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(1*R*,4*R*,7*R*,8*R*,9*R*)-8-Benzyloxy-7-benzyloxymethyl-2,5,10-trioxa-tricyclo[5.2.1.$0^{4,8}$]decan-9-ol

Pawan K. Sharma, Poul Nielsen and Andrew D. Bond*

University of Southern Denmark, Department of Physics and Chemistry, Campusvej 55, 5230 Odense, Denmark
Correspondence e-mail: adb@chem.sdu.dk

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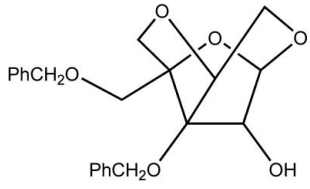
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.063; data-to-parameter ratio = 7.7.

The title compound, $C_{22}H_{24}O_6$, has been prepared in nine synthetic steps from 1,2:5,6-di-*O*-isopropylidene-α-D-glucofuranose. It is expected to constitute a binding pocket for metal ions. The hydroxy group at the 9-position is involved in an intramolecular hydrogen bond with an O atom of the (benzyloxy)methyl substituent, forming a pseudo-six-membered ring. In the crystal structure, the benzene ring of the (benzyloxy)methyl substituent approaches the tricylic binding pocket of a neighbouring molecule, forming a C—H···O contact.

Related literature

For related literature, see: Freitag *et al.* (2004); Sekiguchi *et al.* (2006); Sharma & Nielsen (2004).



Experimental

Crystal data

$C_{22}H_{24}O_6$
M_r = 384.41
Orthorhombic, $P2_12_12_1$
a = 9.4559 (3) Å
b = 10.8048 (4) Å
c = 18.0620 (6) Å
V = 1845.38 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 180 (2) K
0.35 × 0.35 × 0.20 mm

Data collection

Bruker–Nonius X8 APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.865, T_{max} = 0.980
16553 measured reflections
1975 independent reflections
1554 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.063
S = 0.97
1975 reflections
257 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O6	0.90 (3)	1.79 (3)	2.664 (2)	163 (3)
C15—H15A···O2^{i}	0.95	2.64	3.468 (3)	146

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

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: KP2133).

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supplementary materials

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(1*R*,4*R*,7*R*,8*R*,9*R*)-8-Benzyloxy-7-benzyloxymethyl-2,5,10-trioxatricyclo[5.2.1.0^{4,8}]decan-9-ol

P. K. Sharma, P. Nielsen and A. D. Bond

Comment

As a part of our ongoing research on conformationally restricted nucleosides and related compounds (Freitag *et al.*, 2004; Sharma & Nielsen, 2004) the title compound was prepared in nine synthetic steps from commercially available 1,2:5,6-di-*O*-isopropylidene-α-*D*-glucofuranose. The compound is expected to constitute a binding pocket for metal ions. The hydroxyl group at the 9-position is involved in an intramolecular hydrogen bond with an O atom of the (benzyloxy)methyl substituent. In the crystal, the benzene ring of the (benzyloxy)methyl substituent approaches the tricylic binding pocket of a neighbouring molecule in a side-on manner, forming a C—H···O contact [H···O, 2.64 and H···O 3.468 (3) Å].

Experimental

The title compound was prepared in nine synthetic steps from commercially available 1,2:5,6-di-*O*-isopropylidene-α-*D*-glucofuranose. From this starting material, the known compound 3-*O*-benzyl-4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-3-*C*-vinyl-α-*D*-ribofuranose was obtained in five steps (Sekiguchi *et al.*, 2006). Benzylation of the pro-*S* hydroxymethyl group followed by mesylation of the remaining free hydroxymethyl group yielded 3-*O*-benzyl-4-*C*-benzyloxymethyl-1,2-*O*-isopropylidene-5-O-methansulfunyl-3-C– vinyl-α-*D*-ribofuranose, which was successively treated with $RuCl_3.xH_2O/NaIO_4$ and $NaBH_4$ (Sharma & Nielsen, 2004) to yield the tricyclic title compound.

Refinement

H atoms bound to C atoms were placed geometrically and refined using a riding model with C—H = 0.95–1.00 Å and with U_{iso}(H) = 1.2U_{eq}(C). The H atom of the hydroxyl group was located in a difference Fourier map and refined with an isotropic displacement parameter, without restraint. In the absence of significant anomalous scattering effects, Friedel pairs (1570 measured) were merged as equivalent data. The absolute structure is assigned on the basis of unchanging chirality of the 1,2:5,6-di-*O*-isopropylidene-α-*D*-glucofuranose starting material.

Figures

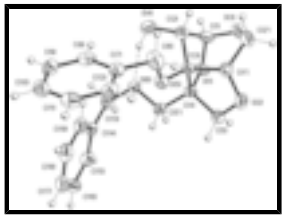


Fig. 1. Molecular structure of the title compound showing displacement ellipsoids at the 50% probability level for non-H atoms. The dashed line indicates an intramolecular O—H···O hydrogen bond.

(1*R*,4*R*,7*R*,8*R*,9*R*)-8-(Benzyloxy)-7- (benzyloxymethyl)-2,5,10-trioxatricyclo[5.2.1.$0^{4,8}$]decan-9-ol

Crystal data

$C_{22}H_{24}O_6$	F_{000} = 816
M_r = 384.41	D_x = 1.384 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4020 reflections
a = 9.4559 (3) Å	θ = 2.4–21.1º
b = 10.8048 (4) Å	μ = 0.10 mm^{-1}
c = 18.0620 (6) Å	T = 180 (2) K
V = 1845.38 (11) Å^3	Block, colourless
Z = 4	0.35 × 0.35 × 0.20 mm

Data collection

Bruker–Nonius X8 APEXII CCD diffractometer	1975 independent reflections
Radiation source: fine-focus sealed tube	1554 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 180(2) K	θ_{max} = 25.6º
thin–slice ω and φ scans	θ_{min} = 3.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −11→11
T_{min} = 0.865, T_{max} = 0.980	k = −13→10
16553 measured reflections	l = −15→21

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.063	$\Delta\rho_{max}$ = 0.11 e Å^{-3}
S = 0.97	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
1975 reflections	Extinction correction: none
257 parameters	Absolute structure: In the absence of significant anomalous scattering effects, Friedel opposites (1570 measured) have been merged.
Primary atom site location: structure-invariant direct methods	Flack parameter: ?
Secondary atom site location: difference Fourier map	Rogers parameter: ?
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.31999 (14)	0.32447 (13)	0.38560 (7)	0.0337 (4)
O2	0.32776 (16)	0.58002 (15)	0.31636 (7)	0.0407 (4)
O3	0.36347 (17)	0.31654 (16)	0.25819 (8)	0.0468 (4)
O4	0.62645 (16)	0.25576 (13)	0.40265 (9)	0.0372 (4)
H4	0.590 (3)	0.275 (3)	0.4471 (15)	0.080 (10)*
O5	0.61495 (14)	0.52440 (12)	0.40763 (7)	0.0264 (3)
O6	0.48368 (14)	0.33819 (13)	0.51986 (7)	0.0299 (4)
C1	0.4084 (2)	0.2757 (2)	0.32887 (11)	0.0378 (6)
H1A	0.4067	0.1832	0.3307	0.045*
C2	0.5564 (2)	0.3221 (2)	0.34630 (11)	0.0312 (5)
H2A	0.6151	0.3224	0.3003	0.037*
C3	0.5156 (2)	0.45471 (18)	0.36712 (10)	0.0239 (5)
C4	0.3784 (2)	0.43887 (18)	0.41337 (10)	0.0241 (5)
C5	0.2874 (2)	0.5486 (2)	0.39023 (10)	0.0327 (5)
H5A	0.1860	0.5262	0.3920	0.039*
H5B	0.3036	0.6196	0.4238	0.039*
C1'	0.4575 (2)	0.5201 (2)	0.29674 (10)	0.0320 (5)
H1'A	0.5271	0.5836	0.2797	0.038*
C2'	0.4298 (2)	0.4292 (2)	0.23455 (11)	0.0442 (7)
H2'A	0.3687	0.4696	0.1971	0.053*
H2'B	0.5207	0.4088	0.2103	0.053*
C5'	0.3885 (2)	0.43260 (18)	0.49704 (10)	0.0268 (5)
H5'A	0.4212	0.5134	0.5164	0.032*
H5'B	0.2936	0.4159	0.5180	0.032*
C6	0.7473 (2)	0.5465 (2)	0.37005 (11)	0.0414 (6)
H6A	0.7369	0.6158	0.3346	0.050*
H6B	0.7763	0.4718	0.3422	0.050*
C7	0.8564 (2)	0.5779 (2)	0.42712 (10)	0.0271 (5)
C8	0.9042 (2)	0.4876 (2)	0.47596 (11)	0.0306 (5)
H8A	0.8692	0.4054	0.4720	0.037*
C9	1.0021 (2)	0.5159 (2)	0.53018 (11)	0.0330 (5)
H9A	1.0329	0.4537	0.5637	0.040*
C10	1.0549 (2)	0.6345 (2)	0.53563 (12)	0.0345 (6)

H10A	1.1210	0.6546	0.5734	0.041*
C11	1.0120 (2)	0.7231 (2)	0.48650 (12)	0.0354 (6)
H11A	1.0506	0.8041	0.4893	0.043*
C12	0.9124 (2)	0.6955 (2)	0.43248 (11)	0.0317 (5)
H12A	0.8825	0.7581	0.3990	0.038*
C13	0.4875 (2)	0.3209 (2)	0.59906 (10)	0.0320 (5)
H13A	0.5545	0.2533	0.6109	0.038*
H13B	0.3926	0.2951	0.6163	0.038*
C14	0.5312 (2)	0.4361 (2)	0.64016 (10)	0.0271 (5)
C15	0.4519 (2)	0.4825 (2)	0.69786 (11)	0.0355 (5)
H15A	0.3691	0.4398	0.7132	0.043*
C16	0.4912 (3)	0.5904 (2)	0.73382 (12)	0.0437 (6)
H16A	0.4357	0.6211	0.7736	0.052*
C17	0.6106 (3)	0.6533 (2)	0.71189 (13)	0.0459 (7)
H17A	0.6372	0.7279	0.7360	0.055*
C18	0.6916 (3)	0.6072 (2)	0.65464 (13)	0.0417 (6)
H18A	0.7742	0.6501	0.6392	0.050*
C19	0.6526 (2)	0.4986 (2)	0.61982 (11)	0.0341 (5)
H19A	0.7101	0.4665	0.5812	0.041*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0280 (8)	0.0360 (8)	0.0371 (8)	−0.0061 (7)	0.0051 (7)	−0.0152 (7)
O2	0.0394 (9)	0.0570 (10)	0.0256 (7)	0.0191 (8)	0.0011 (7)	0.0061 (8)
O3	0.0424 (10)	0.0617 (11)	0.0362 (9)	−0.0018 (9)	−0.0029 (8)	−0.0199 (9)
O4	0.0391 (9)	0.0341 (9)	0.0384 (9)	0.0112 (8)	0.0040 (8)	0.0006 (8)
O5	0.0220 (7)	0.0313 (8)	0.0257 (7)	−0.0031 (7)	0.0034 (6)	−0.0003 (6)
O6	0.0349 (8)	0.0301 (8)	0.0247 (7)	0.0081 (7)	0.0007 (7)	0.0005 (6)
C1	0.0371 (14)	0.0399 (14)	0.0364 (13)	0.0029 (12)	0.0030 (11)	−0.0161 (11)
C2	0.0305 (12)	0.0343 (13)	0.0289 (11)	0.0034 (11)	0.0043 (10)	−0.0056 (10)
C3	0.0209 (11)	0.0281 (12)	0.0226 (10)	−0.0007 (10)	0.0013 (9)	−0.0022 (9)
C4	0.0235 (11)	0.0222 (11)	0.0265 (10)	−0.0012 (10)	0.0014 (9)	−0.0056 (9)
C5	0.0313 (12)	0.0420 (14)	0.0247 (10)	0.0079 (11)	0.0015 (10)	0.0003 (10)
C1'	0.0278 (12)	0.0429 (13)	0.0253 (11)	0.0062 (11)	0.0010 (10)	0.0006 (10)
C2'	0.0373 (14)	0.0697 (18)	0.0258 (12)	0.0115 (14)	−0.0030 (11)	−0.0041 (13)
C5'	0.0249 (11)	0.0277 (11)	0.0276 (11)	0.0019 (10)	0.0031 (9)	0.0006 (10)
C6	0.0296 (12)	0.0633 (17)	0.0315 (12)	−0.0118 (13)	0.0074 (10)	0.0002 (11)
C7	0.0199 (11)	0.0339 (12)	0.0273 (11)	−0.0025 (10)	0.0070 (9)	0.0003 (10)
C8	0.0307 (12)	0.0237 (12)	0.0375 (12)	−0.0032 (10)	0.0124 (10)	−0.0011 (10)
C9	0.0304 (12)	0.0350 (13)	0.0335 (12)	0.0043 (11)	0.0033 (10)	0.0087 (11)
C10	0.0302 (12)	0.0442 (15)	0.0292 (12)	−0.0018 (12)	0.0028 (10)	−0.0031 (11)
C11	0.0340 (13)	0.0260 (12)	0.0463 (14)	−0.0078 (11)	0.0082 (12)	−0.0064 (11)
C12	0.0277 (12)	0.0312 (13)	0.0361 (12)	0.0032 (10)	0.0071 (11)	0.0074 (10)
C13	0.0349 (13)	0.0342 (12)	0.0270 (11)	−0.0012 (11)	0.0008 (10)	0.0069 (11)
C14	0.0257 (12)	0.0325 (12)	0.0230 (10)	0.0026 (10)	−0.0023 (9)	0.0073 (10)
C15	0.0309 (12)	0.0436 (14)	0.0320 (12)	0.0031 (12)	0.0042 (10)	0.0067 (12)
C16	0.0538 (16)	0.0460 (16)	0.0314 (13)	0.0147 (14)	0.0023 (12)	−0.0061 (12)

C17	0.0557 (17)	0.0391 (15)	0.0430 (14)	0.0059 (14)	−0.0209 (13)	−0.0020 (12)
C18	0.0371 (14)	0.0421 (15)	0.0458 (14)	−0.0062 (12)	−0.0124 (12)	0.0068 (12)
C19	0.0273 (12)	0.0449 (14)	0.0302 (11)	0.0015 (11)	0.0017 (10)	0.0018 (11)

Geometric parameters (Å, °)

O1—C1	1.423 (2)	C6—C7	1.497 (3)
O1—C4	1.444 (2)	C6—H6A	0.9900
O2—C5	1.428 (2)	C6—H6B	0.9900
O2—C1'	1.432 (3)	C7—C12	1.380 (3)
O3—C1	1.416 (2)	C7—C8	1.391 (3)
O3—C2'	1.435 (3)	C8—C9	1.382 (3)
O4—C2	1.410 (2)	C8—H8A	0.9500
O4—H4	0.90 (3)	C9—C10	1.380 (3)
O5—C3	1.409 (2)	C9—H9A	0.9500
O5—C6	1.444 (2)	C10—C11	1.367 (3)
O6—C5'	1.422 (2)	C10—H10A	0.9500
O6—C13	1.443 (2)	C11—C12	1.389 (3)
C1—C2	1.519 (3)	C11—H11A	0.9500
C1—H1A	1.0000	C12—H12A	0.9500
C2—C3	1.531 (3)	C13—C14	1.507 (3)
C2—H2A	1.0000	C13—H13A	0.9900
C3—C4	1.552 (3)	C13—H13B	0.9900
C3—C1'	1.555 (3)	C14—C15	1.378 (3)
C4—C5'	1.516 (3)	C14—C19	1.381 (3)
C4—C5	1.524 (3)	C15—C16	1.386 (3)
C5—H5A	0.9900	C15—H15A	0.9500
C5—H5B	0.9900	C16—C17	1.376 (3)
C1'—C2'	1.514 (3)	C16—H16A	0.9500
C1'—H1'A	1.0000	C17—C18	1.380 (3)
C2'—H2'A	0.9900	C17—H17A	0.9500
C2'—H2'B	0.9900	C18—C19	1.381 (3)
C5'—H5'A	0.9900	C18—H18A	0.9500
C5'—H5'B	0.9900	C19—H19A	0.9500
C1—O1—C4	110.02 (15)	O6—C5'—H5'B	109.4
C5—O2—C1'	110.63 (15)	C4—C5'—H5'B	109.4
C1—O3—C2'	113.70 (16)	H5'A—C5'—H5'B	108.0
C2—O4—H4	110.6 (18)	O5—C6—C7	108.11 (15)
C3—O5—C6	114.99 (14)	O5—C6—H6A	110.1
C5'—O6—C13	113.35 (15)	C7—C6—H6A	110.1
O3—C1—O1	110.96 (17)	O5—C6—H6B	110.1
O3—C1—C2	111.12 (18)	C7—C6—H6B	110.1
O1—C1—C2	105.63 (16)	H6A—C6—H6B	108.4
O3—C1—H1A	109.7	C12—C7—C8	118.48 (19)
O1—C1—H1A	109.7	C12—C7—C6	121.38 (19)
C2—C1—H1A	109.7	C8—C7—C6	120.14 (19)
O4—C2—C1	114.52 (18)	C9—C8—C7	120.8 (2)
O4—C2—C3	114.62 (16)	C9—C8—H8A	119.6
C1—C2—C3	97.33 (17)	C7—C8—H8A	119.6

O4—C2—H2A	109.9	C10—C9—C8	119.9 (2)
C1—C2—H2A	109.9	C10—C9—H9A	120.0
C3—C2—H2A	109.9	C8—C9—H9A	120.0
O5—C3—C2	117.39 (17)	C11—C10—C9	119.8 (2)
O5—C3—C4	109.67 (14)	C11—C10—H10A	120.1
C2—C3—C4	103.84 (16)	C9—C10—H10A	120.1
O5—C3—C1'	114.69 (16)	C10—C11—C12	120.5 (2)
C2—C3—C1'	108.27 (16)	C10—C11—H11A	119.8
C4—C3—C1'	101.21 (15)	C12—C11—H11A	119.8
O1—C4—C5'	109.39 (16)	C7—C12—C11	120.5 (2)
O1—C4—C5	110.78 (15)	C7—C12—H12A	119.8
C5'—C4—C5	110.10 (16)	C11—C12—H12A	119.8
O1—C4—C3	103.14 (14)	O6—C13—C14	112.82 (16)
C5'—C4—C3	119.30 (16)	O6—C13—H13A	109.0
C5—C4—C3	103.79 (15)	C14—C13—H13A	109.0
O2—C5—C4	106.88 (16)	O6—C13—H13B	109.0
O2—C5—H5A	110.3	C14—C13—H13B	109.0
C4—C5—H5A	110.3	H13A—C13—H13B	107.8
O2—C5—H5B	110.3	C15—C14—C19	118.3 (2)
C4—C5—H5B	110.3	C15—C14—C13	121.56 (19)
H5A—C5—H5B	108.6	C19—C14—C13	120.09 (18)
O2—C1'—C2'	109.19 (17)	C14—C15—C16	121.0 (2)
O2—C1'—C3	107.83 (15)	C14—C15—H15A	119.5
C2'—C1'—C3	111.92 (18)	C16—C15—H15A	119.5
O2—C1'—H1'A	109.3	C17—C16—C15	120.0 (2)
C2'—C1'—H1'A	109.3	C17—C16—H16A	120.0
C3—C1'—H1'A	109.3	C15—C16—H16A	120.0
O3—C2'—C1'	113.87 (17)	C16—C17—C18	119.6 (2)
O3—C2'—H2'A	108.8	C16—C17—H17A	120.2
C1'—C2'—H2'A	108.8	C18—C17—H17A	120.2
O3—C2'—H2'B	108.8	C17—C18—C19	119.9 (2)
C1'—C2'—H2'B	108.8	C17—C18—H18A	120.0
H2'A—C2'—H2'B	107.7	C19—C18—H18A	120.0
O6—C5'—C4	111.14 (16)	C18—C19—C14	121.1 (2)
O6—C5'—H5'A	109.4	C18—C19—H19A	119.4
C4—C5'—H5'A	109.4	C14—C19—H19A	119.4
C2'—O3—C1—O1	90.9 (2)	O5—C3—C1'—O2	−94.83 (19)
C2'—O3—C1—C2	−26.4 (2)	C2—C3—C1'—O2	131.93 (17)
C4—O1—C1—O3	−92.53 (19)	C4—C3—C1'—O2	23.1 (2)
C4—O1—C1—C2	28.0 (2)	O5—C3—C1'—C2'	145.06 (17)
O3—C1—C2—O4	−160.61 (17)	C2—C3—C1'—C2'	11.8 (2)
O1—C1—C2—O4	79.0 (2)	C4—C3—C1'—C2'	−96.99 (19)
O3—C1—C2—C3	78.03 (18)	C1—O3—C2'—C1'	−35.5 (2)
O1—C1—C2—C3	−42.4 (2)	O2—C1'—C2'—O3	−76.8 (2)
C6—O5—C3—C2	62.4 (2)	C3—C1'—C2'—O3	42.5 (2)
C6—O5—C3—C4	−179.48 (16)	C13—O6—C5'—C4	−174.74 (17)
C6—O5—C3—C1'	−66.4 (2)	O1—C4—C5'—O6	63.6 (2)
O4—C2—C3—O5	41.1 (2)	C5—C4—C5'—O6	−174.41 (15)
C1—C2—C3—O5	162.37 (16)	C3—C4—C5'—O6	−54.6 (2)

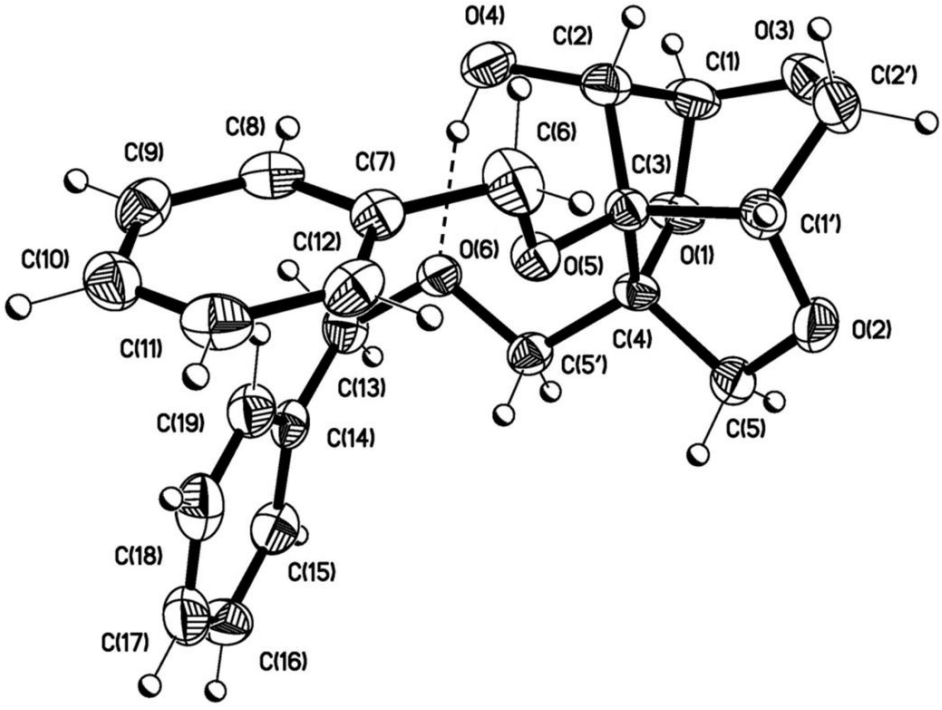
O4—C2—C3—C4	−80.1 (2)	C3—O5—C6—C7	−159.43 (16)
C1—C2—C3—C4	41.16 (17)	O5—C6—C7—C12	−111.0 (2)
O4—C2—C3—C1'	172.89 (17)	O5—C6—C7—C8	69.4 (2)
C1—C2—C3—C1'	−65.83 (18)	C12—C7—C8—C9	2.1 (3)
C1—O1—C4—C5'	−128.44 (18)	C6—C7—C8—C9	−178.29 (17)
C1—O1—C4—C5	110.02 (17)	C7—C8—C9—C10	−0.9 (3)
C1—O1—C4—C3	−0.50 (18)	C8—C9—C10—C11	−1.1 (3)
O5—C3—C4—O1	−152.95 (14)	C9—C10—C11—C12	1.9 (3)
C2—C3—C4—O1	−26.70 (17)	C8—C7—C12—C11	−1.3 (3)
C1'—C3—C4—O1	85.51 (17)	C6—C7—C12—C11	179.11 (18)
O5—C3—C4—C5'	−31.5 (2)	C10—C11—C12—C7	−0.7 (3)
C2—C3—C4—C5'	94.8 (2)	C5'—O6—C13—C14	−59.5 (2)
C1'—C3—C4—C5'	−153.03 (17)	O6—C13—C14—C15	128.2 (2)
O5—C3—C4—C5	91.43 (16)	O6—C13—C14—C19	−51.1 (2)
C2—C3—C4—C5	−142.33 (16)	C19—C14—C15—C16	1.1 (3)
C1'—C3—C4—C5	−30.12 (18)	C13—C14—C15—C16	−178.16 (19)
C1'—O2—C5—C4	−13.6 (2)	C14—C15—C16—C17	0.3 (3)
O1—C4—C5—O2	−82.16 (19)	C15—C16—C17—C18	−0.8 (3)
C5'—C4—C5—O2	156.71 (17)	C16—C17—C18—C19	0.0 (3)
C3—C4—C5—O2	27.93 (19)	C17—C18—C19—C14	1.5 (3)
C5—O2—C1'—C2'	115.25 (19)	C15—C14—C19—C18	−2.0 (3)
C5—O2—C1'—C3	−6.6 (2)	C13—C14—C19—C18	177.30 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O6	0.90 (3)	1.79 (3)	2.664 (2)	163 (3)
C15—H15A···O2^{i}	0.95	2.64	3.468 (3)	146

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

Fig. 1


O(4)
C(2)
O(3)
C(1)
C(2′)
C(8)
C(6)
C(9)
C(7)
C(3)
C(1′)
C(12)
O(6)
O(5)
O(1)
C(10)
C(4)
O(2)
C(11)
C(5′)
C(13)
C(19)
C(14)
C(5)
C(18)
C(15)
C(17)
C(16)