

## S-Phenyl 4-methoxybenzoate

Adel S. El-Azab,<sup>a,b</sup> Alaa A.-M. Abdel-Aziz,<sup>a,c</sup> Hussein I. El-Subbagh,<sup>d</sup> Suchada Chantrapromma<sup>e,†</sup> and Hoong-Kun Fun<sup>f,\*§</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia, <sup>b</sup>Department of Organic Chemistry, Faculty of Pharmacy, Al-Azhar University, Cairo 11884, Egypt, <sup>c</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, University of Mansoura, Mansoura 35516, Egypt, <sup>d</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences and Pharmaceutical Industries, Future University, Cairo 12311, Egypt, <sup>e</sup>Crystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, and <sup>f</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia  
Correspondence e-mail: hkfun@usm.my

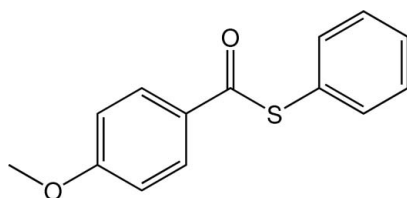
Received 30 January 2012; accepted 7 February 2012

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å; R factor = 0.056; wR factor = 0.199; data-to-parameter ratio = 13.7.

In the molecule of the title thioester,  $\text{C}_{14}\text{H}_{12}\text{O}_2\text{S}$ , the dihedral angle between the phenyl and benzene rings is  $71.8(3)^\circ$ . The methoxy group is essentially coplanar with the benzene ring to which it is bonded, with an r.m.s. deviation of  $0.0065(5)$  Å for the non-H atoms involved. In the crystal, weak  $\text{C}-\text{H}\cdots\pi$  interactions are present.

### Related literature

For background to and applications of thioesters, see: Agapiou & Krische (2003); Choi *et al.* (2003); El-Azab & Abdel-Aziz (2012); Horst *et al.* (2007); Howell *et al.* (2006); Jew *et al.* (2003); Liebeskind & Srogl (2000); McGarvey *et al.* (1986); Ozaki *et al.* (2003); Shah *et al.* (2002); Yang & Drucekhammer (2001). For related structures and the synthesis of similar compounds, see: Barbero *et al.* (2003). For bond-length data, see: Allen *et al.* (1987).



<sup>†</sup> Thomson Reuters ResearcherID: A-5085-2009.

<sup>§</sup> Alternative address: College of Pharmacy (Visiting Professor), King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia. Thomson Reuters ResearcherID: A-3561-2009.

### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{12}\text{O}_2\text{S}$   
 $M_r = 244.31$   
Orthorhombic,  $P2_12_12_1$   
 $a = 5.4478(2)$  Å  
 $b = 8.2149(3)$  Å  
 $c = 27.3841(6)$  Å  
 $V = 1225.52(7)$  Å<sup>3</sup>  
 $Z = 4$   
Cu  $K\alpha$  radiation  
 $\mu = 2.23$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.58 \times 0.22 \times 0.17$  mm

#### Data collection

Bruker SMART APEXII CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2009)  
 $T_{\min} = 0.357$ ,  $T_{\max} = 0.699$   
7810 measured reflections  
2144 independent reflections  
1479 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.050$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.199$   
 $S = 1.22$   
2144 reflections  
156 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
1811 Friedel pairs  
Flack parameter: 0.07 (5)

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3A}\cdots\text{Cg1}^i$	0.93	2.96	3.658 (6)	133

Symmetry code: (i)  $-x - 1, y - \frac{1}{2}, -z + \frac{5}{2}$ .

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

The authors thank the Deanship of Scientific Research and the Research Center of the College of Pharmacy, King Saud University. The authors also thank Universiti Sains Malaysia for Research University grant No. 1001/PFIZIK/811160. HKF thanks King Saud University, Riyadh, Saudi Arabia, for the award of a Visiting Professorship (23 December 2011 to 14 January 2012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5413).

### References

- Agapiou, K. & Krische, M. J. (2003). *Org. Lett.* **5**, 1737–1740.  
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.  
Barbero, M., Degani, I., Dughera, S. & Fochi, R. (2003). *Synthesis*, pp. 1225–1230.  
Bruker (2009). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.  
Choi, J., Imai, E., Mihara, M., Oderaotoshi, Y., Minakata, S. & Komatsu, M. (2003). *J. Org. Chem.* **68**, 6164–6171.  
El-Azab, A. S. & Abdel-Aziz, A. A.-M. (2012). *Phosphorus Sulfur Silicon Relat. Elem.* In the press.

- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Horst, B., Feringa, B. L. & Minnaard, A. J. (2007). *Org. Lett.* **9**, 3013–3015.
- Howell, G. P., Fletcher, S. P., Geurts, K., Horst, B. & Feringa, B. L. (2006). *J. Am. Chem. Soc.* **128**, 14977–14985.
- Jew, S., Park, B., Lim, D., Kim, M. G., Chung, I. K., Kim, J. H., Hong, C. I., Kim, J., Park, H., Lee, J. & Park, H. (2003). *Bioorg. Med. Chem. Lett.* **13**, 609–612.
- Liebeskind, L. S. & Srogl, J. (2000). *J. Am. Chem. Soc.* **122**, 11260–11261.
- McGarvey, G. J., Williams, J. M., Hiner, R. N., Matsubara, Y. & Oh, T. (1986). *J. Am. Chem. Soc.* **108**, 4943–4952.
- Ozaki, S., Adachi, M., Sekiya, S. & Kamikawa, R. (2003). *J. Org. Chem.* **68**, 4586–4589.
- Shah, S. T. A., Khan, K. M., Heinrich, A. M. & Voelter, W. (2002). *Tetrahedron Lett.* **43**, 8281–8283.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Yang, W. & Drueckhammer, D. G. (2001). *J. Am. Chem. Soc.* **123**, 11004–11009.

## supplementary materials

*Acta Cryst.* (2012). E68, o1074–o1075 [doi:10.1107/S1600536812005454]

**S-Phenyl 4-methoxybenzothioate**

**Adel S. El-Azab, Alaa A.-M. Abdel-Aziz, Hussein I. El-Subbagh, Suchada Chantrapromma and Hoong-Kun Fun**

**Comment**

Thioesters are one of the most useful building blocks for organic transformations such as in application of C-C coupling for the synthesis of carbonyl compounds in asymmetric aldol reactions. Recently, the  $\alpha$ - $\beta$ -unsaturated thioester analogs have been successfully applied for asymmetric additions which allow the access to chiral intermediates for the synthesis of more complex compounds. Furthermore, they were used in natural product synthesis and also are acting as biologically relevant substances finding application for *in vivo* tumor suppression (Agapiou & Krische (2003); Barbero *et al.*, 2003; Choi *et al.*, 2003; Horst *et al.*, 2007; Howell *et al.*, 2006; Jew *et al.*, 2003; Liebeskind & Srogl 2000; McGarvey *et al.*, 1986; Ozaki *et al.*, 2003; Shah *et al.*, 2002; Yang & Drueckhammer, 2001). Owing to these applications of thioesters, the title compound (I) was synthesized. The molecule is chiral even though it has no chiral center as its mirror image cannot be superposed onto itself. The absolute configuration and crystal structure are reported. We have examined optically the batch of crystals and the morphology is the same for all the crystals in the batch thereby implying that there is no spontaneous resolution.

In the molecule of (I) shown in Fig. 1, the dihedral angle between the phenyl and benzene rings is 71.8 (3)°. The central O1/C7/S1 plane makes dihedral angles of 10.8 (5) and 81.0 (6)° with the C1–C6 and C8–C13 rings, respectively. The methoxy group of the 4-methoxyphenyl group is essentially co-planar with its bound benzene ring with a r.m.s. deviation of 0.0065 (5) Å for the eight non H atoms (C1/C2/C3/C4/C5/C6/O2/C14) and the torsion angle C14–O2–C4–C3 = -2.1 (8)°. The bond distances in (I) are within normal ranges (Allen *et al.*, 1987).

The crystal structure is consolidated by weak C—H $\cdots$  $\pi$  interactions (Table 1).

**Experimental**

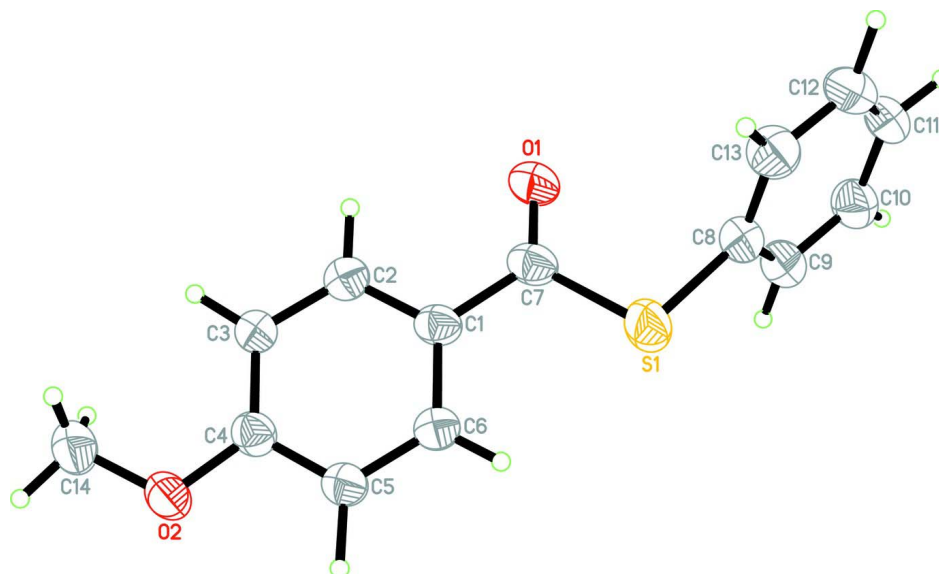
The title compound was synthesized according to El-Azab & Abdel-Aziz (2012). The trifluoroacetic acid (0.4 equiv) was added dropwise to a stirred solution of carboxylic acid (1 equiv) and thiophenol (1 equiv) in dry CH<sub>3</sub>CN (0.01 mol/l) over a period of 15 min at room temperature. After being stirred for 2–5 h at 333 K, the mixture was quenched by adding ammonium chloride solution (5 ml), extracted with ethylacetate, washed with brine and dried over anhydrous sodium sulfate. The product obtained after the evaporation of the solvent was purified by column chromatography using mixture of hexane and CHCl<sub>3</sub> as eluent. The crystal was obtained by slow evaporation of the eluent system hexane and CHCl<sub>3</sub>; m.p. 366–367 K, 97% yield. IR (KBr): 1661 cm<sup>-1</sup> (CO), <sup>1</sup>H NMR (CDCl<sub>3</sub>): d 8.06 (d, 2H, J = 8.5 Hz), 7.55–7.54 (m, 2H), 7.48 (m, 3H), 6.99 (t, 2H, J = 4.0 Hz), 2.90 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>): d 55.6, 113.9, 127.7, 129.2, 129.4, 129.8, 135.2, 164.0, 188.6.

## Refinement

All H atoms were placed in calculated positions with  $d(\text{C—H}) = 0.93$  for aromatic and  $0.96 \text{ \AA}$  for  $\text{CH}_3$  atoms. The  $U_{\text{iso}}$  values were constrained to be  $1.5U_{\text{eq}}$  of the carrier atom for methyl H atoms and  $1.2U_{\text{eq}}$  for the remaining H atoms. A rotating group model was used for the methyl groups. 1811 Friedel pairs were used to determine the absolute configuration.

## Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).



**Figure 1**

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

## S-Phenyl 4-methoxybenzothioate

### Crystal data

$\text{C}_{14}\text{H}_{12}\text{O}_2\text{S}$

$M_r = 244.31$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 5.4478 (2) \text{ \AA}$

$b = 8.2149 (3) \text{ \AA}$

$c = 27.3841 (6) \text{ \AA}$

$V = 1225.52 (7) \text{ \AA}^3$

$Z = 4$

$F(000) = 512$

$D_x = 1.324 \text{ Mg m}^{-3}$

Melting point = 366–367 K

Cu  $K\alpha$  radiation,  $\lambda = 1.54178 \text{ \AA}$

Cell parameters from 2144 reflections

$\theta = 3.2\text{--}69.4^\circ$

$\mu = 2.23 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Needle, colourless

$0.58 \times 0.22 \times 0.17 \text{ mm}$

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer	7810 measured reflections
Radiation source: fine-focus sealed tube	2144 independent reflections
Graphite monochromator	1479 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.050$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$\theta_{\text{max}} = 69.4^\circ$ , $\theta_{\text{min}} = 3.2^\circ$
$T_{\text{min}} = 0.357$ , $T_{\text{max}} = 0.699$	$h = -4 \rightarrow 6$
	$k = -9 \rightarrow 8$
	$l = -32 \rightarrow 29$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2 + 0.2372P]$
$wR(F^2) = 0.199$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.22$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2144 reflections	$\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$
156 parameters	$\Delta\rho_{\text{min}} = -0.28 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXTL</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.025 (3)
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), with 1811 Friedel pairs
	Flack parameter: 0.07 (5)

*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.

**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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.2447 (3)	0.2241 (2)	0.88540 (4)	0.0866 (6)
O1	-0.1014 (8)	0.0079 (5)	0.87109 (10)	0.0848 (13)
O2	-0.0150 (7)	-0.0916 (5)	1.10026 (10)	0.0712 (10)
C1	0.0101 (8)	0.0386 (6)	0.95439 (14)	0.0579 (11)
C2	-0.1770 (8)	-0.0607 (6)	0.97065 (16)	0.0641 (12)
H2A	-0.2939	-0.0981	0.9486	0.077*
C3	-0.1940 (8)	-0.1055 (7)	1.01918 (14)	0.0657 (13)
H3A	-0.3225	-0.1713	1.0297	0.079*
C4	-0.0204 (8)	-0.0527 (6)	1.05180 (14)	0.0596 (11)
C5	0.1682 (8)	0.0475 (6)	1.03636 (15)	0.0637 (12)
H5A	0.2841	0.0853	1.0585	0.076*
C6	0.1830 (8)	0.0911 (7)	0.98763 (15)	0.0625 (12)
H6A	0.3117	0.1568	0.9771	0.075*

C7	0.0229 (9)	0.0742 (7)	0.90125 (15)	0.0653 (13)
C8	0.2346 (9)	0.2180 (7)	0.82059 (16)	0.0684 (13)
C9	0.4109 (10)	0.1329 (7)	0.79629 (16)	0.0773 (15)
H9A	0.5299	0.0757	0.8136	0.093*
C10	0.4122 (11)	0.1319 (8)	0.74530 (17)	0.0827 (17)
H10A	0.5297	0.0722	0.7284	0.099*
C11	0.2390 (10)	0.2194 (7)	0.72047 (17)	0.0779 (14)
H11A	0.2402	0.2198	0.6865	0.094*
C12	0.0654 (11)	0.3056 (9)	0.74480 (18)	0.0860 (18)
H12A	-0.0511	0.3651	0.7275	0.103*
C13	0.0619 (11)	0.3049 (8)	0.79550 (19)	0.0818 (16)
H13A	-0.0574	0.3634	0.8123	0.098*
C14	-0.2089 (11)	-0.1900 (9)	1.11832 (18)	0.096 (2)
H14A	-0.1840	-0.2103	1.1525	0.144*
H14B	-0.2115	-0.2915	1.1010	0.144*
H14C	-0.3624	-0.1347	1.1137	0.144*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.1088 (11)	0.0977 (13)	0.0532 (6)	-0.0329 (9)	-0.0016 (6)	-0.0022 (6)
O1	0.088 (3)	0.107 (4)	0.0589 (17)	-0.019 (2)	-0.0185 (16)	0.0018 (19)
O2	0.083 (2)	0.079 (3)	0.0521 (16)	-0.0038 (17)	-0.0032 (13)	0.0042 (16)
C1	0.058 (2)	0.064 (3)	0.052 (2)	0.0023 (19)	-0.0063 (17)	-0.011 (2)
C2	0.061 (3)	0.066 (4)	0.065 (2)	-0.006 (2)	-0.0035 (18)	0.001 (2)
C3	0.061 (3)	0.083 (4)	0.053 (2)	-0.013 (2)	-0.0014 (17)	0.003 (2)
C4	0.066 (3)	0.060 (3)	0.053 (2)	-0.001 (2)	-0.0001 (17)	-0.006 (2)
C5	0.066 (3)	0.069 (4)	0.056 (2)	-0.008 (2)	-0.0074 (17)	0.000 (2)
C6	0.061 (3)	0.066 (4)	0.060 (2)	-0.009 (2)	-0.0048 (18)	-0.001 (2)
C7	0.066 (3)	0.077 (4)	0.053 (2)	0.008 (2)	-0.0078 (18)	-0.012 (2)
C8	0.069 (3)	0.077 (4)	0.058 (2)	-0.008 (3)	-0.0016 (19)	0.005 (2)
C9	0.077 (3)	0.087 (4)	0.068 (3)	0.001 (3)	-0.003 (2)	0.013 (3)
C10	0.080 (3)	0.102 (5)	0.067 (3)	0.004 (3)	0.007 (2)	0.004 (3)
C11	0.085 (3)	0.096 (4)	0.053 (2)	-0.005 (3)	-0.005 (2)	0.011 (2)
C12	0.081 (4)	0.108 (5)	0.069 (3)	0.006 (3)	-0.015 (3)	0.013 (3)
C13	0.080 (3)	0.086 (5)	0.080 (3)	0.007 (3)	0.002 (2)	0.000 (3)
C14	0.103 (4)	0.120 (6)	0.065 (3)	-0.033 (4)	0.004 (3)	0.014 (3)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

S1—C8	1.776 (4)	C6—H6A	0.9300
S1—C7	1.779 (6)	C8—C9	1.362 (7)
O1—C7	1.199 (5)	C8—C13	1.366 (7)
O2—C4	1.366 (5)	C9—C10	1.397 (6)
O2—C14	1.419 (6)	C9—H9A	0.9300
C1—C6	1.379 (6)	C10—C11	1.367 (7)
C1—C2	1.380 (6)	C10—H10A	0.9300
C1—C7	1.486 (6)	C11—C12	1.356 (8)
C2—C3	1.382 (6)	C11—H11A	0.9300
C2—H2A	0.9300	C12—C13	1.389 (7)

C3—C4	1.371 (6)	C12—H12A	0.9300
C3—H3A	0.9300	C13—H13A	0.9300
C4—C5	1.383 (6)	C14—H14A	0.9600
C5—C6	1.384 (6)	C14—H14B	0.9600
C5—H5A	0.9300	C14—H14C	0.9600
C8—S1—C7	101.7 (2)	C9—C8—S1	118.7 (4)
C4—O2—C14	117.1 (4)	C13—C8—S1	120.6 (4)
C6—C1—C2	118.5 (4)	C8—C9—C10	119.7 (5)
C6—C1—C7	123.6 (4)	C8—C9—H9A	120.2
C2—C1—C7	117.8 (4)	C10—C9—H9A	120.2
C1—C2—C3	121.1 (4)	C11—C10—C9	119.4 (5)
C1—C2—H2A	119.4	C11—C10—H10A	120.3
C3—C2—H2A	119.4	C9—C10—H10A	120.3
C4—C3—C2	119.7 (4)	C12—C11—C10	120.7 (4)
C4—C3—H3A	120.1	C12—C11—H11A	119.6
C2—C3—H3A	120.1	C10—C11—H11A	119.6
O2—C4—C3	125.0 (4)	C11—C12—C13	119.9 (5)
O2—C4—C5	114.9 (4)	C11—C12—H12A	120.0
C3—C4—C5	120.1 (4)	C13—C12—H12A	120.0
C4—C5—C6	119.5 (4)	C8—C13—C12	119.7 (5)
C4—C5—H5A	120.3	C8—C13—H13A	120.2
C6—C5—H5A	120.3	C12—C13—H13A	120.2
C1—C6—C5	121.0 (4)	O2—C14—H14A	109.5
C1—C6—H6A	119.5	O2—C14—H14B	109.5
C5—C6—H6A	119.5	H14A—C14—H14B	109.5
O1—C7—C1	124.0 (5)	O2—C14—H14C	109.5
O1—C7—S1	122.0 (4)	H14A—C14—H14C	109.5
C1—C7—S1	114.0 (3)	H14B—C14—H14C	109.5
C9—C8—C13	120.5 (5)		
C6—C1—C2—C3	0.8 (7)	C6—C1—C7—S1	-12.0 (6)
C7—C1—C2—C3	176.9 (5)	C2—C1—C7—S1	172.1 (3)
C1—C2—C3—C4	-0.9 (8)	C8—S1—C7—O1	-5.6 (5)
C14—O2—C4—C3	-2.2 (8)	C8—S1—C7—C1	173.6 (4)
C14—O2—C4—C5	178.1 (5)	C7—S1—C8—C9	-99.8 (5)
C2—C3—C4—O2	-178.6 (5)	C7—S1—C8—C13	84.1 (5)
C2—C3—C4—C5	1.2 (8)	C13—C8—C9—C10	-1.3 (8)
O2—C4—C5—C6	178.4 (5)	S1—C8—C9—C10	-177.4 (5)
C3—C4—C5—C6	-1.3 (8)	C8—C9—C10—C11	1.4 (9)
C2—C1—C6—C5	-0.9 (8)	C9—C10—C11—C12	-0.6 (9)
C7—C1—C6—C5	-176.8 (5)	C10—C11—C12—C13	-0.3 (9)
C4—C5—C6—C1	1.2 (7)	C9—C8—C13—C12	0.4 (9)
C6—C1—C7—O1	167.1 (5)	S1—C8—C13—C12	176.5 (5)
C2—C1—C7—O1	-8.8 (8)	C11—C12—C13—C8	0.4 (10)

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C1–C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C3-H3A\cdots Cg1^i$	0.93	2.96	3.658 (6)	133

Symmetry code: (i)  $-x-1, y-1/2, -z+5/2$ .