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

Shino Manabe,[a]* Kazuyuki Ishii,[a] Daisuke Hashizume[b] and Yukishige Ito[a]

[a]RIKEN, DRI, (The Institute of Physical and Chemical Research, Discovery Research Institute), Hirosawa, Wako-shi, Saitama 351-0198, Japan, and [b]RIKEN, ADSC, (The Institute of Physical and Chemical Research, Advanced Development and Supporting Center), Hirosawa, Wako-shi, Saitama 351-0198, Japan
Correspondence e-mail: smanabe@riken.jp

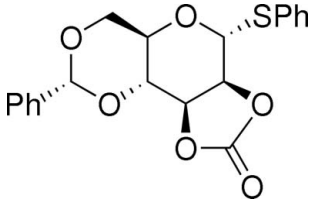
Received 1 May 2007; accepted 5 May 2007

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).

References

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Cremer, D. & Pople, A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Crich, D., Cai, W. & Dai, Z. (2000). *J. Org. Chem.* **65**, 1291–1297.
Crich, D., Viond, A. U., Picione, J. & Wink, D. J. (2005). *Arkivoc*, pp. 339–344.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Manabe, S., Ishii, K. & Ito, Y. (2006). *J. Am. Chem. Soc.* **128**, 10666–10667.
Mendlik, M. T., Coleman, R. S., Qi, G., Lowary, T. L. & Ferguson, M. J. (2006). *Acta Cryst.* E**62**, o2788–o2790.
Mendlik, M. T., Coleman, R. S., Qi, G., Lowary, T. L. & McDonald, R. (2006). *Acta Cryst.* E**62**, o2490–o2492.
Rigaku Corporation (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807022210

supplementary materials

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

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

S. Manabe, K. Ishii, D. Hashizume and Y. Ito

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.

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.

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.

Figures

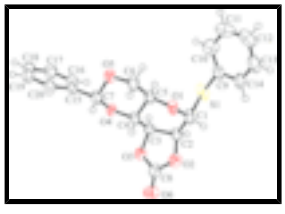


Fig. 1. The molecular structure of (I). Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

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

Crystal data

$C_{20}H_{18}O_6S$	F_{000} = 404
M_r = 386.40	D_x = 1.391 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 11035 reflections
a = 11.5672 (9) Å	θ = 3.5–30.0º
b = 5.7425 (4) Å	μ = 0.21 mm^{-1}
c = 14.6172 (10) Å	T = 200 K
β = 108.143 (2)º	Needle, colourless
V = 922.68 (12) Å^3	0.61 × 0.17 × 0.14 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	4729 independent reflections
Radiation source: normal-focus sealed tube	3073 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
Detector resolution: 10 pixels mm^{-1}	θ_{max} = 30.0º
T = 200 K	θ_{min} = 3.5º
ω scans	h = −16→16
Absorption correction: numerical (NUMABS; Higashi, 1999)	k = −8→7
T_{min} = 0.928, T_{max} = 0.976	l = −20→20
11024 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.1924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.103	$(\Delta/\sigma)_{max} < 0.001$
S = 1.12	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
4729 reflections	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
261 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1790 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.01 (9)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	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)

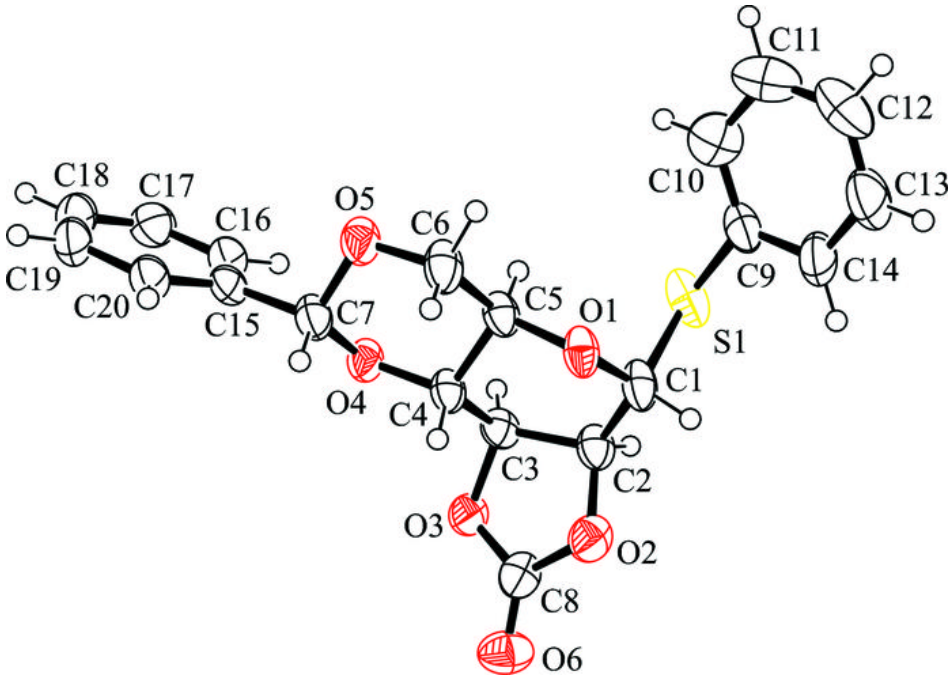
Geometric parameters (Å, °)

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)		

Fig. 1


C11
C12
C10
C13
C9
C14
S1
C18
C17
C16
O5
C6
C19
C20
C15
C7
C5
O1
C1
O4
C4
C3
C2
O3
O2
C8
O6