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(1*R*,4*R*,7*S*)-1,7-Dimethyl-7-(phenylsulfonylmethyl)spiro[bicyclo[2.2.1]heptane-2,2′-1,3-dioxolane]

Ya-Wen Wang and Yu Peng*

Department of Chemistry, State Key Laboratory of Applied Organic Chemstry, College of Chemical Engineering, Lanzhou University, Lanzhou 730000, People's Republic of China
Correspondence e-mail: pengyu@lzu.edu.cn

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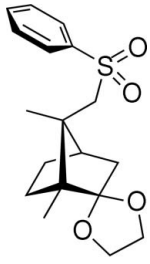
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.083; data-to-parameter ratio = 14.6.

In the title compound, $C_{18}H_{24}O_4S$, the chiral bicyclo[2.2.1]heptane group is not symmetrical due to the influence of the substituents. The angle between the three-atom bridge plane and the four-atom planes of the boat-shaped six-membered ring are 55.07 (19) and 56.24 (19)°. The bridgehead angle is 92.75 (17)°.

Related literature

For related literature, see: Antczak *et al.* (1987); García Martínez *et al.* (2004); Gorichko *et al.* (2002); Kuo & Money (1988); Money (1985); Tanyeli *et al.* (2004); Trost *et al.* (1979); Vaillancourt & Albizati (1993). For related structures, see: Bear & Trotter (1975); Cullen *et al.* (1988); Komarov *et al.* (1997); Takasu *et al.* (2000).



Experimental

Crystal data

$C_{18}H_{24}O_4S$
M_r = 336.43
Orthorhombic, $P2_12_12_1$
a = 10.5420 (2) Å
b = 11.7946 (2) Å
c = 13.2997 (3) Å
V = 1653.67 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.12 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
8969 measured reflections
3080 independent reflections
2595 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.083
S = 1.01
3080 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1307 Friedel pairs
Flack parameter: 0.09 (9)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2344).

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(1*R*,4*R*,7*S*)-1,7-Dimethyl-7-(phenylsulfonylmethyl)spiro[bicyclo-[2.2.1]heptane-2,2′-1,3-dioxolane]

Ya-Wen Wang and Yu Peng

S1. Comment

The uniqueness of the bicyclic structure of camphor is illustrated by a wide variety of intriguing structure transformations that frequently involve fascinating rearrangement processes (Money, 1985; García Martínez *et al.*, 2004). Studies towards these transformations have produced much chemical knowledge on theoretical and mechanistic aspects of organic chemistry in the past century and offered synthetically useful chiral building blocks (Kuo & Money, 1988; Vaillancourt & Albizati, 1993) and chiral ligands (Tanyeli *et al.*, 2004; Gorichko *et al.*, 2002; Komarov *et al.*, 1997) from readily available natural camphor. Some related X-ray structures (Beta & Trotter, 1975; Cullen *et al.*, 1988; Takasu *et al.*, 2000; Antczak *et al.*, 1987) have been obtained.

The chiral bicyclo[2.2.1]heptane group is not symmetrical due to the influence of the substituents. The angles between the three-atom bridge plane, C10, C13, C14 and the four-atom planes (C9, C10, C14, C18 and C10, C11, C12, C14) of the boat-shaped six-membered ring are 55.07 (19) and 56.24 (19)° while the bridgehead angle is 92.75 (17)°.

S2. Experimental

The title compound was prepared by the reaction of sodium benzenesulfinate with (+)-8-bromocamphor (Bear & Trotter, 1975) ketal through the literature method (Trost *et al.*, 1979). Single crystals suitable for X-ray determination were obtained by slow evaporation of a EtOAc solution over a period of several days. IR (film): 3063, 2961, 2883, 1586, 1478, 1448, 1306, 1145, 1084, 1053, 1023, 972, 742, 691 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): 7.93 (d, J=7.2 Hz, 2H), 7.65 (t, J=8.5 Hz, 1H), 7.56 (t, J=8.0 Hz, 2H), 4.12 (d, J=14.7 Hz, 1H), 3.91–3.86 (m, 1H), 3.84–3.81(m, 1H), 3.76–3.70 (m, 2H), 2.90 (d, J=14.7 Hz, 1H), 2.11 (dt, J=3.4, 13.7 Hz, 1H), 1.94–1.89 (m, 1H), 1.77–1.75 (m, 1H), 1.52 (d, J=13.9 Hz, 1H), 1.37–1.26 (m, 3H), 1.23 (s, 3H), 0.89 (s, 3H) p.p.m.; EIMS m/*z* (%): 336 (M^+, 0.6), 321 (3.3), 272 (1), 235 (1), 181 (38), 125 (3), 109 (14), 95 (100); HRMS (ESI): calcd. for $C_{18}H_{25}SO_{4+}$ $[M+H]_+$: 337.1468, found: 337.1460.

S3. Refinement

All H atoms were placed geometrically (C—H values were set to 0.98, 0.97, 0.96 and 0.93 A° for atoms CH, CH_2, CH_3, and CH (phenyl), respectively) and refined with a riding model, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C), or1.5 U_{eq}(O).

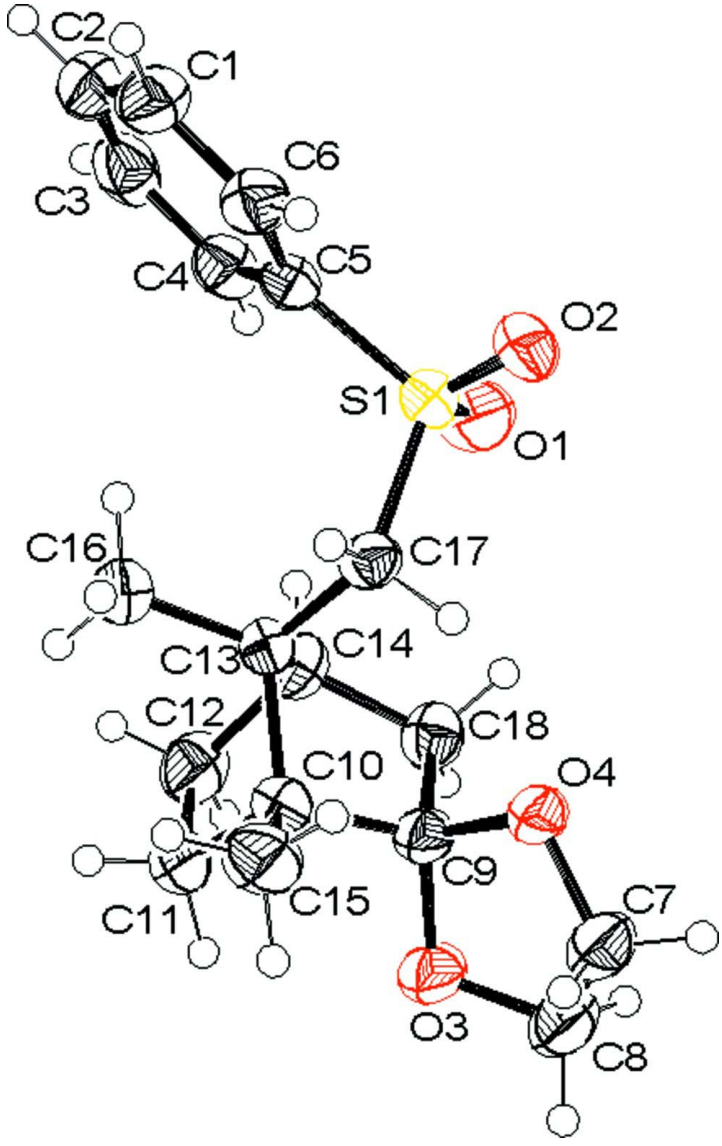

Figure 1

The independent components of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

(1*R*,4*R*,7*S*)-1,7-Dimethyl-7- (phenylsulfonylmethyl)spiro[bicyclo[2.2.1]heptane-2,2′-1,3-dioxolane]

Crystal data

$C_{18}H_{24}O_4S$
$M_r = 336.43$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.5420\ (2)$ Å
$b = 11.7946\ (2)$ Å
$c = 13.2997\ (3)$ Å
$V = 1653.67\ (6)$ Å^3
$Z = 4$
$F(000) = 720$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2482 reflections
$\theta = 2.3–22.9°$
$\mu = 0.21$ mm^{-1}
$T = 294$ K
Block, colorless
0.22 × 0.20 × 0.12 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
8969 measured reflections
3080 independent reflections
2595 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.083$
$S = 1.01$
3080 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.3259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0024 (6)
Absolute structure: Flack (1983), 1307 Friedel pairs
Absolute structure parameter: 0.09 (9)

Special details

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 $F^2 > \sigma(F^2)$ 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}
C1	0.8521 (3)	0.4745 (2)	0.8698 (2)	0.0553 (7)
H1	0.9141	0.4185	0.8671	0.066*
C2	0.7480 (3)	0.4684 (2)	0.8078 (2)	0.0573 (8)
H2	0.7396	0.4083	0.7630	0.069*
C3	0.6567 (3)	0.5508 (2)	0.81181 (19)	0.0559 (7)
H3	0.5869	0.5464	0.7693	0.067*
C4	0.6670 (2)	0.6412 (2)	0.87884 (18)	0.0460 (6)
H4	0.6050	0.6972	0.8814	0.055*
C5	0.7711 (2)	0.64549 (17)	0.94106 (17)	0.0366 (5)
C6	0.8644 (3)	0.5640 (2)	0.93635 (18)	0.0458 (6)
H6	0.9353	0.5690	0.9777	0.055*
C7	0.9448 (3)	1.1891 (2)	1.1304 (2)	0.0520 (7)
H7A	1.0316	1.2009	1.1088	0.062*
H7B	0.9416	1.1890	1.2033	0.062*
C8	0.8581 (3)	1.2769 (2)	1.08728 (18)	0.0543 (7)
H8A	0.7817	1.2846	1.1273	0.065*
H8B	0.8999	1.3500	1.0829	0.065*

C9	0.8317 (2)	1.11268 (18)	0.99706 (16)	0.0393 (6)
C10	0.8975 (2)	1.06072 (19)	0.90376 (17)	0.0386 (6)
C11	0.8356 (3)	1.1177 (2)	0.81204 (18)	0.0526 (7)
H11A	0.8811	1.0990	0.7509	0.063*
H11B	0.8342	1.1995	0.8199	0.063*
C12	0.7000 (3)	1.0694 (2)	0.80945 (18)	0.0545 (7)
H12A	0.6838	1.0296	0.7469	0.065*
H12B	0.6373	1.1289	0.8177	0.065*
C13	0.8356 (2)	0.93875 (18)	0.89830 (16)	0.0352 (5)
C14	0.6987 (2)	0.9872 (2)	0.89958 (17)	0.0420 (6)
H14	0.6319	0.9295	0.8967	0.050*
C15	1.0411 (2)	1.0690 (2)	0.9064 (2)	0.0567 (7)
H15C	1.0757	1.0343	0.8472	0.085*
H15A	1.0726	1.0307	0.9650	0.085*
H15B	1.0657	1.1474	0.9087	0.085*
C16	0.8700 (3)	0.8742 (2)	0.80203 (17)	0.0474 (6)
H16B	0.9595	0.8591	0.8013	0.071*
H16C	0.8478	0.9192	0.7445	0.071*
H16A	0.8242	0.8039	0.8000	0.071*
C17	0.8764 (2)	0.86578 (17)	0.98851 (17)	0.0353 (5)
H17B	0.8897	0.9172	1.0444	0.042*
H17A	0.9587	0.8340	0.9719	0.042*
C18	0.6982 (2)	1.0590 (2)	0.99592 (17)	0.0440 (6)
H18B	0.6847	1.0121	1.0549	0.053*
H18A	0.6329	1.1168	0.9933	0.053*
O1	0.65482 (17)	0.79178 (14)	1.05340 (14)	0.0596 (5)
O2	0.8532 (2)	0.70566 (14)	1.11702 (12)	0.0606 (5)
O3	0.83048 (18)	1.23328 (13)	0.99050 (12)	0.0545 (5)
O4	0.89416 (16)	1.08703 (13)	1.08999 (11)	0.0438 (4)
S1	0.78162 (6)	0.75224 (5)	1.03435 (4)	0.04187 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0658 (19)	0.0410 (14)	0.0590 (17)	0.0034 (14)	0.0122 (16)	−0.0026 (13)
C2	0.077 (2)	0.0501 (16)	0.0452 (15)	−0.0175 (16)	0.0103 (15)	−0.0074 (12)
C3	0.0596 (18)	0.0666 (18)	0.0417 (14)	−0.0257 (17)	−0.0051 (13)	0.0071 (13)
C4	0.0445 (15)	0.0467 (14)	0.0468 (15)	−0.0053 (12)	0.0025 (12)	0.0061 (11)
C5	0.0384 (13)	0.0340 (12)	0.0375 (12)	−0.0076 (11)	0.0056 (11)	0.0016 (9)
C6	0.0477 (16)	0.0437 (13)	0.0461 (15)	−0.0036 (13)	−0.0010 (12)	−0.0001 (11)
C7	0.0631 (18)	0.0451 (14)	0.0476 (15)	−0.0054 (14)	−0.0085 (13)	−0.0096 (13)
C8	0.0682 (18)	0.0419 (15)	0.0529 (15)	0.0028 (13)	−0.0070 (14)	−0.0101 (11)
C9	0.0514 (15)	0.0297 (11)	0.0368 (12)	0.0014 (11)	−0.0056 (11)	0.0007 (9)
C10	0.0434 (14)	0.0358 (12)	0.0366 (13)	−0.0043 (11)	0.0009 (11)	0.0030 (10)
C11	0.080 (2)	0.0418 (14)	0.0361 (13)	−0.0009 (15)	−0.0051 (13)	0.0042 (11)
C12	0.067 (2)	0.0502 (15)	0.0459 (15)	0.0102 (14)	−0.0169 (14)	−0.0006 (12)
C13	0.0398 (13)	0.0350 (11)	0.0307 (11)	−0.0037 (10)	0.0021 (10)	0.0001 (10)
C14	0.0392 (14)	0.0460 (13)	0.0407 (13)	0.0013 (11)	−0.0061 (11)	−0.0040 (11)

C15	0.0490 (16)	0.0571 (17)	0.0639 (18)	−0.0137 (13)	0.0117 (14)	−0.0007 (15)
C16	0.0586 (17)	0.0426 (14)	0.0411 (14)	−0.0023 (13)	0.0081 (12)	−0.0013 (11)
C17	0.0338 (12)	0.0321 (11)	0.0400 (13)	−0.0032 (10)	0.0017 (10)	−0.0028 (9)
C18	0.0429 (15)	0.0452 (13)	0.0439 (13)	0.0074 (12)	0.0008 (11)	−0.0031 (11)
O1	0.0523 (11)	0.0550 (10)	0.0717 (12)	−0.0074 (9)	0.0261 (10)	−0.0081 (9)
O2	0.0968 (15)	0.0496 (10)	0.0354 (9)	−0.0141 (10)	−0.0086 (10)	0.0099 (8)
O3	0.0854 (13)	0.0322 (9)	0.0459 (9)	0.0029 (9)	−0.0093 (9)	−0.0005 (7)
O4	0.0614 (11)	0.0349 (9)	0.0351 (9)	−0.0056 (8)	−0.0094 (8)	−0.0003 (7)
S1	0.0523 (4)	0.0367 (3)	0.0367 (3)	−0.0066 (3)	0.0075 (3)	0.0005 (3)

Geometric parameters (Å, º)

C1—C2	1.375 (4)	C10—C13	1.581 (3)
C1—C6	1.383 (3)	C11—C12	1.540 (4)
C1—H1	0.9300	C11—H11A	0.9700
C2—C3	1.368 (4)	C11—H11B	0.9700
C2—H2	0.9300	C12—C14	1.542 (3)
C3—C4	1.394 (4)	C12—H12A	0.9700
C3—H3	0.9300	C12—H12B	0.9700
C4—C5	1.375 (3)	C13—C16	1.533 (3)
C4—H4	0.9300	C13—C17	1.538 (3)
C5—C6	1.377 (3)	C13—C14	1.553 (3)
C5—S1	1.771 (2)	C14—C18	1.536 (3)
C6—H6	0.9300	C14—H14	0.9800
C7—O4	1.422 (3)	C15—H15C	0.9600
C7—C8	1.496 (3)	C15—H15A	0.9600
C7—H7A	0.9700	C15—H15B	0.9600
C7—H7B	0.9700	C16—H16B	0.9600
C8—O3	1.417 (3)	C16—H16C	0.9600
C8—H8A	0.9700	C16—H16A	0.9600
C8—H8B	0.9700	C17—S1	1.779 (2)
C9—O3	1.425 (3)	C17—H17B	0.9700
C9—O4	1.433 (3)	C17—H17A	0.9700
C9—C18	1.543 (3)	C18—H18B	0.9700
C9—C10	1.548 (3)	C18—H18A	0.9700
C10—C15	1.517 (3)	O1—S1	1.4383 (18)
C10—C11	1.538 (3)	O2—S1	1.4422 (18)
C2—C1—C6	119.9 (3)	C11—C12—H12A	111.2
C2—C1—H1	120.1	C14—C12—H12A	111.2
C6—C1—H1	120.1	C11—C12—H12B	111.2
C3—C2—C1	120.0 (2)	C14—C12—H12B	111.2
C3—C2—H2	120.0	H12A—C12—H12B	109.1
C1—C2—H2	120.0	C16—C13—C17	107.93 (18)
C2—C3—C4	120.9 (3)	C16—C13—C14	114.30 (19)
C2—C3—H3	119.5	C17—C13—C14	117.21 (19)
C4—C3—H3	119.5	C16—C13—C10	113.13 (18)
C5—C4—C3	118.3 (2)	C17—C13—C10	110.99 (18)

C5—C4—H4	120.8	C14—C13—C10	92.75 (17)
C3—C4—H4	120.8	C18—C14—C12	107.56 (18)
C4—C5—C6	121.1 (2)	C18—C14—C13	102.43 (18)
C4—C5—S1	119.86 (18)	C12—C14—C13	102.4 (2)
C6—C5—S1	118.91 (18)	C18—C14—H14	114.4
C5—C6—C1	119.7 (3)	C12—C14—H14	114.4
C5—C6—H6	120.2	C13—C14—H14	114.4
C1—C6—H6	120.2	C10—C15—H15C	109.5
O4—C7—C8	102.25 (19)	C10—C15—H15A	109.5
O4—C7—H7A	111.3	H15C—C15—H15A	109.5
C8—C7—H7A	111.3	C10—C15—H15B	109.5
O4—C7—H7B	111.3	H15C—C15—H15B	109.5
C8—C7—H7B	111.3	H15A—C15—H15B	109.5
H7A—C7—H7B	109.2	C13—C16—H16B	109.5
O3—C8—C7	102.85 (19)	C13—C16—H16C	109.5
O3—C8—H8A	111.2	H16B—C16—H16C	109.5
C7—C8—H8A	111.2	C13—C16—H16A	109.5
O3—C8—H8B	111.2	H16B—C16—H16A	109.5
C7—C8—H8B	111.2	H16C—C16—H16A	109.5
H8A—C8—H8B	109.1	C13—C17—S1	122.12 (16)
O3—C9—O4	105.53 (17)	C13—C17—H17B	106.8
O3—C9—C18	113.6 (2)	S1—C17—H17B	106.8
O4—C9—C18	109.93 (18)	C13—C17—H17A	106.8
O3—C9—C10	110.50 (18)	S1—C17—H17A	106.8
O4—C9—C10	113.71 (18)	H17B—C17—H17A	106.6
C18—C9—C10	103.77 (18)	C14—C18—C9	103.38 (19)
C15—C10—C11	114.4 (2)	C14—C18—H18B	111.1
C15—C10—C9	113.7 (2)	C9—C18—H18B	111.1
C11—C10—C9	105.84 (19)	C14—C18—H18A	111.1
C15—C10—C13	118.1 (2)	C9—C18—H18A	111.1
C11—C10—C13	100.76 (18)	H18B—C18—H18A	109.1
C9—C10—C13	102.27 (17)	C8—O3—C9	107.78 (17)
C10—C11—C12	104.44 (19)	C7—O4—C9	108.65 (17)
C10—C11—H11A	110.9	O1—S1—O2	118.38 (12)
C12—C11—H11A	110.9	O1—S1—C5	107.19 (11)
C10—C11—H11B	110.9	O2—S1—C5	107.22 (10)
C12—C11—H11B	110.9	O1—S1—C17	109.78 (11)
H11A—C11—H11B	108.9	O2—S1—C17	104.73 (11)
C11—C12—C14	102.9 (2)	C5—S1—C17	109.29 (10)

C6—C1—C2—C3	0.0 (4)	C11—C12—C14—C13	−35.5 (2)
C1—C2—C3—C4	−0.4 (4)	C16—C13—C14—C18	−172.69 (19)
C2—C3—C4—C5	−0.1 (4)	C17—C13—C14—C18	59.6 (2)
C3—C4—C5—C6	1.2 (3)	C10—C13—C14—C18	−55.74 (19)
C3—C4—C5—S1	−174.85 (17)	C16—C13—C14—C12	−61.3 (2)
C4—C5—C6—C1	−1.7 (4)	C17—C13—C14—C12	170.99 (18)
S1—C5—C6—C1	174.40 (19)	C10—C13—C14—C12	55.66 (19)
C2—C1—C6—C5	1.1 (4)	C16—C13—C17—S1	−81.5 (2)

O4—C7—C8—O3	−35.5 (3)	C14—C13—C17—S1	49.2 (3)
O3—C9—C10—C15	76.8 (2)	C10—C13—C17—S1	153.97 (16)
O4—C9—C10—C15	−41.6 (3)	C12—C14—C18—C9	−69.3 (2)
C18—C9—C10—C15	−161.0 (2)	C13—C14—C18—C9	38.2 (2)
O3—C9—C10—C11	−49.6 (2)	O3—C9—C18—C14	117.2 (2)
O4—C9—C10—C11	−168.02 (19)	O4—C9—C18—C14	−124.85 (18)
C18—C9—C10—C11	72.6 (2)	C10—C9—C18—C14	−2.9 (2)
O3—C9—C10—C13	−154.66 (19)	C7—C8—O3—C9	31.9 (3)
O4—C9—C10—C13	86.9 (2)	O4—C9—O3—C8	−15.7 (3)
C18—C9—C10—C13	−32.5 (2)	C18—C9—O3—C8	104.8 (2)
C15—C10—C11—C12	164.0 (2)	C10—C9—O3—C8	−139.0 (2)
C9—C10—C11—C12	−69.9 (2)	C8—C7—O4—C9	26.9 (3)
C13—C10—C11—C12	36.2 (2)	O3—C9—O4—C7	−8.1 (2)
C10—C11—C12—C14	−1.0 (3)	C18—C9—O4—C7	−131.0 (2)
C15—C10—C13—C16	−62.9 (3)	C10—C9—O4—C7	113.2 (2)
C11—C10—C13—C16	62.4 (2)	C4—C5—S1—O1	21.5 (2)
C9—C10—C13—C16	171.40 (19)	C6—C5—S1—O1	−154.61 (18)
C15—C10—C13—C17	58.6 (3)	C4—C5—S1—O2	149.62 (19)
C11—C10—C13—C17	−176.12 (19)	C6—C5—S1—O2	−26.5 (2)
C9—C10—C13—C17	−67.1 (2)	C4—C5—S1—C17	−97.4 (2)
C15—C10—C13—C14	179.1 (2)	C6—C5—S1—C17	86.5 (2)
C11—C10—C13—C14	−55.55 (19)	C13—C17—S1—O1	−52.6 (2)
C9—C10—C13—C14	53.46 (19)	C13—C17—S1—O2	179.28 (18)
C11—C12—C14—C18	72.0 (2)	C13—C17—S1—C5	64.7 (2)