$ K
 $0.37 \times 0.16 \times 0.09$ mm

2.2. Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.618$, $T_{\max} = 0.745$

6725 measured reflections
1935 independent reflections
1627 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.076$
 $S = 1.04$
1935 reflections
183 parameters
1 restraint
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.12$ e Å⁻³

$\Delta\rho_{\min} = -0.14$ e Å⁻³
Absolute structure: Flack x
determined using 418 quotients
[$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons
et al., 2013)
Absolute structure parameter:
0.09 (4)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C8-H8\cdots O1^i$	0.98	2.54	3.406 (5)	147
$C16-H16C\cdots O1^{ii}$	0.96	2.47	3.421 (5)	170

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SIR* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *Marvinsketch* (ChemAxon, 2010) and *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5455).

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supporting information

Acta Cryst. (2015). E71, o657–o658 [https://doi.org/10.1107/S2056989015014565]

Crystal structure of 2-methoxy-2-[(4-methoxyphenyl)sulfanyl]-1-phenylethanone

Ignez Caracelli, Paulo R. Olivato, Henrique J. Traesel, Jéssica Valença, Daniel N. S. Rodrigues and Edward R. T. Tiekink

S1. Introduction

As part of our on-going research into the conformational and electronic interactions of β -thio-carbonyl, β -bis-thio-carbonyl and β -thio- β -oxa-carbonyl compounds, *e.g.* N,N-diethyl-2-[(4'-substituted)phenylthio]acetamides, 1-methyl-3-phenylsulfonyl-2-piperidone, 3,3-bis[(4'-substituted)phenylsulfanyl]-1-methyl-2-piperidones, 2-alkylthio-2-alkylsulfinyl-acetophenones, 2-alkylthio-2-phenylsulfonyl-acetophenones, 2-alkylsulfinyl-2-alkylsulfonyl-acetophenones and 2-methoxy-2-[(4'-methylphenyl)sulfanyl]-1-phenylethan-1-one, utilizing spectroscopic, theoretical and X-ray diffraction methods (Distefano *et al.*, 1996; Zukerman-Schpector *et al.*, 2008; Olivato *et al.*, 2013; Vinhato *et al.*, 2013; Zukerman-Schpector *et al.*, 2015) the title compound was synthesized and its crystal structure determined.

S2. Experimental

S2.1. Synthesis and crystallization

4'-Methoxythiophenol (5.0 g, 36 mmol) was reacted with bromine (1.1 ml, 20 mmol) in dichloromethane (250 ml) on an hydrated silica gel support (25 g of SiO₂ and 12 ml of water) to give 4'-methoxyphenyl disulfide (4.0 g, yield = 80%). A white solid was obtained after filtration and evaporation without further purification (Ali & McDermott, 2002). A solution of 2-methoxy acetophenone (0.80 ml, 5.81 mmol, Sigma-Aldrich) in THF (20 ml), was added drop-wise to a cooled (195 K) solution of diisopropylamine (0.90 ml, 6.39 mmol) and butyllithium (4.30 ml, 5.81 mmol) in THF (30 ml). After 30 minutes, a solution of 4'-methoxyphenyl disulfide (1.780 g, 6.39 mmol) with hexamethylphosphoramide (HMPA) (1.0 ml, 5.81 mmol) dissolved in THF (20 ml) was added drop-wise to the enolate solution (Zoretic & Soja, 1976). After stirring for 3 h, water (50 ml) was added at room temperature and extraction with dichloromethane was performed. The organic layer was then treated with saturated solution of ammonium chloride until neutral pH, and then dried over anhydrous magnesium sulfate. A brown oil was obtained after evaporation of the solvent. Purification through flash chromatography with toluene was used to remove the non-polar reactant (disulfide) then acetone to give a mixture of both acetophenones (product and reactant). Crystallization was performed by vapour diffusion of *n*-hexane into a chloroform solution held at 283 K to give pure product (0.3 g, yield = 40%). Suitable crystals for X-ray diffraction were obtained by same pathway; m.pt: 393.5-394.2 K. IR (cm⁻¹): ν (C=O) 1695 (CCl₄). ¹H NMR (CDCl₃, 500 MHz, δ p.p.m.): 3.68 (s, 3H), 3.78 (s, 3H), 5.76 (s, 1H), 6.80–6.82 (m, 2H), 7.24–7.26 (m, 2H), 7.43–7.46 (m, 2H), 7.56–7.59 (m, 1H), 7.94–7.95 (m, 2H). Analysis for C₁₆H₁₆O₃S: calculated (%): C 66.64, H 5.59; found (%): C 66.52, H 5.53. High-Resolution MS calculated (M⁺): 288.0820; found (M⁺): 288.0821.

S2.2. Refinement

Carbon-bound H-atoms were placed in calculated positions ($C-H = 0.93-0.98 \text{ \AA}$) and were included in the refinement in the riding model approximation, with $U_{iso}(H) = 1.2-1.5U_{eq}(C)$.

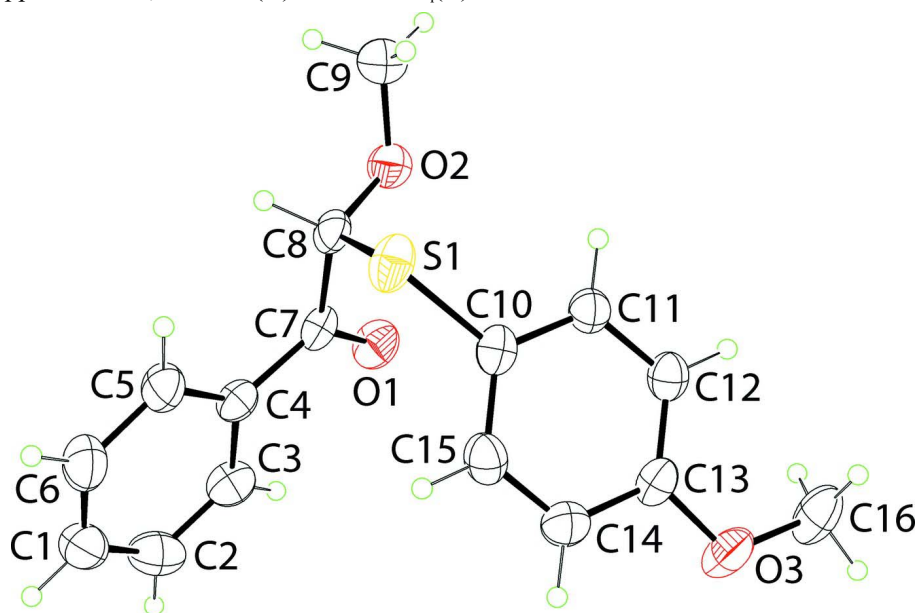


Figure 1

The molecular structure of the title compound showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

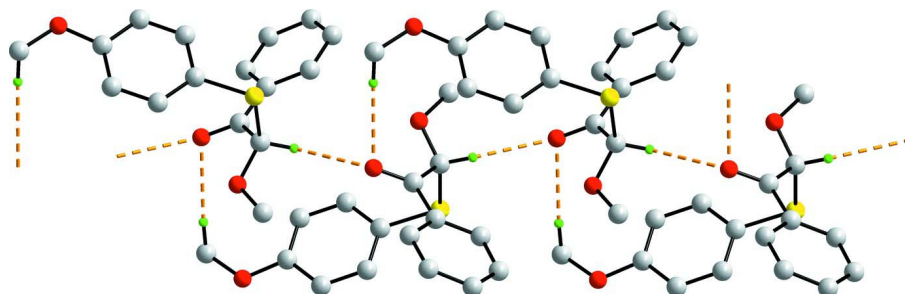


Figure 2

The supramolecular chain in the title compound sustained by $C-H\cdots O$ interactions shown as orange dashed lines. Hydrogen atoms not participating in $C-H\cdots O$ interactions have been omitted for reasons of clarity.

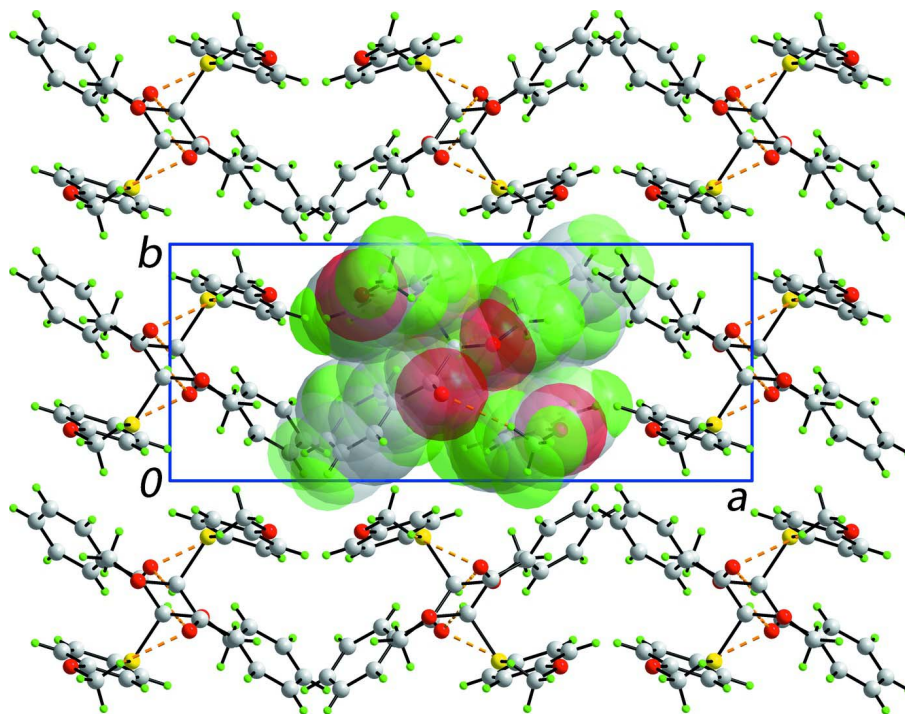


Figure 3

Unit-cell contents of the title compound shown in projection down the c axis. Intermolecular C—H \cdots O interactions are shown as orange dashed lines. One supramolecular chain has been highlighted in space-filling mode.

2-Methoxy-2-[(4-methoxyphenyl)sulfanyl]-1-phenylethanone

Crystal data

$C_{16}H_{16}O_3S$

$M_r = 288.35$

Orthorhombic, $Pca2_1$

$a = 18.769$ (3) Å

$b = 7.643$ (1) Å

$c = 10.0578$ (16) Å

$V = 1442.8$ (4) Å³

$Z = 4$

$F(000) = 608$

$D_x = 1.327$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2745 reflections

$\theta = 2.2$ – 25.1°

$\mu = 0.23$ mm⁻¹

$T = 296$ K

Irregular, colourless

$0.37 \times 0.16 \times 0.09$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.618$, $T_{\max} = 0.745$

6725 measured reflections

1935 independent reflections

1627 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -22 \rightarrow 22$

$k = -8 \rightarrow 9$

$l = -7 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.076$

$S = 1.04$

1935 reflections

183 parameters
 1 restraint
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.2623P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.12 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack x determined using
 418 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*,
 2013)
 Absolute structure parameter: 0.09 (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.

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	0.56536 (5)	0.23724 (10)	0.74255 (12)	0.0585 (3)
O1	0.53351 (13)	0.6345 (3)	0.9109 (3)	0.0608 (6)
O2	0.44516 (10)	0.4243 (3)	0.7959 (3)	0.0588 (6)
O3	0.67048 (13)	0.2149 (3)	1.2961 (3)	0.0702 (8)
C1	0.7294 (2)	0.8300 (5)	0.6168 (5)	0.0670 (11)
H1	0.7687	0.8842	0.5784	0.080*
C2	0.70618 (18)	0.8808 (4)	0.7391 (5)	0.0707 (11)
H2	0.7294	0.9710	0.7834	0.085*
C3	0.64887 (17)	0.8002 (4)	0.7975 (4)	0.0566 (9)
H3	0.6338	0.8355	0.8814	0.068*
C4	0.61332 (15)	0.6666 (4)	0.7325 (4)	0.0441 (7)
C5	0.63593 (19)	0.6186 (5)	0.6074 (4)	0.0587 (9)
H5	0.6117	0.5320	0.5608	0.070*
C6	0.6949 (2)	0.6995 (5)	0.5506 (4)	0.0696 (11)
H6	0.7108	0.6644	0.4672	0.083*
C7	0.55159 (15)	0.5857 (4)	0.8007 (3)	0.0439 (7)
C8	0.51146 (15)	0.4382 (3)	0.7343 (4)	0.0455 (7)
H8	0.5041	0.4685	0.6407	0.055*
C9	0.3949 (2)	0.3296 (5)	0.7185 (4)	0.0718 (12)
H9A	0.4129	0.2143	0.7012	0.108*
H9B	0.3871	0.3894	0.6358	0.108*
H9C	0.3507	0.3213	0.7663	0.108*
C10	0.59396 (18)	0.2334 (4)	0.9103 (4)	0.0448 (8)
C11	0.55035 (17)	0.1718 (4)	1.0103 (4)	0.0474 (8)
H11	0.5045	0.1348	0.9897	0.057*
C12	0.57361 (17)	0.1641 (4)	1.1405 (4)	0.0493 (9)
H12	0.5434	0.1230	1.2068	0.059*
C13	0.64116 (18)	0.2170 (4)	1.1714 (4)	0.0491 (9)
C14	0.68553 (18)	0.2783 (4)	1.0714 (4)	0.0610 (10)
H14	0.7316	0.3143	1.0919	0.073*
C15	0.66189 (18)	0.2860 (4)	0.9429 (4)	0.0550 (9)
H15	0.6921	0.3273	0.8767	0.066*

C16	0.6275 (2)	0.1561 (6)	1.4024 (4)	0.0749 (11)
H16A	0.6538	0.1639	1.4841	0.112*
H16B	0.6138	0.0367	1.3871	0.112*
H16C	0.5856	0.2277	1.4083	0.112*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0873 (6)	0.0513 (4)	0.0370 (5)	0.0083 (4)	−0.0003 (5)	−0.0065 (5)
O1	0.0732 (14)	0.0705 (15)	0.0387 (16)	0.0031 (13)	0.0019 (12)	−0.0129 (13)
O2	0.0561 (13)	0.0760 (15)	0.0444 (16)	−0.0089 (11)	0.0015 (13)	−0.0003 (13)
O3	0.0628 (15)	0.0992 (19)	0.0486 (18)	0.0162 (14)	−0.0127 (15)	0.0049 (15)
C1	0.056 (2)	0.067 (2)	0.078 (4)	−0.0075 (19)	−0.006 (2)	0.015 (2)
C2	0.061 (2)	0.061 (2)	0.090 (4)	−0.0085 (17)	−0.010 (3)	−0.010 (3)
C3	0.061 (2)	0.0537 (18)	0.055 (3)	0.0065 (17)	−0.007 (2)	−0.0090 (18)
C4	0.0491 (16)	0.0415 (14)	0.042 (2)	0.0075 (13)	−0.0069 (16)	−0.0003 (17)
C5	0.073 (2)	0.064 (2)	0.039 (2)	−0.0115 (18)	−0.0002 (19)	−0.0035 (18)
C6	0.075 (2)	0.083 (3)	0.051 (3)	−0.001 (2)	0.009 (2)	0.008 (2)
C7	0.0561 (17)	0.0455 (16)	0.030 (2)	0.0080 (14)	−0.0052 (17)	0.0020 (15)
C8	0.0552 (17)	0.0530 (16)	0.0282 (17)	−0.0006 (14)	−0.0009 (16)	0.0002 (18)
C9	0.070 (2)	0.081 (2)	0.065 (3)	−0.020 (2)	−0.009 (2)	0.002 (2)
C10	0.0572 (19)	0.0356 (16)	0.041 (2)	0.0100 (14)	0.0040 (16)	−0.0001 (15)
C11	0.0507 (18)	0.0478 (18)	0.044 (2)	−0.0021 (14)	0.0007 (16)	0.0018 (16)
C12	0.0536 (19)	0.0496 (19)	0.045 (2)	0.0071 (15)	0.0068 (16)	0.0041 (16)
C13	0.053 (2)	0.055 (2)	0.040 (2)	0.0139 (16)	−0.0016 (18)	0.0033 (16)
C14	0.0455 (18)	0.075 (2)	0.063 (3)	0.0020 (17)	−0.004 (2)	0.008 (2)
C15	0.055 (2)	0.060 (2)	0.050 (3)	0.0023 (17)	0.0125 (19)	0.0059 (18)
C16	0.083 (2)	0.103 (3)	0.039 (3)	0.027 (3)	−0.001 (2)	0.005 (2)

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

S1—C10	1.771 (4)	C7—C8	1.511 (4)
S1—C8	1.841 (3)	C8—H8	0.9800
O1—C7	1.217 (4)	C9—H9A	0.9600
O2—C8	1.394 (3)	C9—H9B	0.9600
O2—C9	1.421 (4)	C9—H9C	0.9600
O3—C13	1.370 (4)	C10—C15	1.376 (5)
O3—C16	1.413 (5)	C10—C11	1.380 (5)
C1—C2	1.361 (6)	C11—C12	1.381 (5)
C1—C6	1.363 (6)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.367 (5)
C2—C3	1.372 (5)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.387 (5)
C3—C4	1.384 (4)	C14—C15	1.368 (6)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.377 (5)	C15—H15	0.9300
C4—C7	1.482 (4)	C16—H16A	0.9600
C5—C6	1.390 (5)	C16—H16B	0.9600

C5—H5	0.9300	C16—H16C	0.9600
C6—H6	0.9300		
C10—S1—C8	102.90 (15)	O2—C9—H9A	109.5
C8—O2—C9	112.8 (3)	O2—C9—H9B	109.5
C13—O3—C16	117.8 (3)	H9A—C9—H9B	109.5
C2—C1—C6	119.8 (4)	O2—C9—H9C	109.5
C2—C1—H1	120.1	H9A—C9—H9C	109.5
C6—C1—H1	120.1	H9B—C9—H9C	109.5
C1—C2—C3	120.7 (4)	C15—C10—C11	118.4 (3)
C1—C2—H2	119.7	C15—C10—S1	120.2 (3)
C3—C2—H2	119.7	C11—C10—S1	121.4 (3)
C2—C3—C4	120.4 (4)	C10—C11—C12	121.2 (3)
C2—C3—H3	119.8	C10—C11—H11	119.4
C4—C3—H3	119.8	C12—C11—H11	119.4
C5—C4—C3	118.6 (3)	C13—C12—C11	119.8 (3)
C5—C4—C7	123.6 (3)	C13—C12—H12	120.1
C3—C4—C7	117.8 (3)	C11—C12—H12	120.1
C4—C5—C6	120.2 (4)	C12—C13—O3	125.3 (3)
C4—C5—H5	119.9	C12—C13—C14	119.5 (4)
C6—C5—H5	119.9	O3—C13—C14	115.2 (3)
C1—C6—C5	120.2 (4)	C15—C14—C13	120.3 (4)
C1—C6—H6	119.9	C15—C14—H14	119.8
C5—C6—H6	119.9	C13—C14—H14	119.8
O1—C7—C4	120.8 (3)	C14—C15—C10	120.8 (3)
O1—C7—C8	119.4 (3)	C14—C15—H15	119.6
C4—C7—C8	119.8 (3)	C10—C15—H15	119.6
O2—C8—C7	107.8 (2)	O3—C16—H16A	109.5
O2—C8—S1	114.0 (2)	O3—C16—H16B	109.5
C7—C8—S1	109.2 (2)	H16A—C16—H16B	109.5
O2—C8—H8	108.6	O3—C16—H16C	109.5
C7—C8—H8	108.6	H16A—C16—H16C	109.5
S1—C8—H8	108.6	H16B—C16—H16C	109.5
C6—C1—C2—C3	0.9 (6)	C4—C7—C8—S1	74.1 (3)
C1—C2—C3—C4	−0.5 (5)	C10—S1—C8—O2	−74.0 (3)
C2—C3—C4—C5	−1.1 (5)	C10—S1—C8—C7	46.6 (3)
C2—C3—C4—C7	−179.6 (3)	C8—S1—C10—C15	−101.2 (3)
C3—C4—C5—C6	2.2 (5)	C8—S1—C10—C11	81.4 (3)
C7—C4—C5—C6	−179.3 (3)	C15—C10—C11—C12	0.6 (4)
C2—C1—C6—C5	0.2 (6)	S1—C10—C11—C12	178.0 (2)
C4—C5—C6—C1	−1.9 (6)	C10—C11—C12—C13	−0.5 (5)
C5—C4—C7—O1	−179.3 (3)	C11—C12—C13—O3	−179.7 (3)
C3—C4—C7—O1	−0.8 (4)	C11—C12—C13—C14	0.2 (5)
C5—C4—C7—C8	2.1 (4)	C16—O3—C13—C12	−1.1 (5)
C3—C4—C7—C8	−179.4 (3)	C16—O3—C13—C14	179.1 (3)
C9—O2—C8—C7	161.9 (3)	C12—C13—C14—C15	0.1 (5)
C9—O2—C8—S1	−76.7 (3)	O3—C13—C14—C15	179.9 (3)

O1—C7—C8—O2	19.8 (4)	C13—C14—C15—C10	0.0 (5)
C4—C7—C8—O2	−161.5 (2)	C11—C10—C15—C14	−0.3 (5)
O1—C7—C8—S1	−104.5 (3)	S1—C10—C15—C14	−177.8 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C8—H8 \cdots O1 ⁱ	0.98	2.54	3.406 (5)	147
C16—H16C \cdots O1 ⁱⁱ	0.96	2.47	3.421 (5)	170

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