Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

S-Phenyl 4,6-*O*-benzylidene-2,3-*O*-carbonyl-1-thia-α-D-mannopyranoside

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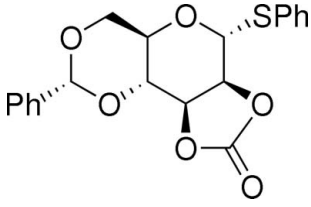
Received 1 May 2007; accepted 5 May 2007

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 18.1.

In the title compound, $C_{20}H_{18}O_6S$, the pyranoside ring adopts a distorted conformation (*E*2 oriented $^4C_1$). The presence of a fused *cis*-carbonate alters the conformation of the pyranose ring from the normal $^4C_1$ chair conformation.

Related literature

For related literature, see: Cremer & Pople (1975); Crich *et al.* (2000, 2005); Manabe *et al.* (2006); Mendlik, Coleman, Qi, Lowary & Ferguson (2006); Mendlik, Coleman, Qi, Lowary & McDonald (2006).



Experimental

Crystal data

$C_{20}H_{18}O_6S$
M_r = 386.40
Monoclinic, $P2_1$
a = 11.5672 (9) Å
b = 5.7425 (4) Å
c = 14.6172 (10) Å
β = 108.143 (2)°
V = 922.68 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 200 K
0.61 × 0.17 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.928, T_{max} = 0.976
11024 measured reflections
4729 independent reflections
3073 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.12
4729 reflections
261 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 1790 Friedel pairs
Flack parameter: −0.01 (9)

Table 1
Selected torsion angles (°).

C1—C2—C3—C4	−31.8 (3)	C4—C5—O1—C1	68.7 (2)
C2—C3—C4—C5	48.3 (3)	C5—O1—C1—C2	−51.0 (3)
C3—C4—C5—O1	−66.7 (2)	O1—C1—C2—C3	32.3 (4)

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the RIKEN matching fund for PRESTO, the President's Discretionary Fund from RIKEN and Grants-in-Aid for Scientific Research (C) (grant No. 19590032) from the Japan Society for the Promotion of Science.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2162).

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  doi:10.1107/S1600536807022210

supporting information

Acta Cryst. (2007). E**63**, o3028 [https://doi.org/10.1107/S1600536807022210]

S-Phenyl 4,6-*O*-benzylidene-2,3-*O*-carbonyl-1-thia-*α*-D-mannopyranoside

Shino Manabe, Kazuyuki Ishii, Daisuke Hashizume and Yukishige Ito

S1. Comment

As part of our recent investigation into the development of *α*-selective glycosyl donors of 2-amino-2-deoxy sugars (Manabe *et al.*, 2006), we became interested in the relationship between pyranose conformation and selectivity in the glycosylation reaction. The title compound, (I), is an *α*-selective glycosylation donor of mannose, as reported by Crich *et al.* (2000). As the first part of this study, we examined the conformation of the mannopyranose ring by X-ray crystal structure analysis.

The glycosyl donor exhibits high *α*-selectivity despite the lack of a participating group at the 2-position. The pyranose ring of mannose, O1/C1—C5, is distorted probably due to the presence of the 2,3-*cis* carbonate; this is supported by deviations in the torsion angles around the C1—C2, C2—C3 and C3—C4 bonds from the ideal values for a chair conformation. The same phenomenon was observed in the case of rhamnose (Crich *et al.*, 2005) and daunosamine (Mendlik, Coleman, Qi, Lowary & McDonald, 2006; Mendlik, Coleman, Qi, Lowary & Ferguson, 2006) containing 2,3-*cis* carbonate. The Cremer-Pople puckering parameters (Cremer & Pople, 1975), Q = 0.546 (2) Å, θ = 153.3 (3)° and φ = 56.0 (6)°, clearly indicate a large distortion of the ring.

S2. Experimental

The compound was prepared as described by Crich *et al.* (2000). The compound was dissolved in EtOAc at room temperature and hexane was added. The solution was kept at room temperature in a sealed flask for a few days to give single crystals suitable for X-ray analysis.

S3. Refinement

All H atoms were found on a difference map and were subsequently treated as riding atoms with C—H distances of 1.00, 0.99 and 0.95 Å for methyne, methylene and phenyl, respectively. The U_{iso}'s of H atoms were fixed to have 1.2U_{eq} of the parent atoms. Floating origin restraint was applied to fix the X-ray 'center of gravity′ of the structure in the *b* axis direction.

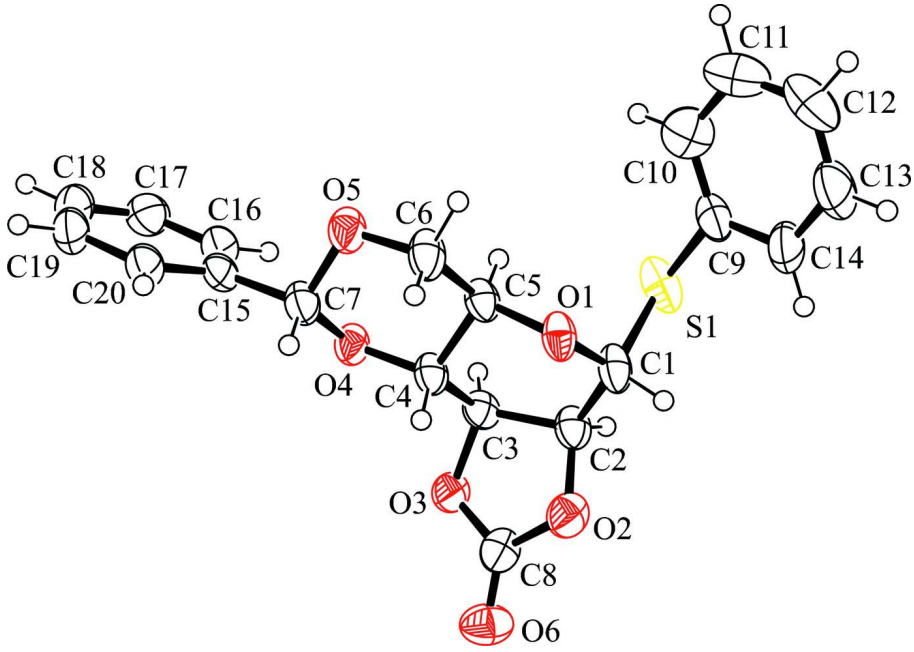

Figure 1

The molecular structure of (I). Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

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$c = 14.6172\ (10)$ Å
$\beta = 108.143\ (2)°$
$V = 922.68\ (12)$ Å^3
$Z = 2$
$F(000) = 404$
$D_x = 1.391$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11035 reflections
$\theta = 3.5–30.0°$
$\mu = 0.21$ mm^{-1}
$T = 200$ K
Needle, colourless
0.61 × 0.17 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.928$, $T_{max} = 0.976$
11024 measured reflections
4729 independent reflections
3073 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.5°$
$h = -16\rightarrow16$
$k = -8\rightarrow7$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.103$
$S = 1.12$
4729 reflections
261 parameters
1 restraint

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.1924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983), 1790 Friedel pairs
Absolute structure parameter: −0.01 (9)

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	0.17264 (6)	0.11075 (16)	0.08559 (5)	0.0574 (2)
O1	0.29605 (13)	0.3564 (3)	0.24474 (11)	0.0408 (4)
O2	0.40038 (15)	0.6337 (3)	0.09979 (12)	0.0494 (4)
O3	0.56776 (14)	0.4206 (3)	0.12945 (12)	0.0430 (4)
O4	0.60166 (12)	0.1151 (4)	0.30258 (10)	0.0406 (4)
O5	0.51693 (15)	−0.0002 (3)	0.42029 (12)	0.0508 (5)
O6	0.57299 (18)	0.7955 (3)	0.08992 (14)	0.0579 (5)
C1	0.2575 (2)	0.3698 (5)	0.14384 (16)	0.0443 (6)
H1	0.2029	0.5082	0.1241	0.053*
C2	0.3601 (2)	0.3930 (5)	0.09890 (17)	0.0416 (6)
H2	0.3310	0.3353	0.0310	0.050*
C3	0.47901 (19)	0.2723 (5)	0.15248 (16)	0.0372 (5)
H3	0.4813	0.1114	0.1269	0.045*
C4	0.50209 (19)	0.2671 (5)	0.25987 (16)	0.0376 (5)
H4	0.5225	0.4275	0.2866	0.045*
C5	0.38772 (19)	0.1826 (4)	0.27995 (16)	0.0383 (6)
H5	0.3603	0.0312	0.2464	0.046*
C6	0.4145 (2)	0.1536 (6)	0.38735 (16)	0.0501 (7)
H61	0.4336	0.3063	0.4200	0.060*
H62	0.3431	0.0867	0.4016	0.060*
C7	0.62117 (19)	0.0930 (5)	0.40294 (15)	0.0427 (5)
H7	0.6404	0.2490	0.4344	0.051*
C8	0.5184 (2)	0.6310 (5)	0.10486 (16)	0.0433 (6)
C9	0.05254 (19)	0.1003 (6)	0.13747 (16)	0.0465 (6)
C10	0.0427 (3)	−0.0881 (6)	0.1929 (2)	0.0643 (8)
H10	0.1040	−0.2047	0.2092	0.077*
C11	−0.0592 (4)	−0.1047 (7)	0.2248 (3)	0.0749 (10)
H11	−0.0677	−0.2352	0.2621	0.090*

C12	−0.1470 (3)	0.0653 (8)	0.2029 (2)	0.0746 (11)
H12	−0.2166	0.0512	0.2240	0.089*
C13	−0.1339 (3)	0.2529 (7)	0.1511 (3)	0.0774 (10)
H13	−0.1934	0.3728	0.1378	0.093*
C14	−0.0349 (2)	0.2732 (7)	0.1171 (2)	0.0662 (9)
H14	−0.0273	0.4050	0.0801	0.079*
C15	0.7251 (2)	−0.0704 (5)	0.44491 (17)	0.0419 (6)
C16	0.7468 (2)	−0.2562 (5)	0.3924 (2)	0.0480 (6)
H16	0.6987	−0.2757	0.3271	0.058*
C17	0.8387 (2)	−0.4147 (6)	0.4347 (2)	0.0549 (7)
H17	0.8538	−0.5416	0.3983	0.066*
C18	0.9080 (2)	−0.3870 (6)	0.5300 (2)	0.0561 (7)
H18	0.9704	−0.4960	0.5592	0.067*
C19	0.8873 (2)	−0.2032 (6)	0.5828 (2)	0.0542 (7)
H19	0.9349	−0.1859	0.6483	0.065*
C20	0.7966 (2)	−0.0419 (5)	0.54035 (19)	0.0486 (7)
H20	0.7834	0.0872	0.5765	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0351 (3)	0.0882 (5)	0.0482 (3)	−0.0078 (4)	0.0120 (3)	−0.0205 (4)
O1	0.0273 (8)	0.0620 (12)	0.0335 (7)	0.0073 (8)	0.0103 (6)	−0.0036 (8)
O2	0.0434 (9)	0.0552 (12)	0.0556 (10)	0.0120 (10)	0.0241 (8)	0.0092 (10)
O3	0.0322 (9)	0.0491 (10)	0.0528 (10)	0.0080 (8)	0.0204 (7)	0.0102 (9)
O4	0.0284 (7)	0.0538 (10)	0.0412 (8)	0.0067 (9)	0.0132 (6)	0.0089 (9)
O5	0.0321 (9)	0.0774 (14)	0.0445 (9)	0.0049 (8)	0.0143 (7)	0.0172 (9)
O6	0.0673 (13)	0.0510 (12)	0.0670 (13)	−0.0018 (11)	0.0379 (11)	0.0051 (10)
C1	0.0265 (11)	0.0667 (18)	0.0390 (12)	0.0065 (11)	0.0091 (9)	−0.0007 (12)
C2	0.0316 (12)	0.0558 (16)	0.0390 (11)	0.0035 (11)	0.0134 (10)	0.0009 (12)
C3	0.0311 (11)	0.0423 (14)	0.0424 (12)	0.0020 (10)	0.0177 (9)	−0.0010 (11)
C4	0.0257 (11)	0.0482 (14)	0.0392 (11)	0.0039 (10)	0.0107 (9)	0.0002 (11)
C5	0.0270 (11)	0.0529 (17)	0.0362 (11)	0.0009 (10)	0.0116 (9)	−0.0023 (10)
C6	0.0307 (12)	0.083 (2)	0.0391 (11)	0.0079 (13)	0.0138 (9)	0.0079 (13)
C7	0.0295 (11)	0.0576 (16)	0.0394 (11)	−0.0008 (13)	0.0086 (9)	0.0021 (13)
C8	0.0423 (13)	0.0529 (16)	0.0393 (11)	0.0099 (14)	0.0196 (10)	0.0040 (13)
C9	0.0290 (11)	0.0686 (17)	0.0389 (11)	−0.0036 (14)	0.0062 (9)	−0.0032 (15)
C10	0.069 (2)	0.0591 (19)	0.0671 (18)	0.0010 (16)	0.0241 (16)	−0.0063 (17)
C11	0.092 (3)	0.068 (2)	0.078 (2)	−0.025 (2)	0.046 (2)	−0.0040 (19)
C12	0.0486 (17)	0.102 (3)	0.080 (2)	−0.0230 (19)	0.0310 (16)	−0.019 (2)
C13	0.0349 (15)	0.109 (3)	0.090 (2)	0.0075 (18)	0.0208 (16)	0.016 (2)
C14	0.0320 (14)	0.094 (3)	0.0696 (18)	0.0094 (16)	0.0113 (13)	0.0295 (19)
C15	0.0262 (11)	0.0549 (16)	0.0449 (12)	−0.0050 (11)	0.0114 (10)	0.0083 (12)
C16	0.0354 (13)	0.0547 (16)	0.0506 (14)	−0.0028 (12)	0.0086 (11)	0.0054 (14)
C17	0.0475 (15)	0.0525 (18)	0.0655 (16)	0.0012 (14)	0.0186 (13)	0.0062 (16)
C18	0.0362 (13)	0.0650 (18)	0.0650 (16)	0.0071 (15)	0.0126 (12)	0.0187 (18)
C19	0.0327 (13)	0.072 (2)	0.0524 (15)	0.0002 (14)	0.0048 (11)	0.0135 (15)
C20	0.0334 (13)	0.0604 (18)	0.0499 (14)	−0.0016 (12)	0.0100 (11)	0.0072 (13)

Geometric parameters (Å, º)

S1—C9	1.779 (2)	C7—C15	1.498 (4)
S1—C1	1.839 (3)	C7—H7	1.0000
O1—C1	1.404 (3)	C9—C10	1.378 (4)
O1—C5	1.430 (3)	C9—C14	1.382 (4)
O2—C8	1.344 (3)	C10—C11	1.399 (4)
O2—C2	1.457 (3)	C10—H10	0.9500
O3—C8	1.337 (3)	C11—C12	1.373 (5)
O3—C3	1.452 (3)	C11—H11	0.9500
O4—C7	1.419 (2)	C12—C13	1.352 (5)
O4—C4	1.425 (3)	C12—H12	0.9500
O5—C7	1.412 (3)	C13—C14	1.388 (4)
O5—C6	1.435 (3)	C13—H13	0.9500
O6—C8	1.194 (3)	C14—H14	0.9500
C1—C2	1.531 (3)	C15—C16	1.383 (4)
C1—H1	1.0000	C15—C20	1.392 (3)
C2—C3	1.522 (3)	C16—C17	1.389 (4)
C2—H2	1.0000	C16—H16	0.9500
C3—C4	1.508 (3)	C17—C18	1.384 (4)
C3—H3	1.0000	C17—H17	0.9500
C4—C5	1.521 (3)	C18—C19	1.371 (4)
C4—H4	1.0000	C18—H18	0.9500
C5—C6	1.512 (3)	C19—C20	1.392 (4)
C5—H5	1.0000	C19—H19	0.9500
C6—H61	0.9900	C20—H20	0.9500
C6—H62	0.9900		
C9—S1—C1	101.82 (12)	O4—C7—C15	109.2 (2)
C1—O1—C5	111.96 (18)	O5—C7—H7	109.7
C8—O2—C2	107.8 (2)	O4—C7—H7	109.7
C8—O3—C3	108.61 (18)	C15—C7—H7	109.7
C7—O4—C4	110.76 (17)	O6—C8—O3	124.0 (2)
C7—O5—C6	111.6 (2)	O6—C8—O2	124.5 (3)
O1—C1—C2	114.86 (19)	O3—C8—O2	111.5 (2)
O1—C1—S1	113.0 (2)	C10—C9—C14	120.1 (3)
C2—C1—S1	104.18 (18)	C10—C9—S1	119.7 (2)
O1—C1—H1	108.2	C14—C9—S1	120.0 (2)
C2—C1—H1	108.2	C9—C10—C11	118.8 (3)
S1—C1—H1	108.2	C9—C10—H10	120.6
O2—C2—C3	101.07 (19)	C11—C10—H10	120.6
O2—C2—C1	111.5 (2)	C12—C11—C10	120.9 (4)
C3—C2—C1	115.9 (2)	C12—C11—H11	119.6
O2—C2—H2	109.3	C10—C11—H11	119.6
C3—C2—H2	109.3	C13—C12—C11	119.5 (3)
C1—C2—H2	109.3	C13—C12—H12	120.2
O3—C3—C4	110.13 (19)	C11—C12—H12	120.2
O3—C3—C2	101.81 (19)	C12—C13—C14	121.1 (3)

C4—C3—C2	112.54 (18)	C12—C13—H13	119.5
O3—C3—H3	110.7	C14—C13—H13	119.5
C4—C3—H3	110.7	C9—C14—C13	119.5 (3)
C2—C3—H3	110.7	C9—C14—H14	120.2
O4—C4—C3	108.98 (18)	C13—C14—H14	120.2
O4—C4—C5	110.68 (19)	C16—C15—C20	119.6 (2)
C3—C4—C5	108.93 (18)	C16—C15—C7	121.2 (2)
O4—C4—H4	109.4	C20—C15—C7	119.2 (2)
C3—C4—H4	109.4	C15—C16—C17	120.3 (3)
C5—C4—H4	109.4	C15—C16—H16	119.9
O1—C5—C6	109.87 (18)	C17—C16—H16	119.9
O1—C5—C4	107.45 (18)	C18—C17—C16	119.8 (3)
C6—C5—C4	109.03 (18)	C18—C17—H17	120.1
O1—C5—H5	110.1	C16—C17—H17	120.1
C6—C5—H5	110.1	C19—C18—C17	120.4 (3)
C4—C5—H5	110.1	C19—C18—H18	119.8
O5—C6—C5	107.28 (19)	C17—C18—H18	119.8
O5—C6—H61	110.3	C18—C19—C20	120.1 (3)
C5—C6—H61	110.3	C18—C19—H19	120.0
O5—C6—H62	110.3	C20—C19—H19	120.0
C5—C6—H62	110.3	C15—C20—C19	119.9 (3)
H61—C6—H62	108.5	C15—C20—H20	120.1
O5—C7—O4	110.46 (17)	C19—C20—H20	120.1
O5—C7—C15	108.1 (2)		

C1—C2—C3—C4	−31.8 (3)	C6—O5—C7—O4	−64.2 (3)
C2—C3—C4—C5	48.3 (3)	C6—O5—C7—C15	176.4 (2)
C3—C4—C5—O1	−66.7 (2)	C4—O4—C7—O5	60.5 (3)
C4—C5—O1—C1	68.7 (2)	C4—O4—C7—C15	179.2 (2)
C5—O1—C1—C2	−51.0 (3)	C3—O3—C8—O6	173.5 (2)
O1—C1—C2—C3	32.3 (4)	C3—O3—C8—O2	−6.1 (3)
C5—O1—C1—S1	68.3 (2)	C2—O2—C8—O6	166.1 (2)
C9—S1—C1—O1	56.67 (19)	C2—O2—C8—O3	−14.3 (3)
C9—S1—C1—C2	−177.99 (17)	C1—S1—C9—C10	−117.4 (2)
C8—O2—C2—C3	27.0 (2)	C1—S1—C9—C14	66.7 (2)
C8—O2—C2—C1	150.79 (18)	C14—C9—C10—C11	2.4 (5)
O1—C1—C2—O2	−82.7 (3)	S1—C9—C10—C11	−173.5 (2)
S1—C1—C2—O2	153.16 (16)	C9—C10—C11—C12	−1.1 (5)
S1—C1—C2—C3	−91.9 (2)	C10—C11—C12—C13	−1.0 (5)
C8—O3—C3—C4	−97.1 (2)	C11—C12—C13—C14	2.0 (6)
C8—O3—C3—C2	22.5 (2)	C10—C9—C14—C13	−1.4 (5)
O2—C2—C3—O3	−28.9 (2)	S1—C9—C14—C13	174.4 (3)
C1—C2—C3—O3	−149.6 (2)	C12—C13—C14—C9	−0.8 (5)
O2—C2—C3—C4	89.0 (2)	O5—C7—C15—C16	87.1 (3)
C7—O4—C4—C3	−176.1 (2)	O4—C7—C15—C16	−33.1 (3)
C7—O4—C4—C5	−56.3 (3)	O5—C7—C15—C20	−89.1 (3)
O3—C3—C4—O4	−78.0 (2)	O4—C7—C15—C20	150.7 (2)
C2—C3—C4—O4	169.2 (2)	C20—C15—C16—C17	0.5 (4)

O3—C3—C4—C5	161.14 (19)	C7—C15—C16—C17	−175.7 (3)
C1—O1—C5—C6	−172.8 (2)	C15—C16—C17—C18	0.5 (4)
O4—C4—C5—O1	173.50 (18)	C16—C17—C18—C19	−0.5 (4)
O4—C4—C5—C6	54.5 (3)	C17—C18—C19—C20	−0.4 (4)
C3—C4—C5—C6	174.3 (2)	C16—C15—C20—C19	−1.4 (4)
C7—O5—C6—C5	61.3 (3)	C7—C15—C20—C19	174.8 (2)
O1—C5—C6—O5	−172.92 (19)	C18—C19—C20—C15	1.4 (4)
C4—C5—C6—O5	−55.4 (3)		