Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2-Di-*C*-methoxy-1,4:3,6-dianhydro-mannitol

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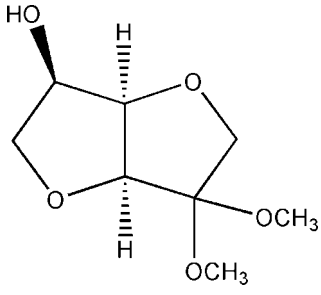
Received 23 June 2007; accepted 8 July 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.051; wR factor = 0.138; data-to-parameter ratio = 6.7.

The title compound, $C_8H_{14}O_5$, is a 1,4:3,6-dianhydro-D-fructose derivative. Its structure consists of two fused tetrahydrofuran rings with a *cis* ring junction, giving a V-shaped molecule with an angle between the two rings of 129.9°. Intermolecular O—H···O hydrogen bonds help stabilize the crystal structure.

Related literature

Bioactivity of sugar derivatives: Stutz (1999); Chang *et al.* (2001).



Experimental

Crystal data

$C_8H_{14}O_5$
M_r = 190.19
Monoclinic, $P2_1$
a = 6.4996 (13) Å
b = 6.3375 (13) Å
c = 10.983 (2) Å
β = 93.07 (3)°
V = 451.77 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 291 (2) K
0.20 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS-IV diffractometer
Absorption correction: none
1418 measured reflections
829 independent reflections
772 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.138
S = 1.04
829 reflections
123 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*E*···O4^{i}	0.91 (14)	2.33 (13)	3.123 (6)	145 (9)

Symmetry code: (i) $x-1, y, z$.

Data collection: *R-AXIS* (Molecular Structure Corporation, 1993); cell refinement: *R-AXIS*; data reduction: *R-AXIS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1993); software used to prepare material for publication: *TEXSAN*.

We gratefully acknowledge financial support from the National Natural Science Foundation of P. R. China (No. 20572103).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2143).

References

Chang, C. W. T., Hui, Y. & Elchert, B. (2001). *Tetrahedron Lett.* **42**, 7019–7023.
Molecular Structure Corporation (1993). *TEXSAN* (Version 1.6) and *R-AXIS* (Version 4.02). MSC, The Woodlands, Texas, USA.
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 doi:10.1107/S1600536807033387

supplementary materials

Acta Cryst. (2007). E**63**, o3653 [**doi:10.1107/S1600536807033387**]

2,2-Di-*C*-methoxy-1,4:3,6-dianhydromannitol

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Comment

Sugar derivatives are an important class of compounds having a broad spectrum of applications in the chemical, biochemical, medicinal(Chang *et al.*, 2001), and pharmaceutical fields (Stutz, 1999), Here we report the structure of a novel Sugar derivative.

The molecular structure of title compound is shown in Fig.1. Torsion angle C(2)—C(3)—C(4)—C(5) is −129.9°·Intermolecular O3–H···O4 hydrogen bonds links the molecules into chains along the *a* axis.

Experimental

1,4:3,6-dianhydro-D-fructose, having three known chiral centers, was dissolved in MeOH. Catalytic amount of H_2SO_4 was added and the mixture was stirred at room temperature for 4 h,and evaporated under reduced pressure to dryness. The residue was recrystallization from MeOH,to give title compound as a colorless crystal.

Refinement

The absolute configuration could not be determined from the experimental data, therefore, the Friedel equivalents were merged before refinement. The absolute configuration was set from the starting material of known configurataion.

Figures

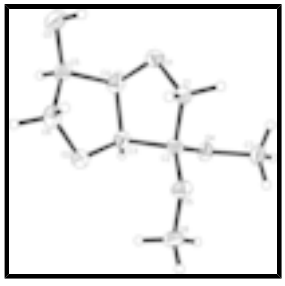

Fig. 1. The molecular structure of I, with 30% probability displacement ellipsoids and hydrogen atoms shown as spheres of arbitrary radii

Fig. 2. The Molecular stacking of title compound along the *a* axis showing the intermolecular hydrogen bonds.

2,2-Di-*C*-methoxy-1,4:3,6-dianhydromannitol

Crystal data

$C_8H_{14}O_5$	F_{000} = 204
M_r = 190.19	D_x = 1.398 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.4996 (13) Å	Cell parameters from 389 reflections
b = 6.3375 (13) Å	θ = 2–25.1º
c = 10.983 (2) Å	μ = 0.12 mm^{-1}
β = 93.07 (3)º	T = 291 (2) K
V = 451.77 (16) Å^3	Prism, colorless
Z = 2	0.20 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS-IV diffractometer	772 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.045
Monochromator: graphite	θ_{max} = 25.0º
T = 291(2) K	θ_{min} = 1.9º
Oscillation frames scans	h = 0→7
Absorption correction: None	k = −7→7
1418 measured reflections	l = −13→13
829 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2 + 0.0821P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.138	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
829 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
123 parameters	Extinction coefficient: 0.32 (5)
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
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.

Because the absolute configuration was established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration, we have merged the Friedels in the refinement.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0086 (5)	0.4646 (6)	0.1232 (3)	0.0643 (9)
O2	0.1615 (4)	0.4646 (6)	0.4086 (2)	0.0658 (9)
O3	−0.2707 (5)	0.2344 (7)	0.2434 (4)	0.0799 (11)
O4	0.4505 (4)	0.6120 (5)	0.1554 (2)	0.0534 (8)
O5	0.3034 (4)	0.8296 (5)	0.2983 (3)	0.0526 (8)
C1	0.0757 (7)	0.6726 (7)	0.1524 (4)	0.0559 (11)
H1A	−0.0253	0.7449	0.1992	0.067*
H1B	0.0954	0.7526	0.0786	0.067*
C2	0.2786 (6)	0.6500 (6)	0.2271 (3)	0.0453 (9)
C3	0.2496 (6)	0.4386 (7)	0.2940 (4)	0.0481 (10)
H3A	0.3798	0.3607	0.3029	0.058*
C4	0.0928 (6)	0.3198 (7)	0.2124 (3)	0.0543 (10)
H4A	0.1568	0.1992	0.1733	0.065*
C5	−0.0701 (6)	0.2466 (7)	0.2976 (4)	0.0543 (10)
H5A	−0.0308	0.1077	0.3304	0.065*
C6	−0.0468 (6)	0.4083 (9)	0.3988 (4)	0.0647 (13)
H6A	−0.1315	0.5311	0.3794	0.078*
H6B	−0.0887	0.3488	0.4750	0.078*
C7	0.5017 (8)	0.7814 (8)	0.0763 (4)	0.0684 (13)
H7A	0.6192	0.7426	0.0319	0.103*
H7B	0.5333	0.9054	0.1239	0.103*
H7C	0.3868	0.8098	0.0201	0.103*
C8	0.4823 (6)	0.8327 (9)	0.3786 (4)	0.0630 (12)
H8A	0.4872	0.9629	0.4233	0.095*
H8B	0.6028	0.8208	0.3322	0.095*
H8C	0.4777	0.7166	0.4344	0.095*
H3E	−0.298 (15)	0.36 (2)	0.204 (8)	0.18 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0798 (19)	0.0572 (19)	0.0542 (15)	−0.0192 (16)	−0.0124 (13)	0.0022 (16)
O2	0.0693 (17)	0.078 (2)	0.0499 (14)	−0.0169 (18)	0.0038 (12)	0.0008 (17)
O3	0.0611 (18)	0.074 (2)	0.103 (3)	−0.0198 (18)	−0.0077 (16)	0.016 (2)
O4	0.0644 (17)	0.0408 (15)	0.0562 (14)	−0.0050 (13)	0.0141 (12)	0.0020 (14)
O5	0.0541 (15)	0.0410 (15)	0.0622 (16)	0.0028 (14)	−0.0034 (12)	−0.0060 (15)
C1	0.061 (2)	0.045 (3)	0.060 (2)	−0.0047 (19)	−0.0137 (18)	0.010 (2)
C2	0.049 (2)	0.042 (2)	0.0446 (18)	0.0019 (16)	−0.0024 (15)	0.0011 (18)
C3	0.0427 (17)	0.044 (2)	0.057 (2)	0.0065 (17)	0.0017 (15)	0.011 (2)
C4	0.068 (2)	0.036 (2)	0.060 (2)	−0.0005 (19)	0.0112 (19)	−0.006 (2)
C5	0.057 (2)	0.042 (2)	0.064 (2)	−0.0064 (18)	0.0012 (17)	0.008 (2)
C6	0.064 (3)	0.065 (3)	0.067 (3)	−0.001 (2)	0.018 (2)	0.005 (2)
C7	0.091 (3)	0.052 (3)	0.063 (2)	−0.015 (2)	0.014 (2)	0.009 (2)
C8	0.062 (2)	0.062 (3)	0.064 (2)	−0.012 (2)	−0.0107 (18)	−0.007 (3)

Geometric parameters (Å, °)

O1—C1	1.420 (6)	C3—C4	1.521 (6)
O1—C4	1.429 (5)	C3—H3A	0.9800
O2—C6	1.399 (5)	C4—C5	1.522 (6)
O2—C3	1.419 (5)	C4—H4A	0.9800
O3—C5	1.406 (5)	C5—C6	1.514 (7)
O3—H3E	0.91 (14)	C5—H5A	0.9800
O4—C2	1.422 (5)	C6—H6A	0.9700
O4—C7	1.431 (5)	C6—H6B	0.9700
O5—C2	1.385 (5)	C7—H7A	0.9600
O5—C8	1.421 (4)	C7—H7B	0.9600
C1—C2	1.523 (5)	C7—H7C	0.9600
C1—H1A	0.9700	C8—H8A	0.9600
C1—H1B	0.9700	C8—H8B	0.9600
C2—C3	1.545 (6)	C8—H8C	0.9600
C1—O1—C4	109.9 (3)	C3—C4—H4A	110.9
C6—O2—C3	109.7 (3)	C5—C4—H4A	110.9
C5—O3—H3E	108 (7)	O3—C5—C6	113.7 (4)
C2—O4—C7	115.1 (3)	O3—C5—C4	114.6 (3)
C2—O5—C8	115.4 (3)	C6—C5—C4	101.5 (3)
O1—C1—C2	106.3 (3)	O3—C5—H5A	108.9
O1—C1—H1A	110.5	C6—C5—H5A	108.9
C2—C1—H1A	110.5	C4—C5—H5A	108.9
O1—C1—H1B	110.5	O2—C6—C5	106.7 (4)
C2—C1—H1B	110.5	O2—C6—H6A	110.4
H1A—C1—H1B	108.7	C5—C6—H6A	110.4
O5—C2—O4	112.4 (3)	O2—C6—H6B	110.4
O5—C2—C1	107.4 (3)	C5—C6—H6B	110.4
O4—C2—C1	113.7 (3)	H6A—C6—H6B	108.6

O5—C2—C3	117.2 (3)	O4—C7—H7A	109.5
O4—C2—C3	103.6 (3)	O4—C7—H7B	109.5
C1—C2—C3	102.3 (3)	H7A—C7—H7B	109.5
O2—C3—C4	106.9 (3)	O4—C7—H7C	109.5
O2—C3—C2	112.7 (3)	H7A—C7—H7C	109.5
C4—C3—C2	104.1 (3)	H7B—C7—H7C	109.5
O2—C3—H3A	110.9	O5—C8—H8A	109.5
C4—C3—H3A	110.9	O5—C8—H8B	109.5
C2—C3—H3A	110.9	H8A—C8—H8B	109.5
O1—C4—C3	107.8 (3)	O5—C8—H8C	109.5
O1—C4—C5	111.3 (3)	H8A—C8—H8C	109.5
C3—C4—C5	104.7 (3)	H8B—C8—H8C	109.5
O1—C4—H4A	110.9		
C4—O1—C1—C2	25.6 (4)	O4—C2—C3—C4	−93.3 (3)
C8—O5—C2—O4	−56.7 (4)	C1—C2—C3—C4	25.1 (4)
C8—O5—C2—C1	177.6 (3)	C1—O1—C4—C3	−8.7 (4)
C8—O5—C2—C3	63.2 (4)	C1—O1—C4—C5	105.6 (4)
C7—O4—C2—O5	−56.8 (4)	O2—C3—C4—O1	108.3 (4)
C7—O4—C2—C1	65.4 (4)	C2—C3—C4—O1	−11.2 (4)
C7—O4—C2—C3	175.7 (3)	O2—C3—C4—C5	−10.4 (4)
O1—C1—C2—O5	−155.2 (3)	C2—C3—C4—C5	−129.9 (3)
O1—C1—C2—O4	79.9 (4)	O1—C4—C5—O3	32.0 (5)
O1—C1—C2—C3	−31.2 (4)	C3—C4—C5—O3	148.3 (4)
C6—O2—C3—C4	−10.7 (5)	O1—C4—C5—C6	−91.0 (4)
C6—O2—C3—C2	103.1 (4)	C3—C4—C5—C6	25.3 (4)
O5—C2—C3—O2	26.8 (4)	C3—O2—C6—C5	27.8 (5)
O4—C2—C3—O2	151.2 (3)	O3—C5—C6—O2	−156.3 (4)
C1—C2—C3—O2	−90.3 (4)	C4—C5—C6—O2	−32.7 (5)
O5—C2—C3—C4	142.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3E···O4^{i}	0.91 (14)	2.33 (13)	3.123 (6)	145 (9)

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

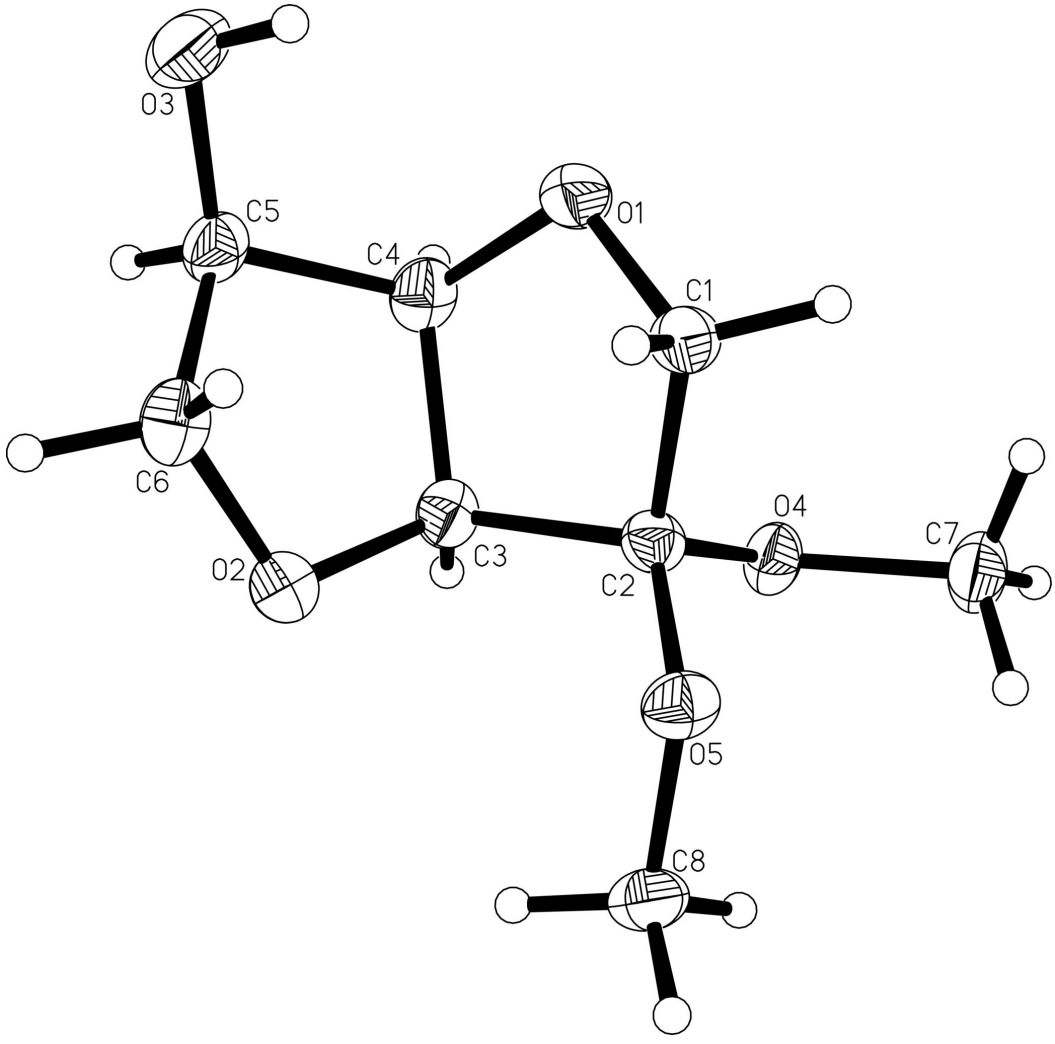

Fig. 2