Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methoxy-4-methyl-1-[1-(phenylsulfonyl)propan-2-yl]benzene

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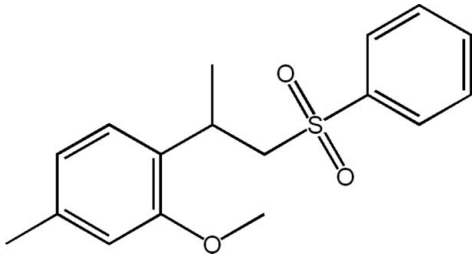
Received 27 August 2011; accepted 3 September 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.187; data-to-parameter ratio = 14.3.

The title molecule, $C_{17}H_{20}O_3S$, displays a U-shaped structure; the two benzene rings are nearly parallel and partially overlapped to each other, the dihedral angle and centroid-to-centroid distance being 15.0 (2)° and 3.723 (2) Å. In the crystal, weak intermolecular C—H···O hydrogen bonds link the molecules, forming supramolecular chains running along the *a* axis.

Related literature

For propargylic sulfides as precusors of indene derivatives, see: Peng *et al.* (2007). For a related structure, see: Xi *et al.* (2004).



Experimental

Crystal data

$C_{17}H_{20}O_3S$
M_r = 304.39
Monoclinic, $P2_1/c$
a = 9.101 (1) Å
b = 12.2579 (14) Å
c = 15.9251 (17) Å
β = 118.307 (1)°
V = 1564.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 K
0.42 × 0.27 × 0.13 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.915, T_{max} = 0.973
7654 measured reflections
2754 independent reflections
1641 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.187
S = 1.08
2754 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11B···O2^{i}	0.96	2.59	3.503 (6)	159

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

Financial support from the Fundamental Research Funds for the Central Universities in NWSUAF (QN2009048) and the Excellent Young Funds (211020712) is greatly appreciated.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5314).

References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Peng, L., Zhang, X., Zhang, S. & Wang, J. (2007). *J. Org. Chem.* **72**, 1192–1197.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Xi, C., Lai, C., Chen, C. & Wang, R. (2004). *Synlett*, **9**, 1595–1597.

supporting information

Acta Cryst. (2011). E**67**, o2589 [https://doi.org/10.1107/S1600536811035987]

2-Methoxy-4-methyl-1-[1-(phenylsulfonyl)propan-2-yl]benzene

Bao-Jun Shi, Li-Chun Ding, Gang Chen and Zhen-Ting Du

S1. Comment

Propargylic sulfides have been studied as the precusor of indene derivatives (Peng *et al.* 2007). As a result of our program of screening of new indene derivatives, we obtained a intermediate compound $C_{17}H_{20}O_3S$ (I) and the synthesis and structure are reported here.

There are two benzene rings in the title compound and they exhibit face-to-face conformation. The dihedral angle between the two benzene rings is 12.0 (2)°. The molecules of **I** are crystalized in $P2_1/c$ space group which is different from that of 2–phenyl–1–(*p*–toluenesulfonyl)propan–2–ol (*Pbca*, Xi *et al.*, 2004). In the crystal structure there is an intermolecular C—H···O hydrogen-bonding interaction (Table 1), which is helpful to the stabilization of the packing.

S2. Experimental

A mixture of 1-(1-bromopropan-2-yl)-4-methylbenzene (1.0 g, 4.7 mmol) and sodium benzenesulfinate (0.83 g, 5.6 mmol) in dry DMF (20 mL) was stirred over night at 80°C. When the reaction was completed, 50 mL water was added to the mixture and was extracted with ethyl acetate. The ethyl acetate layer was washed by 50 mL water, then 15 mL saturated sodium chloride and over anhydrous sodium sulfate and was separated on silica gel column chromatography with a gradient of petroleum ether and ethyl acetate as eluent to yield 1.3 g the title compound. The compound was then dissolved in ethyl acetate, and colorless crystals were formed on slow evaporation at room temperature over one week.

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.93 Å and N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C, N).

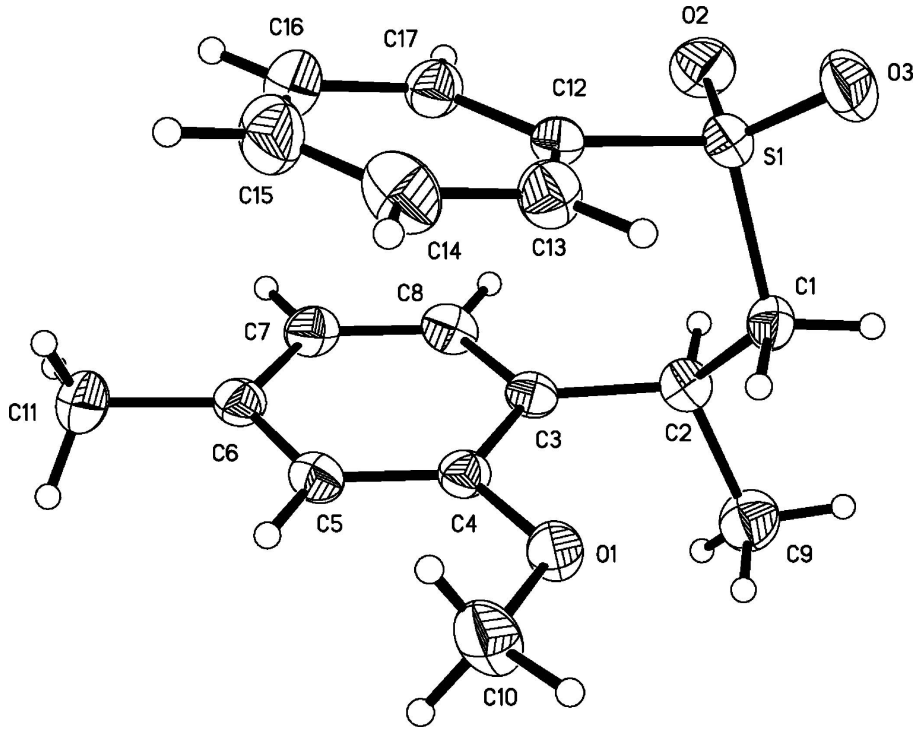


Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

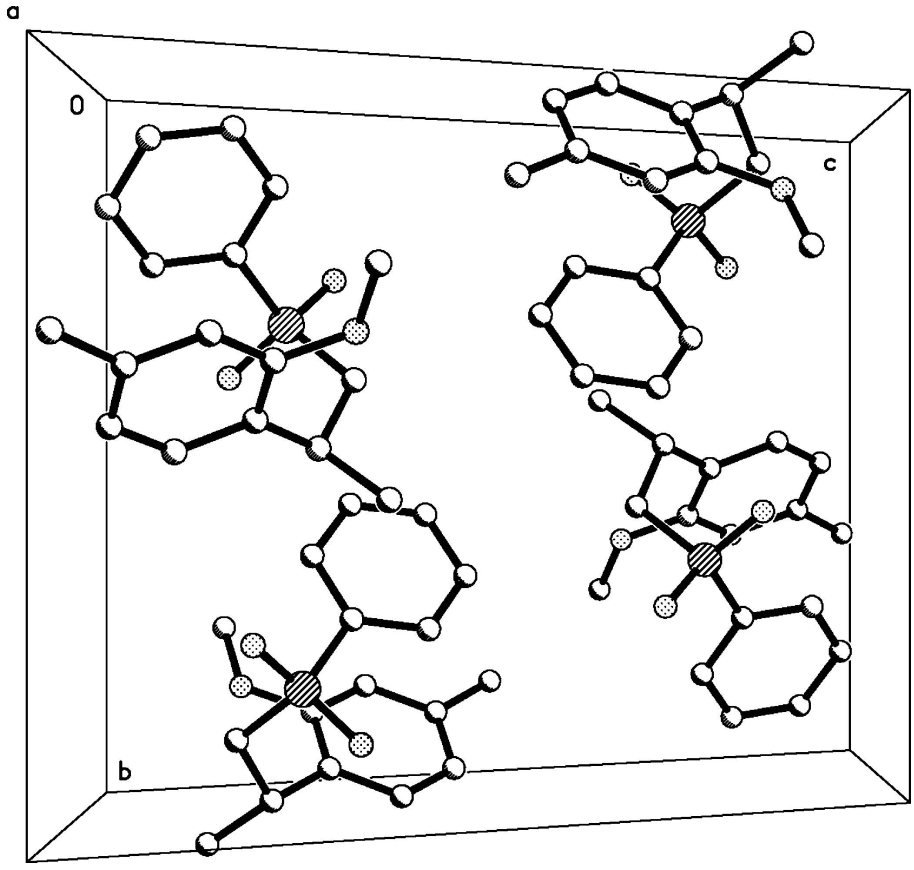


Figure 2

The molecular packing of (I) viewed along the *a* axis, with hydrogen bonds shown as dashed lines.

2-Methoxy-4-methyl-1-[1-(phenylsulfonyl)propan-2-yl]benzene

Crystal data

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$c = 15.9251\ (17)$ Å
$\beta = 118.307\ (1)°$
$V = 1564.1\ (3)$ Å^3
$Z = 4$
$F(000) = 648$
$D_x = 1.293$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1375 reflections
$\theta = 2.5–23.0°$
$\mu = 0.21$ mm^{-1}
$T = 298$ K
Block, colorless
0.42 × 0.27 × 0.13 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.915$, $T_{max} = 0.973$
7654 measured reflections
2754 independent reflections
1641 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
$h = -10\rightarrow10$
$k = -14\rightarrow14$
$l = -11\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.187$
$S = 1.08$
2754 reflections
193 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0032P)^2 + 0.4143P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.9829 (3)	0.3534 (2)	0.33678 (17)	0.0512 (7)
O2	0.3680 (3)	0.4052 (2)	0.16790 (19)	0.0622 (8)
O3	0.4268 (4)	0.2682 (2)	0.2938 (2)	0.0677 (9)
S1	0.48398 (11)	0.33304 (8)	0.23977 (7)	0.0450 (3)
C1	0.6540 (4)	0.4104 (3)	0.3246 (2)	0.0419 (9)
H1A	0.6215	0.4415	0.3693	0.050*
H1B	0.7460	0.3608	0.3601	0.050*
C2	0.7182 (4)	0.5027 (3)	0.2863 (3)	0.0431 (9)
H2	0.6230	0.5508	0.2496	0.052*
C3	0.7823 (4)	0.4663 (3)	0.2192 (2)	0.0372 (9)
C4	0.9128 (4)	0.3909 (3)	0.2449 (3)	0.0394 (9)
C5	0.9644 (4)	0.3587 (3)	0.1804 (3)	0.0434 (9)
H5	1.0517	0.3091	0.1993	0.052*
C6	0.8891 (4)	0.3985 (3)	0.0877 (3)	0.0429 (9)
C7	0.7631 (4)	0.4745 (3)	0.0628 (3)	0.0470 (10)
H7	0.7123	0.5040	0.0016	0.056*
C8	0.7120 (4)	0.5070 (3)	0.1277 (3)	0.0453 (10)
H8	0.6270	0.5583	0.1091	0.054*
C9	0.8460 (5)	0.5702 (3)	0.3700 (3)	0.0619 (12)
H9A	0.9400	0.5253	0.4095	0.093*
H9B	0.7955	0.5973	0.4069	0.093*
H9C	0.8825	0.6305	0.3460	0.093*
C10	1.1077 (5)	0.2713 (4)	0.3645 (3)	0.0709 (13)
H10A	1.0622	0.2083	0.3246	0.106*
H10B	1.1445	0.2514	0.4298	0.106*

H10C	1.2005	0.2987	0.3579	0.106*
C11	0.9425 (5)	0.3583 (4)	0.0172 (3)	0.0630 (12)
H11A	0.9019	0.2854	−0.0021	0.095*
H11B	1.0621	0.3586	0.0463	0.095*
H11C	0.8975	0.4053	−0.0376	0.095*
C12	0.5631 (4)	0.2425 (3)	0.1847 (3)	0.0381 (9)
C13	0.6598 (5)	0.1548 (3)	0.2355 (3)	0.0529 (10)
H13	0.6851	0.1441	0.2987	0.063*
C14	0.7178 (6)	0.0837 (3)	0.1916 (4)	0.0674 (13)
H14	0.7839	0.0248	0.2255	0.081*
C15	0.6790 (6)	0.0988 (4)	0.0979 (4)	0.0694 (13)
H15	0.7183	0.0496	0.0687	0.083*
C16	0.5828 (5)	0.1856 (4)	0.0468 (3)	0.0628 (12)
H16	0.5575	0.1958	−0.0165	0.075*
C17	0.5239 (5)	0.2579 (3)	0.0910 (3)	0.0481 (10)
H17	0.4578	0.3168	0.0572	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0449 (15)	0.0676 (16)	0.0393 (15)	0.0191 (13)	0.0185 (13)	0.0142 (13)
O2	0.0437 (16)	0.0711 (17)	0.0598 (18)	0.0197 (13)	0.0147 (15)	0.0003 (15)
O3	0.074 (2)	0.0761 (18)	0.077 (2)	−0.0205 (16)	0.0555 (18)	−0.0102 (17)
S1	0.0406 (6)	0.0526 (6)	0.0480 (6)	−0.0027 (4)	0.0259 (5)	−0.0040 (5)
C1	0.044 (2)	0.0461 (19)	0.039 (2)	0.0018 (16)	0.0228 (18)	−0.0041 (17)
C2	0.045 (2)	0.0388 (19)	0.047 (2)	0.0029 (16)	0.0223 (19)	0.0027 (17)
C3	0.0347 (19)	0.0327 (17)	0.043 (2)	−0.0027 (15)	0.0171 (18)	0.0024 (16)
C4	0.036 (2)	0.043 (2)	0.037 (2)	−0.0035 (16)	0.0158 (18)	0.0027 (17)
C5	0.036 (2)	0.045 (2)	0.048 (2)	0.0028 (16)	0.0190 (19)	0.0011 (18)
C6	0.040 (2)	0.046 (2)	0.044 (2)	−0.0085 (16)	0.0200 (18)	−0.0016 (17)
C7	0.046 (2)	0.054 (2)	0.036 (2)	−0.0035 (18)	0.0164 (19)	0.0102 (18)
C8	0.042 (2)	0.041 (2)	0.051 (2)	0.0014 (16)	0.021 (2)	0.0116 (18)
C9	0.069 (3)	0.054 (2)	0.065 (3)	−0.009 (2)	0.034 (3)	−0.012 (2)
C10	0.058 (3)	0.095 (3)	0.063 (3)	0.039 (2)	0.032 (2)	0.035 (3)
C11	0.067 (3)	0.082 (3)	0.046 (2)	−0.005 (2)	0.031 (2)	−0.008 (2)
C12	0.035 (2)	0.0393 (18)	0.040 (2)	−0.0058 (15)	0.0178 (17)	−0.0037 (17)
C13	0.054 (2)	0.057 (2)	0.049 (2)	0.0062 (19)	0.025 (2)	0.008 (2)
C14	0.067 (3)	0.047 (2)	0.097 (4)	0.013 (2)	0.046 (3)	0.007 (3)
C15	0.079 (3)	0.058 (3)	0.085 (4)	0.000 (2)	0.050 (3)	−0.017 (3)
C16	0.070 (3)	0.072 (3)	0.052 (3)	−0.004 (2)	0.033 (2)	−0.012 (2)
C17	0.049 (2)	0.051 (2)	0.043 (2)	−0.0013 (18)	0.021 (2)	0.0019 (19)

Geometric parameters (Å, º)

O1—C4	1.369 (4)	C8—H8	0.9300
O1—C10	1.422 (4)	C9—H9A	0.9600
O2—S1	1.435 (3)	C9—H9B	0.9600
O3—S1	1.438 (3)	C9—H9C	0.9600

S1—C12	1.766 (4)	C10—H10A	0.9600
S1—C1	1.771 (3)	C10—H10B	0.9600
C1—C2	1.527 (5)	C10—H10C	0.9600
C1—H1A	0.9700	C11—H11A	0.9600
C1—H1B	0.9700	C11—H11B	0.9600
C2—C3	1.507 (5)	C11—H11C	0.9600
C2—C9	1.530 (5)	C12—C17	1.372 (5)
C2—H2	0.9800	C12—C13	1.382 (5)
C3—C8	1.378 (5)	C13—C14	1.370 (6)
C3—C4	1.404 (5)	C13—H13	0.9300
C4—C5	1.375 (5)	C14—C15	1.374 (6)
C5—C6	1.389 (5)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.373 (6)
C6—C7	1.382 (5)	C15—H15	0.9300
C6—C11	1.501 (5)	C16—C17	1.388 (5)
C7—C8	1.379 (5)	C16—H16	0.9300
C7—H7	0.9300	C17—H17	0.9300

C4—O1—C10	117.9 (3)	C2—C9—H9A	109.5
O2—S1—O3	118.67 (18)	C2—C9—H9B	109.5
O2—S1—C12	108.05 (17)	H9A—C9—H9B	109.5
O3—S1—C12	107.38 (16)	C2—C9—H9C	109.5
O2—S1—C1	108.94 (16)	H9A—C9—H9C	109.5
O3—S1—C1	105.84 (17)	H9B—C9—H9C	109.5
C12—S1—C1	107.48 (17)	O1—C10—H10A	109.5
C2—C1—S1	117.0 (2)	O1—C10—H10B	109.5
C2—C1—H1A	108.0	H10A—C10—H10B	109.5
S1—C1—H1A	108.0	O1—C10—H10C	109.5
C2—C1—H1B	108.0	H10A—C10—H10C	109.5
S1—C1—H1B	108.0	H10B—C10—H10C	109.5
H1A—C1—H1B	107.3	C6—C11—H11A	109.5
C3—C2—C1	114.4 (3)	C6—C11—H11B	109.5
C3—C2—C9	112.8 (3)	H11A—C11—H11B	109.5
C1—C2—C9	109.2 (3)	C6—C11—H11C	109.5
C3—C2—H2	106.6	H11A—C11—H11C	109.5
C1—C2—H2	106.6	H11B—C11—H11C	109.5
C9—C2—H2	106.6	C17—C12—C13	120.6 (4)
C8—C3—C4	116.8 (4)	C17—C12—S1	119.8 (3)
C8—C3—C2	120.0 (3)	C13—C12—S1	119.6 (3)
C4—C3—C2	123.2 (3)	C14—C13—C12	119.3 (4)
O1—C4—C5	123.4 (3)	C14—C13—H13	120.4
O1—C4—C3	115.7 (3)	C12—C13—H13	120.4
C5—C4—C3	120.9 (3)	C13—C14—C15	120.4 (4)
C4—C5—C6	121.5 (3)	C13—C14—H14	119.8
C4—C5—H5	119.3	C15—C14—H14	119.8
C6—C5—H5	119.3	C16—C15—C14	120.7 (4)
C7—C6—C5	117.8 (4)	C16—C15—H15	119.6
C7—C6—C11	121.7 (4)	C14—C15—H15	119.6

C5—C6—C11	120.5 (3)	C15—C16—C17	119.1 (4)
C8—C7—C6	120.6 (4)	C15—C16—H16	120.5
C8—C7—H7	119.7	C17—C16—H16	120.5
C6—C7—H7	119.7	C12—C17—C16	119.9 (4)
C3—C8—C7	122.4 (3)	C12—C17—H17	120.0
C3—C8—H8	118.8	C16—C17—H17	120.0
C7—C8—H8	118.8		

O2—S1—C1—C2	−39.9 (3)	C5—C6—C7—C8	−1.6 (5)
O3—S1—C1—C2	−168.6 (3)	C11—C6—C7—C8	177.5 (3)
C12—S1—C1—C2	76.9 (3)	C4—C3—C8—C7	1.4 (5)
S1—C1—C2—C3	−60.9 (4)	C2—C3—C8—C7	−178.4 (3)
S1—C1—C2—C9	171.6 (3)	C6—C7—C8—C3	−0.1 (5)
C1—C2—C3—C8	121.4 (3)	O2—S1—C12—C17	7.0 (3)
C9—C2—C3—C8	−112.9 (4)	O3—S1—C12—C17	136.1 (3)
C1—C2—C3—C4	−58.5 (4)	C1—S1—C12—C17	−110.4 (3)
C9—C2—C3—C4	67.2 (4)	O2—S1—C12—C13	−171.0 (3)
C10—O1—C4—C5	−4.4 (5)	O3—S1—C12—C13	−41.9 (3)
C10—O1—C4—C3	175.7 (3)	C1—S1—C12—C13	71.6 (3)
C8—C3—C4—O1	178.7 (3)	C17—C12—C13—C14	0.7 (6)
C2—C3—C4—O1	−1.4 (5)	S1—C12—C13—C14	178.7 (3)
C8—C3—C4—C5	−1.2 (5)	C12—C13—C14—C15	−0.7 (6)
C2—C3—C4—C5	178.7 (3)	C13—C14—C15—C16	0.5 (7)
O1—C4—C5—C6	179.6 (3)	C14—C15—C16—C17	−0.5 (7)
C3—C4—C5—C6	−0.5 (5)	C13—C12—C17—C16	−0.7 (5)
C4—C5—C6—C7	1.9 (5)	S1—C12—C17—C16	−178.6 (3)
C4—C5—C6—C11	−177.3 (3)	C15—C16—C17—C12	0.5 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O2^{i}	0.96	2.59	3.503 (6)	159

Symmetry code: (i) *x*+1, *y*, *z*.