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Methyl 5-*O*-triphenylmethyl-*α*-D-arabinofuranoside

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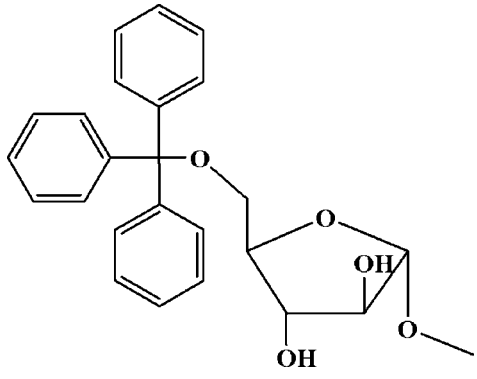
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.082; data-to-parameter ratio = 7.5.

In the title compound, $C_{25}H_{26}O_5$, the five-membered arabinofuranoside ring displays an envelope conformation. Intramolecular O—H···O hydrogen bonding helps to stabilize the molecular structure, and intermolecular O—H···O hydrogen bonding links the molecules into infinite helical supramolecular chains along the a axis.

Related literature

For synthesis, see Mikhailopulo & Sivets (1999).



Experimental

Crystal data

$C_{25}H_{26}O_5$
M_r = 406.46
Orthorhombic, $P2_12_12_1$
a = 7.4286 (15) Å
b = 8.1298 (16) Å
c = 34.101 (7) Å
V = 2059.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.50 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.946, T_{max} = 0.992
6994 measured reflections
2110 independent reflections
1522 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.082
S = 1.01
2110 reflections
281 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O5	0.863 (19)	2.10 (3)	2.896 (3)	153 (4)
O4—H4O···O3^{i}	0.83 (4)	2.06 (4)	2.877 (3)	168 (4)

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

Data collection: *RAPID-AUTO* (Rigaku, 2000); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2257).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Mikhailopulo, I. A. & Sivets, G. (1999). *Helv. Chim. Acta*, **82**, 2052–2065.
Rigaku (2000). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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Methyl 5-*O*-triphenylmethyl-*α*-D-arabinofuranoside

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Comment

The skeleton of the title compound, is composed of three benzene rings and a five-membered heterocyclic ring. And the five-membered ring have envelope conformations, with atom C2 at the flap of the envelope. It lie 0.484 (3) Å. The resultant puckering causes significant contractions of the C1—C2—C3 angles.

The title compound contains both intramolecular and intermolecular O—H···O hydrogen bonds. The intramolecule O—H···O hydrogen bonds join the compound to form a cage, and the intermolecule O—H···O hydrogen bonds link the molecules into infinite helical chains along the *a* axis.

Experimental

The title compound was synthesized according to the procedure of Mikhailopulo & Sivets (1999). The title compound is obtained from methyl alpha/beta-*D*-arabinofuranoside, which reacted with trityl chloride in the presence of 4-(dimethylamino)pyridine in anhydride pyridine at 333–343 K for 6 h, after treatment and column chromatography (hexene-ethyl acetate 1:1, Rf 0.42) yield 45% as a white solid. The compound was crystallized from hexane-ethyl acetate (1:1) to yield colorless block-like crystals after a week at room temperature.

Refinement

The hydroxyl H atoms were initially located in a difference Fourier map, and the position was allowed refined freely along with an isotropic displacement parameter. All other H-atoms were refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic, 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, and 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3. And the methyl H was allowed to rotate freely about its C—C bond. In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

Figures

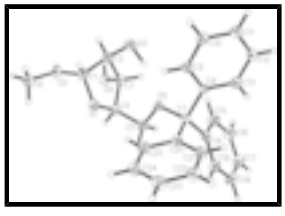

Fig. 1. A view of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

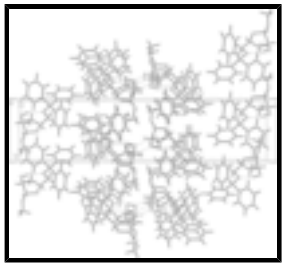

Fig. 2. The molecular packing of (I) viewed along the *a* axis. Dashed lines indicate hydrogen bonding interactions.

Methyl 5-*O*-triphenylmethyl-α-*D*-arabinofuranoside

Crystal data

$C_{25}H_{26}O_5$	F_{000} = 864
M_r = 406.46	D_x = 1.311 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 6994 reflections
a = 7.4286 (15) Å	θ = 2.4–25.0º
b = 8.1298 (16) Å	μ = 0.09 mm^{-1}
c = 34.101 (7) Å	T = 295 (2) K
V = 2059.5 (7) Å^3	Block, colorless
Z = 4	0.50 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2110 independent reflections
Radiation source: fine-focus sealed tube	1522 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
Detector resolution: 10 pixels mm^{-1}	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 2.4º
ω scans	h = −8→8
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −9→9
T_{min} = 0.946, T_{max} = 0.992	l = −40→40
6994 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.082	$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 0.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$

2110 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
281 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0260 (15)

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 $F^2 > \sigma(F^2)$ 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	0.5208 (3)	0.5222 (3)	0.08813 (6)	0.0407 (6)
O2	0.4450 (3)	0.6557 (3)	0.02943 (6)	0.0469 (6)
O3	0.6178 (4)	0.2463 (3)	0.03120 (7)	0.0498 (7)
H3O	0.646 (6)	0.221 (5)	0.0550 (7)	0.080 (15)*
O4	0.1565 (3)	0.3851 (3)	0.04668 (7)	0.0424 (6)
H4O	0.143 (6)	0.362 (6)	0.0231 (10)	0.081 (16)*
O5	0.5912 (3)	0.2009 (2)	0.11522 (5)	0.0309 (5)
C1	0.5460 (5)	0.5315 (4)	0.04707 (9)	0.0367 (8)
H1	0.6740	0.5455	0.0409	0.044*
C2	0.4782 (5)	0.3666 (4)	0.03127 (10)	0.0361 (8)
H2	0.4307	0.3808	0.0047	0.043*
C3	0.3270 (4)	0.3232 (4)	0.05910 (8)	0.0329 (8)
H3	0.3210	0.2038	0.0629	0.039*
C4	0.3786 (4)	0.4081 (4)	0.09739 (8)	0.0340 (8)
H4	0.2744	0.4705	0.1069	0.041*
C5	0.4398 (4)	0.2931 (4)	0.12950 (8)	0.0342 (8)
H5A	0.4740	0.3555	0.1526	0.041*
H5B	0.3428	0.2190	0.1366	0.041*
C6	0.5213 (6)	0.8169 (4)	0.03313 (10)	0.0532 (11)
H6A	0.4504	0.8940	0.0184	0.080*
H6B	0.6422	0.8162	0.0232	0.080*
H6C	0.5223	0.8486	0.0602	0.080*
C7	0.6897 (4)	0.1002 (4)	0.14349 (8)	0.0287 (7)
C8	0.8065 (4)	−0.0140 (4)	0.11786 (8)	0.0272 (7)
C9	0.9242 (4)	0.0581 (4)	0.09055 (8)	0.0344 (8)
H9	0.9268	0.1719	0.0878	0.041*

C10	1.0355 (5)	−0.0378 (4)	0.06784 (9)	0.0373 (8)
H10	1.1104	0.0116	0.0495	0.045*
C11	1.0372 (5)	−0.2078 (4)	0.07207 (9)	0.0382 (8)
H11	1.1138	−0.2720	0.0569	0.046*
C12	0.9242 (5)	−0.2801 (4)	0.09896 (9)	0.0389 (9)
H12	0.9236	−0.3939	0.1018	0.047*
C13	0.8107 (5)	−0.1839 (4)	0.12205 (9)	0.0360 (8)
H13	0.7367	−0.2341	0.1405	0.043*
C14	0.5546 (4)	0.0034 (4)	0.16861 (8)	0.0283 (7)
C15	0.4268 (4)	−0.0927 (4)	0.15044 (9)	0.0403 (8)
H15	0.4244	−0.0973	0.1232	0.048*
C16	0.3028 (5)	−0.1820 (4)	0.17135 (11)	0.0485 (9)
H16	0.2173	−0.2451	0.1583	0.058*
C17	0.3051 (5)	−0.1779 (4)	0.21152 (11)	0.0484 (9)
H17	0.2228	−0.2397	0.2258	0.058*
C18	0.4296 (5)	−0.0822 (5)	0.23045 (9)	0.0482 (10)
H18	0.4312	−0.0787	0.2577	0.058*
C19	0.5529 (4)	0.0092 (4)	0.20932 (8)	0.0368 (8)
H19	0.6354	0.0752	0.2225	0.044*
C20	0.8215 (4)	0.2061 (4)	0.16746 (8)	0.0292 (7)
C21	0.9461 (4)	0.1301 (4)	0.19168 (9)	0.0377 (8)
H21	0.9453	0.0160	0.1938	0.045*
C22	1.0720 (5)	0.2198 (4)	0.21282 (10)	0.0434 (9)
H22	1.1545	0.1660	0.2288	0.052*
C23	1.0741 (5)	0.3882 (5)	0.20995 (10)	0.0488 (10)
H23	1.1571	0.4493	0.2243	0.059*
C24	0.9544 (5)	0.4649 (4)	0.18615 (10)	0.0496 (10)
H24	0.9563	0.5791	0.1843	0.060*
C25	0.8290 (5)	0.3765 (4)	0.16445 (9)	0.0393 (8)
H25	0.7499	0.4315	0.1479	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0557 (15)	0.0316 (12)	0.0348 (12)	−0.0128 (12)	−0.0050 (11)	−0.0004 (10)
O2	0.0522 (15)	0.0348 (13)	0.0538 (14)	−0.0066 (13)	−0.0080 (14)	0.0111 (12)
O3	0.0535 (17)	0.0537 (16)	0.0423 (14)	0.0193 (14)	0.0049 (13)	−0.0082 (14)
O4	0.0360 (13)	0.0459 (14)	0.0453 (14)	−0.0008 (13)	−0.0086 (13)	−0.0014 (13)
O5	0.0290 (11)	0.0362 (11)	0.0274 (10)	0.0041 (11)	0.0000 (10)	0.0036 (10)
C1	0.0394 (19)	0.0359 (18)	0.0348 (18)	−0.0026 (18)	−0.0024 (18)	0.0045 (16)
C2	0.038 (2)	0.0373 (19)	0.0326 (18)	0.0037 (17)	−0.0051 (16)	−0.0032 (16)
C3	0.0318 (17)	0.0281 (16)	0.0387 (18)	0.0008 (16)	−0.0057 (15)	−0.0022 (15)
C4	0.0365 (19)	0.0364 (18)	0.0293 (16)	0.0012 (17)	0.0005 (15)	−0.0027 (15)
C5	0.0310 (17)	0.0401 (18)	0.0313 (16)	0.0024 (18)	0.0041 (15)	0.0025 (15)
C6	0.070 (3)	0.0360 (19)	0.053 (2)	−0.008 (2)	0.000 (2)	0.0026 (18)
C7	0.0275 (16)	0.0317 (16)	0.0268 (15)	−0.0019 (17)	−0.0012 (14)	0.0045 (15)
C8	0.0279 (17)	0.0272 (16)	0.0266 (16)	−0.0010 (15)	−0.0030 (15)	−0.0016 (15)
C9	0.0351 (19)	0.0325 (18)	0.0355 (17)	−0.0028 (16)	0.0047 (17)	0.0049 (15)

C10	0.0305 (18)	0.043 (2)	0.0383 (18)	−0.0027 (17)	0.0033 (17)	0.0045 (16)
C11	0.0379 (19)	0.0405 (19)	0.0362 (18)	0.0052 (18)	0.0019 (18)	−0.0058 (17)
C12	0.043 (2)	0.0292 (17)	0.0451 (19)	0.0038 (18)	−0.0015 (18)	−0.0005 (16)
C13	0.0361 (19)	0.0360 (18)	0.0361 (19)	−0.0024 (17)	0.0023 (17)	0.0023 (17)
C14	0.0262 (16)	0.0291 (16)	0.0295 (16)	−0.0009 (17)	0.0023 (14)	0.0038 (15)
C15	0.0337 (18)	0.053 (2)	0.0346 (18)	−0.011 (2)	0.0013 (16)	0.0028 (18)
C16	0.039 (2)	0.050 (2)	0.057 (2)	−0.014 (2)	0.0022 (19)	0.003 (2)
C17	0.039 (2)	0.047 (2)	0.059 (2)	−0.008 (2)	0.011 (2)	0.017 (2)
C18	0.053 (2)	0.060 (2)	0.0310 (17)	−0.001 (2)	0.0077 (18)	0.0144 (19)
C19	0.0364 (18)	0.0429 (19)	0.0311 (17)	−0.0034 (19)	−0.0024 (16)	0.0024 (17)
C20	0.0275 (16)	0.0304 (17)	0.0298 (16)	−0.0046 (16)	0.0021 (15)	0.0008 (15)
C21	0.0364 (19)	0.0338 (18)	0.0428 (18)	0.0004 (17)	−0.0047 (18)	−0.0015 (16)
C22	0.0326 (19)	0.053 (2)	0.0442 (19)	0.000 (2)	−0.0094 (18)	−0.0020 (19)
C23	0.047 (2)	0.052 (2)	0.048 (2)	−0.014 (2)	−0.010 (2)	−0.009 (2)
C24	0.060 (3)	0.0329 (19)	0.056 (2)	−0.014 (2)	−0.009 (2)	−0.0010 (18)
C25	0.043 (2)	0.0362 (18)	0.0391 (19)	−0.0064 (19)	−0.0057 (18)	0.0043 (16)

Geometric parameters (Å, °)

O1—C1	1.415 (3)	C10—C11	1.390 (4)
O1—C4	1.441 (4)	C10—H10	0.9300
O2—C1	1.395 (4)	C11—C12	1.375 (4)
O2—C6	1.434 (4)	C11—H11	0.9300
O3—C2	1.425 (4)	C12—C13	1.394 (4)
O3—H3O	0.863 (19)	C12—H12	0.9300
O4—C3	1.427 (4)	C13—H13	0.9300
O4—H4O	0.83 (4)	C14—C15	1.377 (4)
O5—C5	1.437 (4)	C14—C19	1.389 (4)
O5—C7	1.461 (3)	C15—C16	1.372 (4)
C1—C2	1.530 (4)	C15—H15	0.9300
C1—H1	0.9800	C16—C17	1.371 (4)
C2—C3	1.512 (4)	C16—H16	0.9300
C2—H2	0.9800	C17—C18	1.370 (5)
C3—C4	1.526 (4)	C17—H17	0.9300
C3—H3	0.9800	C18—C19	1.382 (4)
C4—C5	1.510 (4)	C18—H18	0.9300
C4—H4	0.9800	C19—H19	0.9300
C5—H5A	0.9700	C20—C21	1.386 (4)
C5—H5B	0.9700	C20—C25	1.390 (4)
C6—H6A	0.9600	C21—C22	1.388 (4)
C6—H6B	0.9600	C21—H21	0.9300
C6—H6C	0.9600	C22—C23	1.373 (5)
C7—C14	1.536 (4)	C22—H22	0.9300
C7—C20	1.539 (4)	C23—C24	1.356 (5)
C7—C8	1.543 (4)	C23—H23	0.9300
C8—C13	1.388 (4)	C24—C25	1.390 (4)
C8—C9	1.405 (4)	C24—H24	0.9300
C9—C10	1.375 (4)	C25—H25	0.9300
C9—H9	0.9300		

C1—O1—C4	110.4 (2)	C10—C9—H9	119.7
C1—O2—C6	114.3 (3)	C8—C9—H9	119.7
C2—O3—H3O	110 (3)	C9—C10—C11	120.7 (3)
C3—O4—H4O	108 (3)	C9—C10—H10	119.6
C5—O5—C7	117.4 (2)	C11—C10—H10	119.6
O2—C1—O1	113.3 (3)	C12—C11—C10	119.3 (3)
O2—C1—C2	107.8 (3)	C12—C11—H11	120.4
O1—C1—C2	105.0 (3)	C10—C11—H11	120.4
O2—C1—H1	110.2	C11—C12—C13	120.4 (3)
O1—C1—H1	110.2	C11—C12—H12	119.8
C2—C1—H1	110.2	C13—C12—H12	119.8
O3—C2—C3	112.4 (3)	C8—C13—C12	120.9 (3)
O3—C2—C1	111.2 (3)	C8—C13—H13	119.6
C3—C2—C1	103.2 (3)	C12—C13—H13	119.6
O3—C2—H2	109.9	C15—C14—C19	117.5 (3)
C3—C2—H2	109.9	C15—C14—C7	119.4 (3)
C1—C2—H2	109.9	C19—C14—C7	123.1 (3)
O4—C3—C2	113.0 (2)	C16—C15—C14	122.0 (3)
O4—C3—C4	108.5 (3)	C16—C15—H15	119.0
C2—C3—C4	104.2 (3)	C14—C15—H15	119.0
O4—C3—H3	110.3	C17—C16—C15	119.9 (3)
C2—C3—H3	110.3	C17—C16—H16	120.1
C4—C3—H3	110.3	C15—C16—H16	120.1
O1—C4—C5	109.7 (2)	C16—C17—C18	119.6 (3)
O1—C4—C3	106.7 (2)	C16—C17—H17	120.2
C5—C4—C3	114.6 (3)	C18—C17—H17	120.2
O1—C4—H4	108.6	C17—C18—C19	120.5 (3)
C5—C4—H4	108.6	C17—C18—H18	119.8
C3—C4—H4	108.6	C19—C18—H18	119.8
O5—C5—C4	108.3 (2)	C18—C19—C14	120.6 (3)
O5—C5—H5A	110.0	C18—C19—H19	119.7
C4—C5—H5A	110.0	C14—C19—H19	119.7
O5—C5—H5B	110.0	C21—C20—C25	117.5 (3)
C4—C5—H5B	110.0	C21—C20—C7	119.4 (3)
H5A—C5—H5B	108.4	C25—C20—C7	122.9 (3)
O2—C6—H6A	109.5	C20—C21—C22	121.7 (3)
O2—C6—H6B	109.5	C20—C21—H21	119.2
H6A—C6—H6B	109.5	C22—C21—H21	119.2
O2—C6—H6C	109.5	C23—C22—C21	119.7 (4)
H6A—C6—H6C	109.5	C23—C22—H22	120.2
H6B—C6—H6C	109.5	C21—C22—H22	120.2
O5—C7—C14	109.2 (2)	C24—C23—C22	119.6 (3)
O5—C7—C20	110.8 (2)	C24—C23—H23	120.2
C14—C7—C20	114.0 (2)	C22—C23—H23	120.2
O5—C7—C8	104.2 (2)	C23—C24—C25	121.3 (3)
C14—C7—C8	112.1 (3)	C23—C24—H24	119.3
C20—C7—C8	106.2 (2)	C25—C24—H24	119.3
C13—C8—C9	118.0 (3)	C20—C25—C24	120.2 (3)
C13—C8—C7	123.5 (3)	C20—C25—H25	119.9

C9—C8—C7	118.3 (3)	C24—C25—H25	119.9
C10—C9—C8	120.7 (3)		
C6—O2—C1—O1	79.8 (4)	C9—C10—C11—C12	0.8 (6)
C6—O2—C1—C2	−164.6 (3)	C10—C11—C12—C13	−0.7 (5)
C4—O1—C1—O2	91.9 (3)	C9—C8—C13—C12	−1.9 (5)
C4—O1—C1—C2	−25.4 (3)	C7—C8—C13—C12	−177.6 (3)
O2—C1—C2—O3	151.1 (3)	C11—C12—C13—C8	1.3 (5)
O1—C1—C2—O3	−87.9 (3)	O5—C7—C14—C15	53.9 (4)
O2—C1—C2—C3	−88.2 (3)	C20—C7—C14—C15	178.4 (3)
O1—C1—C2—C3	32.8 (3)	C8—C7—C14—C15	−60.9 (4)
O3—C2—C3—O4	−150.2 (3)	O5—C7—C14—C19	−125.3 (3)
C1—C2—C3—O4	89.9 (3)	C20—C7—C14—C19	−0.8 (4)
O3—C2—C3—C4	92.3 (3)	C8—C7—C14—C19	119.9 (3)
C1—C2—C3—C4	−27.7 (3)	C19—C14—C15—C16	−0.9 (5)
C1—O1—C4—C5	132.3 (3)	C7—C14—C15—C16	179.9 (3)
C1—O1—C4—C3	7.6 (3)	C14—C15—C16—C17	−0.5 (6)
O4—C3—C4—O1	−107.2 (3)	C15—C16—C17—C18	1.1 (6)
C2—C3—C4—O1	13.5 (3)	C16—C17—C18—C19	−0.3 (5)
O4—C3—C4—C5	131.3 (3)	C17—C18—C19—C14	−1.1 (5)
C2—C3—C4—C5	−108.1 (3)	C15—C14—C19—C18	1.7 (5)
C7—O5—C5—C4	170.8 (2)	C7—C14—C19—C18	−179.2 (3)
O1—C4—C5—O5	−62.1 (3)	O5—C7—C20—C21	−170.5 (3)
C3—C4—C5—O5	57.8 (3)	C14—C7—C20—C21	66.0 (4)
C5—O5—C7—C14	45.8 (3)	C8—C7—C20—C21	−57.9 (4)
C5—O5—C7—C20	−80.5 (3)	O5—C7—C20—C25	5.8 (4)
C5—O5—C7—C8	165.7 (2)	C14—C7—C20—C25	−117.7 (4)
O5—C7—C8—C13	−128.3 (3)	C8—C7—C20—C25	118.4 (3)
C14—C7—C8—C13	−10.4 (4)	C25—C20—C21—C22	1.2 (5)
C20—C7—C8—C13	114.6 (3)	C7—C20—C21—C22	177.7 (3)
O5—C7—C8—C9	56.1 (3)	C20—C21—C22—C23	0.2 (5)
C14—C7—C8—C9	174.0 (3)	C21—C22—C23—C24	−0.8 (6)
C20—C7—C8—C9	−61.0 (3)	C22—C23—C24—C25	0.0 (6)
C13—C8—C9—C10	2.1 (5)	C21—C20—C25—C24	−1.9 (5)
C7—C8—C9—C10	177.9 (3)	C7—C20—C25—C24	−178.3 (3)
C8—C9—C10—C11	−1.6 (5)	C23—C24—C25—C20	1.4 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3O···O5	0.863 (19)	2.10 (3)	2.896 (3)	153 (4)
O4—H4O···O3^{i}	0.83 (4)	2.06 (4)	2.877 (3)	168 (4)

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

Fig. 1

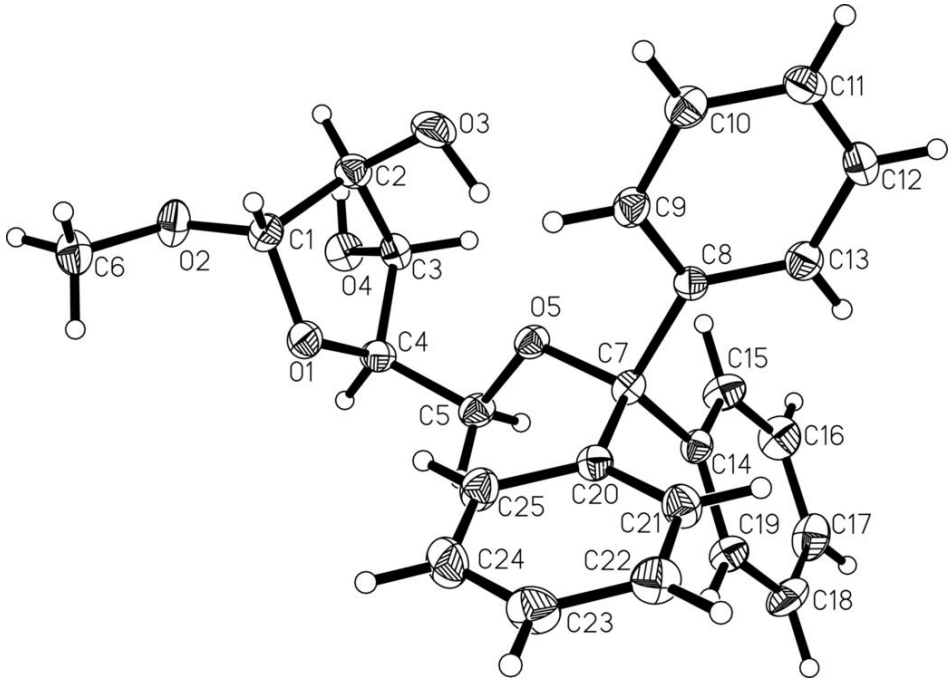
C11
C10
O3
C2
C12
C9
C1
C6
O2
O4
C3
C8
C13
O5
C4
C7
C15
O1
C5
C16
C14
C25
C20
C21
C19
C17
C24
C22
C18
C23

Fig. 2