Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Benzhydryl phenyl sulfone

Mahiuddin Baidya, Herbert Mayr and Peter Mayer*

Ludwig-Maximilians-Universität, Department, Butenandtstrasse 5–13, 81377 München, Germany
Correspondence e-mail: pemay@cup.uni-muenchen.de

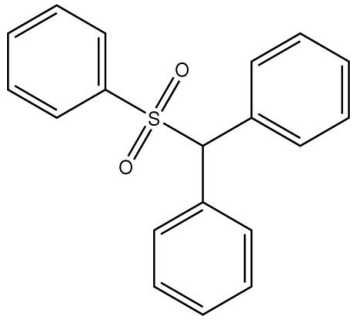
Received 3 November 2009; accepted 23 November 2009

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.075; data-to-parameter ratio = 17.6.

In the title compound, $C_{19}H_{16}O_2S$, the sulfur-bound phenyl group is approximately parallel to one of the two phenyl rings of the benzhydryl group, making a dihedral angle of 12.53 (10)°, and forms a dihedral angle of 41.25 (9)° with the other phenyl ring. In the crystal, weak C—H···O interactions form a two-dimensional network propagating along the *bc* plane.

Related literature

For background to the sulfone anion, see: da Silva Corrêa *et al.* (1968); Mayr *et al.* (2001, 2008). For a related structure, see: Li *et al.* (2005). For graph-set analysis of hydrogen-bond networks, see: Bernstein *et al.* (1995); Etter *et al.* (1990).



Experimental

Crystal data

$C_{19}H_{16}O_2S$
M_r = 308.40
Orthorhombic, $Pca2_1$
a = 16.3250 (4) Å
b = 5.7979 (1) Å
c = 16.4983 (4) Å
V = 1561.58 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 200 K
0.20 × 0.10 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
11675 measured reflections
3499 independent reflections
3136 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.075
S = 1.04
3499 reflections
199 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 1646 Friedel pairs
Flack parameter: −0.03 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{i}	1.00	2.46	3.449 (2)	171
C4—H4···O1^{ii}	0.95	2.66	3.390 (2)	134
C7—H7···O2^{i}	0.95	2.68	3.543 (2)	152

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

Data collection: *COLLECT* (Hooft, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009).

The authors thank Professor Peter Klüfers for generous allocation of diffractometer time.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2011).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hooft, R. W. W. (2004). *COLLECT*. Bruker–Nonius BV, Delft, The Netherlands.
Li, Y.-S. & Su, W.-K. (2005). *Acta Cryst.* E**61**, o2450–o2451.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Mayr, H., Bug, T., Gotta, M. F., Hering, N., Irrgang, B., Janker, B., Kempf, B., Loos, R., Ofial, A. R., Remennikov, G. & Schimmel, H. (2001). *J. Am. Chem. Soc.* **123**, 9500–9512.
Mayr, H. & Ofial, A. R. (2008). *J. Phys. Org. Chem.* **21**, 584–595.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Silva Corrêa, C. M. M. da, Lindsay, A. S. & Waters, W. A. (1968). *J. Chem. Soc C.*, pp. 1872–1874.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2009). E**65**, o3224 [doi:10.1107/S1600536809050363]

Benzhydryl phenyl sulfone

Mahiuddin Baidya, Herbert Mayr and Peter Mayer

S1. Comment

During our studies on the ambident reactivity of the phenylsulfinate anion we used diarylcarbenium ions (Ar_2CH^+) as reference electrophiles [Mayr *et al.* (2001, 2008)] and, hence, obtained the title compound from a reaction of sodium benzenesulfinate with benzhydryl chloride (Ph_2CHCl) in dimethyl sulfoxide.

The asymmetric unit of the title compound contains one complete molecule, which is shown in Figure 1. The sulfur-bound phenyl group is approximately parallel to one of the two phenyl rings of the benzhydryl group with an dihedral angle of 12.53 (10)°. The other one forms a dihedral angle of 41.25 (9)° with the phenyl group bound to the sulfur atom.

Three weak C–H···O interactions are found (Table 1) which lead to the formation of a two-dimensional network that propagates along the *bc* plane (Fig. 2). Contacts of this type have been described for a structure of a related sulfone [Li *et al.* (2005)]. In terms of graph-set analysis [Bernstein *et al.* (1995), Etter *et al.* (1990)], the descriptors on the unitary level are $C_1^1(4)$ for the H1···O2 interaction, $C_1^1(6)$ for the H7···O2 interaction, and $C_1^1(7)$ for the H4···O1 interaction.

S2. Experimental

Benzhydryl Phenyl Sulfone was obtained by heating a mixture of sodium benzenesulfinate (0.21 g, 1.3 mmol) and benzhydryl chloride (0.26 g, 1.3 mmol) in DMSO at 70 °C. After completion of the reaction (4 h), the reaction mixture was cooled to room temperature, diluted with water, and extracted with ethyl acetate. The organic phase was washed several times with water and dried ($MgSO_4$). A viscous oil was obtained after evaporation of the solvent under reduced pressure that solidified on standing. After column chromatography (silica gel, isohexane/EtOAc = 9/1), benzhydryl phenyl sulfone was isolated as colorless solid (0.33 g, 82%). A small amount of the title compound was dissolved in ethyl acetate. The solvent was allowed to evaporate slowly at room temperature. After 2 days crystals had formed that were suitable for X-ray analysis. mp 189 °C (186–187 °C [da Silva Corrêa *et al.* (1968)]).

S3. Refinement

All H atoms were found in difference maps. C-bonded H atoms were positioned geometrically (C—H = 1.00 Å for aliphatic, 0.95 Å for aromatic H) and treated as riding on their parent atoms [U_{iso}(H) = 1.2U_{eq}(C)].

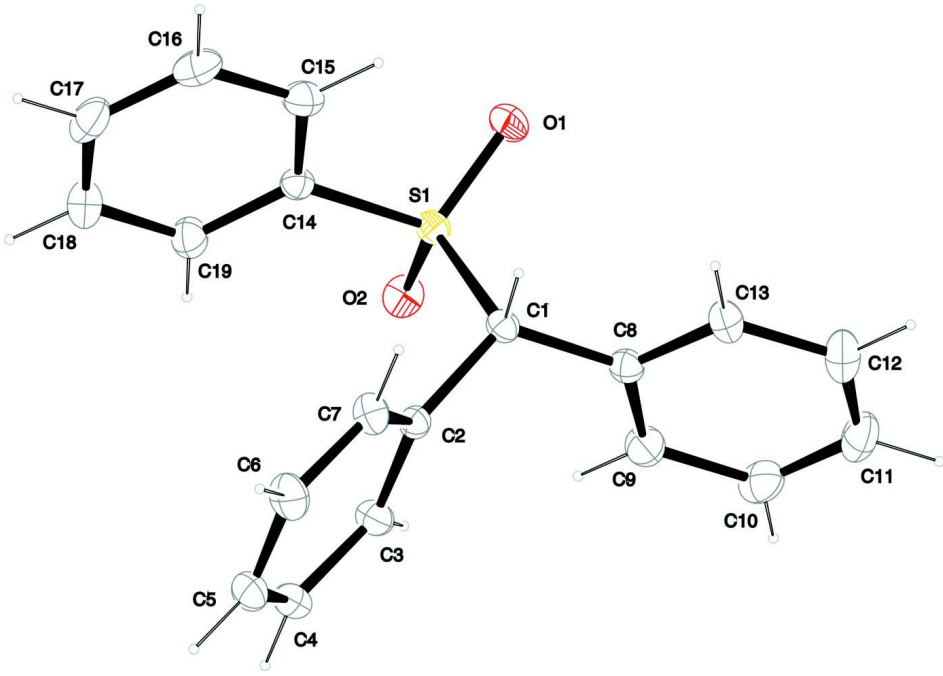


Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

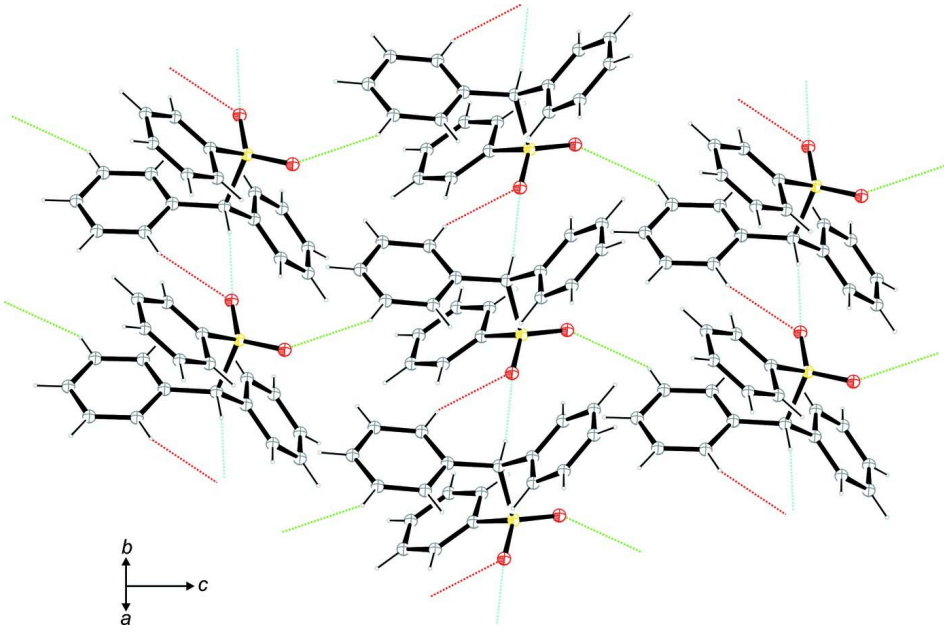


Figure 2

Weak intermolecular hydrogen bonds of the type C–H···O leading to a two-dimensional network that propagates along the *bc* plane (viewing direction approximately along [110]). Color scheme for dashed lines: blue: H1···O2 contacts, red: H7···O2 contacts, green: H4···O1 contacts.

Benzhydryl phenyl sulfone

Crystal data

$C_{19}H_{16}O_2S$
$M_r = 308.40$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 16.3250$ (4) Å
$b = 5.7979$ (1) Å
$c = 16.4983$ (4) Å
$V = 1561.58$ (6) Å^3
$Z = 4$
$F(000) = 648$
$D_x = 1.312$ (1) Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6504 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.21$ mm^{-1}
$T = 200$ K
Rod, colourless
0.20 × 0.10 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
MONTEL, graded multilayered X-ray optics monochromator
Detector resolution: 9 pixels mm^{-1}
CCD; rotation images; thick slices, phi/ω–scan
11675 measured reflections
3499 independent reflections
3136 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -21 \rightarrow 21$
$k = -7 \rightarrow 6$
$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.075$
$S = 1.04$
3499 reflections
199 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.2163P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983), 1646 Friedel pairs
Absolute structure parameter: −0.03 (6)

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.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.06340 (2)	0.12898 (6)	0.26302 (3)	0.02887 (10)
O1	0.08669 (8)	0.1945 (2)	0.34378 (7)	0.0408 (3)
O2	0.03981 (7)	−0.10715 (19)	0.24877 (8)	0.0384 (3)

C1	−0.01788 (10)	0.3229 (3)	0.23092 (10)	0.0276 (3)
H1	0.0034	0.4820	0.2409	0.033*
C2	−0.03155 (9)	0.3073 (3)	0.14009 (10)	0.0272 (3)
C3	−0.06491 (11)	0.1160 (3)	0.10143 (11)	0.0347 (4)
H3	−0.0816	−0.0139	0.1324	0.042*
C4	−0.07391 (11)	0.1141 (3)	0.01781 (12)	0.0405 (4)
H4	−0.0964	−0.0180	−0.0080	0.049*
C5	−0.05082 (12)	0.2999 (4)	−0.02807 (12)	0.0428 (4)
H5	−0.0576	0.2970	−0.0853	0.051*
C6	−0.01740 (12)	0.4927 (4)	0.00955 (13)	0.0451 (5)
H6	−0.0008	0.6218	−0.0218	0.054*
C7	−0.00847 (11)	0.4955 (3)	0.09276 (11)	0.0363 (4)
H7	0.0138	0.6283	0.1182	0.044*
C8	−0.09145 (10)	0.2969 (3)	0.28610 (9)	0.0304 (4)
C9	−0.14154 (12)	0.1021 (3)	0.28814 (12)	0.0431 (4)
H9	−0.1290	−0.0274	0.2551	0.052*
C10	−0.20970 (13)	0.0971 (4)	0.33832 (13)	0.0500 (5)
H10	−0.2444	−0.0343	0.3383	0.060*
C11	−0.22748 (13)	0.2805 (4)	0.38811 (13)	0.0531 (5)
H11	−0.2740	0.2751	0.4227	0.064*
C12	−0.17763 (14)	0.4719 (4)	0.38771 (14)	0.0547 (5)
H12	−0.1895	0.5985	0.4223	0.066*
C13	−0.10994 (12)	0.4802 (3)	0.33668 (11)	0.0406 (4)
H13	−0.0760	0.6133	0.3365	0.049*
C14	0.14411 (10)	0.2005 (3)	0.19613 (10)	0.0292 (3)
C15	0.18653 (11)	0.4044 (3)	0.20890 (12)	0.0407 (4)
H15	0.1739	0.5002	0.2539	0.049*
C16	0.24784 (12)	0.4662 (3)	0.15468 (14)	0.0479 (5)
H16	0.2775	0.6055	0.1623	0.057*
C17	0.26549 (12)	0.3259 (4)	0.09010 (13)	0.0503 (5)
H17	0.3075	0.3691	0.0532	0.060*
C18	0.22315 (13)	0.1231 (4)	0.07798 (14)	0.0517 (5)
H18	0.2364	0.0267	0.0333	0.062*
C19	0.16122 (12)	0.0598 (3)	0.13093 (12)	0.0403 (4)
H19	0.1311	−0.0782	0.1224	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03180 (18)	0.02898 (18)	0.02584 (18)	0.00027 (14)	−0.00044 (18)	0.00176 (17)
O1	0.0447 (7)	0.0530 (8)	0.0247 (6)	0.0025 (6)	−0.0042 (5)	0.0005 (5)
O2	0.0408 (6)	0.0273 (6)	0.0471 (9)	−0.0006 (4)	0.0029 (6)	0.0047 (5)
C1	0.0315 (8)	0.0251 (8)	0.0263 (8)	−0.0019 (6)	0.0000 (7)	−0.0014 (6)
C2	0.0257 (7)	0.0301 (8)	0.0258 (8)	0.0028 (6)	0.0008 (6)	0.0011 (6)
C3	0.0384 (9)	0.0357 (9)	0.0301 (9)	−0.0062 (7)	−0.0017 (7)	−0.0001 (7)
C4	0.0394 (9)	0.0507 (11)	0.0312 (10)	−0.0053 (8)	−0.0032 (8)	−0.0060 (8)
C5	0.0423 (10)	0.0597 (12)	0.0262 (9)	0.0046 (9)	−0.0005 (8)	0.0006 (8)
C6	0.0561 (13)	0.0471 (11)	0.0321 (9)	0.0014 (9)	0.0063 (9)	0.0098 (7)

C7	0.0440 (10)	0.0316 (9)	0.0334 (9)	−0.0002 (7)	0.0045 (7)	0.0013 (7)
C8	0.0327 (8)	0.0324 (8)	0.0261 (9)	0.0015 (6)	−0.0017 (6)	0.0028 (6)
C9	0.0433 (10)	0.0450 (11)	0.0410 (11)	−0.0093 (8)	0.0040 (8)	−0.0017 (8)
C10	0.0403 (10)	0.0638 (13)	0.0460 (12)	−0.0138 (9)	0.0040 (9)	0.0146 (10)
C11	0.0409 (10)	0.0738 (14)	0.0445 (12)	0.0098 (10)	0.0133 (9)	0.0159 (11)
C12	0.0575 (13)	0.0597 (13)	0.0470 (12)	0.0113 (10)	0.0174 (10)	−0.0022 (10)
C13	0.0465 (10)	0.0412 (10)	0.0340 (10)	0.0044 (8)	0.0048 (8)	−0.0049 (8)
C14	0.0270 (8)	0.0333 (8)	0.0273 (8)	0.0008 (6)	−0.0026 (7)	0.0016 (7)
C15	0.0384 (10)	0.0429 (10)	0.0409 (11)	−0.0064 (8)	−0.0044 (8)	−0.0039 (8)
C16	0.0340 (9)	0.0507 (11)	0.0589 (13)	−0.0111 (9)	−0.0065 (9)	0.0088 (10)
C17	0.0320 (9)	0.0683 (13)	0.0505 (12)	0.0027 (9)	0.0089 (9)	0.0144 (10)
C18	0.0466 (11)	0.0625 (13)	0.0459 (12)	0.0048 (9)	0.0128 (10)	−0.0074 (10)
C19	0.0402 (9)	0.0394 (9)	0.0414 (11)	0.0016 (8)	0.0045 (8)	−0.0056 (8)

Geometric parameters (Å, º)

S1—O1	1.4366 (13)	C9—C10	1.387 (3)
S1—O2	1.4415 (12)	C9—H9	0.9500
S1—C14	1.7681 (17)	C10—C11	1.374 (3)
S1—C1	1.8180 (16)	C10—H10	0.9500
C1—C8	1.514 (2)	C11—C12	1.376 (3)
C1—C2	1.518 (2)	C11—H11	0.9500
C1—H1	1.0000	C12—C13	1.390 (3)
C2—C3	1.390 (2)	C12—H12	0.9500
C2—C7	1.394 (2)	C13—H13	0.9500
C3—C4	1.387 (3)	C14—C19	1.379 (2)
C3—H3	0.9500	C14—C15	1.386 (2)
C4—C5	1.369 (3)	C15—C16	1.389 (3)
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.390 (3)	C16—C17	1.371 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.381 (3)	C17—C18	1.378 (3)
C6—H6	0.9500	C17—H17	0.9500
C7—H7	0.9500	C18—C19	1.386 (3)
C8—C13	1.385 (2)	C18—H18	0.9500
C8—C9	1.395 (3)	C19—H19	0.9500
O1—S1—O2	118.23 (7)	C10—C9—C8	120.08 (19)
O1—S1—C14	108.64 (8)	C10—C9—H9	120.0
O2—S1—C14	108.67 (8)	C8—C9—H9	120.0
O1—S1—C1	107.45 (8)	C11—C10—C9	120.67 (19)
O2—S1—C1	110.16 (7)	C11—C10—H10	119.7
C14—S1—C1	102.53 (8)	C9—C10—H10	119.7
C8—C1—C2	118.10 (14)	C10—C11—C12	119.74 (19)
C8—C1—S1	110.02 (11)	C10—C11—H11	120.1
C2—C1—S1	110.99 (11)	C12—C11—H11	120.1
C8—C1—H1	105.6	C11—C12—C13	120.05 (19)
C2—C1—H1	105.6	C11—C12—H12	120.0

S1—C1—H1	105.6	C13—C12—H12	120.0
C3—C2—C7	118.25 (15)	C8—C13—C12	120.79 (18)
C3—C2—C1	123.92 (15)	C8—C13—H13	119.6
C7—C2—C1	117.83 (14)	C12—C13—H13	119.6
C4—C3—C2	120.27 (16)	C19—C14—C15	121.46 (17)
C4—C3—H3	119.9	C19—C14—S1	119.94 (13)
C2—C3—H3	119.9	C15—C14—S1	118.53 (13)
C5—C4—C3	120.94 (18)	C14—C15—C16	118.82 (18)
C5—C4—H4	119.5	C14—C15—H15	120.6
C3—C4—H4	119.5	C16—C15—H15	120.6
C4—C5—C6	119.59 (18)	C17—C16—C15	119.91 (18)
C4—C5—H5	120.2	C17—C16—H16	120.0
C6—C5—H5	120.2	C15—C16—H16	120.0
C7—C6—C5	119.67 (18)	C16—C17—C18	120.89 (19)
C7—C6—H6	120.2	C16—C17—H17	119.6
C5—C6—H6	120.2	C18—C17—H17	119.6
C6—C7—C2	121.27 (17)	C17—C18—C19	120.03 (19)
C6—C7—H7	119.4	C17—C18—H18	120.0
C2—C7—H7	119.4	C19—C18—H18	120.0
C13—C8—C9	118.64 (17)	C14—C19—C18	118.88 (18)
C13—C8—C1	117.33 (15)	C14—C19—H19	120.6
C9—C8—C1	124.03 (15)	C18—C19—H19	120.6

O1—S1—C1—C8	−61.76 (13)	C13—C8—C9—C10	1.9 (3)
O2—S1—C1—C8	68.31 (13)	C1—C8—C9—C10	−177.35 (17)
C14—S1—C1—C8	−176.16 (11)	C8—C9—C10—C11	−1.8 (3)
O1—S1—C1—C2	165.65 (11)	C9—C10—C11—C12	0.6 (3)
O2—S1—C1—C2	−64.28 (13)	C10—C11—C12—C13	0.5 (3)
C14—S1—C1—C2	51.25 (12)	C9—C8—C13—C12	−0.9 (3)
C8—C1—C2—C3	−59.0 (2)	C1—C8—C13—C12	178.46 (18)
S1—C1—C2—C3	69.33 (18)	C11—C12—C13—C8	−0.3 (3)
C8—C1—C2—C7	121.61 (17)	O1—S1—C14—C19	144.32 (14)
S1—C1—C2—C7	−110.03 (15)	O2—S1—C14—C19	14.45 (16)
C7—C2—C3—C4	0.6 (3)	C1—S1—C14—C19	−102.16 (15)
C1—C2—C3—C4	−178.76 (17)	O1—S1—C14—C15	−38.52 (16)
C2—C3—C4—C5	−0.5 (3)	O2—S1—C14—C15	−168.39 (13)
C3—C4—C5—C6	0.4 (3)	C1—S1—C14—C15	75.01 (15)
C4—C5—C6—C7	−0.5 (3)	C19—C14—C15—C16	−0.3 (3)
C5—C6—C7—C2	0.7 (3)	S1—C14—C15—C16	−177.45 (15)
C3—C2—C7—C6	−0.7 (3)	C14—C15—C16—C17	−0.2 (3)
C1—C2—C7—C6	178.68 (17)	C15—C16—C17—C18	0.0 (3)
C2—C1—C8—C13	−120.05 (16)	C16—C17—C18—C19	0.7 (3)
S1—C1—C8—C13	111.14 (15)	C15—C14—C19—C18	1.0 (3)
C2—C1—C8—C9	59.2 (2)	S1—C14—C19—C18	178.09 (15)
S1—C1—C8—C9	−69.59 (19)	C17—C18—C19—C14	−1.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	1.00	2.46	3.449 (2)	171
C4—H4···O1^{ii}	0.95	2.66	3.390 (2)	134
C7—H7···O2^{i}	0.95	2.68	3.543 (2)	152

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