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3-*O*-*tert*-Butyldimethylsilyl-2,2′:5,6-di-*O*-isopropylidene-2-*C*-hydroxymethyl-D-1,4-gluconolactone

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.040
Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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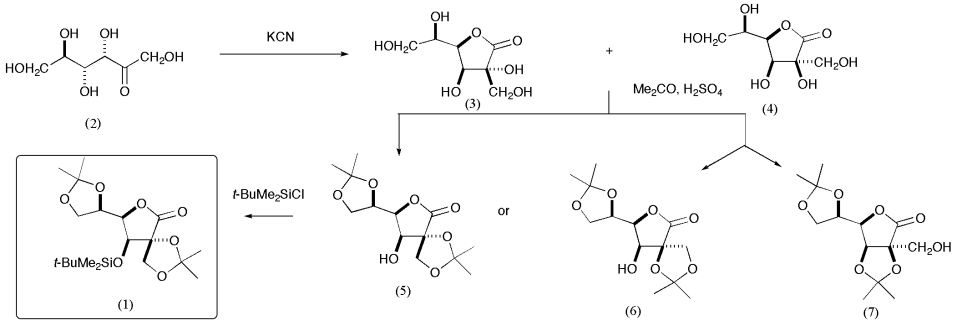
The title compound, $C_{19}H_{34}O_7Si$, is derived from the minor component of a Kiliani reaction on D-fructose. Its crystal structure has been determined in order to confirm its structure and stereochemistry.

Comment

Carbohydrates provide the most diverse set of building blocks for the synthesis of enantiomerically pure compounds (Bols, 1996). At present, all these scaffolds have linear carbon chains and there are no accessible branched sugar chirons (Hanessian, 1983). Such materials, if readily and cheaply available, are likely to have many uses. In particular, they will provide efficient access to highly functionalized compounds containing non-linear carbon chains. While the carbon linear extension of an aldose with cyanide to provide a higher sugar (the Kiliani ascension) has long been developed as an industrial process (Hudson, 1945), the cyanohydrin reaction with ketoses is barely reported. The Kiliani reaction of cyanide with D-fructose was first studied long ago (Kiliani, 1885, 1928) but has only been reported subsequently very rarely (Gorin & Perlin, 1958). In practice, the Kiliani reaction of D-fructose (2) proceeds in good yield to give a mixture of the two diastereomers (3) and (4) which cannot easily be separated. However, direct treatment of this crude material produced the diacetonide (7) as the major product, which crystallized relatively easily. A second diacetonide was also isolated which could have been either of the diacetonides (5) or (6). This unknown product was converted to a crystalline *tert*-butyldimethylsilyl ether (1), the structure and stereochemistry of which were unequivocally determined by X-ray crystallographic analysis. This firmly established that the minor component in the acetonation reaction was the *gluco*-diacectonide (5).



Experimental

The diacetonide (1) was prepared from fructose (2) (Hotchkiss *et al.*, 2004). The title material was crystallized from methanol as colourless plates.

Crystal data

$C_{19}H_{34}O_7Si$
$M_r = 402.56$
Orthorhombic, $P2_12_12_1$
$a = 6.4765\ (2)$ Å
$b = 13.2189\ (2)$ Å
$c = 25.7075\ (6)$ Å
$V = 2200.88\ (9)$ Å^3
$Z = 4$
$D_x = 1.215$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12716 reflections
$\theta = 5$–28°
$\mu = 0.14$ mm^{-1}
$T = 150$ K
Fragment, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.95$, $T_{max} = 0.97$
12716 measured reflections
4801 independent reflections
4025 reflections with $I > 3\ s(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.5^\circ$
$h = -8 \rightarrow 8$
$k = -17 \rightarrow 17$
$l = -33 \rightarrow 33$

Refinement

Refinement on F
$R = 0.037$
R = missing
$wR = 0.040$
$S = 1.11$
4025 reflections
245 parameters
H-atom parameters not refined
Weighting scheme: see text
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983), 1960 Friedel pairs
Flack parameter = 0.04 (12)

The weighting scheme used a Chebychev polynomial (Watkin, 1994, Prince, 1982): $w = \{1 - [(F_o - F_c)/6\sigma(F)]^2\}^2/[0.682T_0(x) + 0.0517T_1(x) + 0.322T_2(x)]$, where $x = F_c/F_{max}$. All H atoms were positioned geometrically (C—H = 1.0 Å), and refined as riding, with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *COLLECT* and *DENZO* (Otwinowski & Minor, 1997); data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ATOMS for Windows* (Shape Software, 2002); software used to prepare material for publication: *CRYSTALS*.

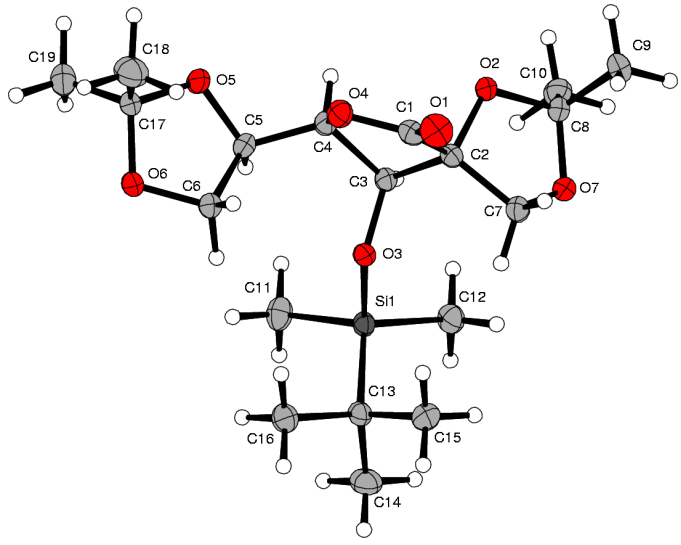


Figure 1
View of the title molecule, showing displacement ellipsoids at the 40% probability level. H atoms are shown as spheres of arbitrary radius.

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2,2:5,6-Di-*O*-isopropylidene-2-*C*-hydroxymethyl-D-glucono-1,4-lactone

Crystal data

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4025 reflections with $I > 3s(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.5°$, $\theta_{min} = 5.2°$
$h = -8 \rightarrow 8$
$k = -17 \rightarrow 17$
$l = -33 \rightarrow 33$

Refinement

Refinement on F
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.040$
$S = 1.11$
4025 reflections
245 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
Method, part 1, Chebychev polynomial (Watkin, 1994; *P*rince, 1982): [*w*eight] = 1.0/[$A_0T_0(x)$ + $A_1T_1(x)$ ··· + A_{n-1}]$T_{n-1}(x)$], where A_i are the Chebychev coefficients listed below and x = F /F_{max}; Method = Robust Weighting (*P*rince, 1982); W = [*w*eight] [1-(δF/6*σF)^2]^2, *w*ith A_i are 0.682, 0.0517 and 0.322
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983), 1960 Friedel pairs
Absolute structure parameter: 0.04 (12)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4926 (3)	0.53606 (15)	0.65813 (8)	0.0294
C2	0.3245 (3)	0.60741 (14)	0.63831 (7)	0.0250
C3	0.1536 (3)	0.53363 (13)	0.62149 (7)	0.0233
C4	0.1835 (3)	0.45070 (14)	0.66269 (7)	0.0256
C5	0.1052 (3)	0.34631 (14)	0.64869 (7)	0.0290
C6	0.2326 (4)	0.28319 (14)	0.61049 (8)	0.0311
C7	0.3930 (3)	0.68839 (15)	0.60018 (8)	0.0298
O1	0.6740 (2)	0.55148 (12)	0.66145 (6)	0.0404
O2	0.2560 (2)	0.66510 (9)	0.68228 (5)	0.0276
O3	0.19790 (19)	0.49591 (10)	0.57091 (5)	0.0236
O4	0.4057 (2)	0.44775 (10)	0.67221 (6)	0.0307
O5	0.1073 (3)	0.28604 (10)	0.69480 (5)	0.0391
O6	0.1906 (3)	0.18228 (10)	0.62718 (5)	0.0323
O7	0.2507 (2)	0.76772 (10)	0.61047 (5)	0.0303
C8	0.2105 (3)	0.76835 (14)	0.66506 (8)	0.0280
C9	0.3552 (4)	0.83863 (15)	0.69389 (9)	0.0371
C10	−0.0146 (3)	0.79115 (16)	0.67321 (8)	0.0350
Si1	0.03555 (8)	0.50884 (4)	0.52065 (2)	0.0236
C11	−0.1794 (3)	0.41558 (16)	0.52733 (9)	0.0366
C12	−0.0733 (3)	0.63982 (14)	0.51977 (9)	0.0328
C13	0.1963 (3)	0.48244 (14)	0.46134 (7)	0.0259
C14	0.0658 (4)	0.50093 (18)	0.41223 (8)	0.0399
C15	0.3853 (4)	0.55315 (17)	0.45984 (8)	0.0355
C16	0.2708 (4)	0.37175 (15)	0.46185 (8)	0.0354
C17	0.1740 (4)	0.18483 (14)	0.68259 (8)	0.0309
C18	0.3799 (5)	0.1662 (2)	0.70760 (10)	0.0483
C19	0.0099 (4)	0.11074 (17)	0.69883 (10)	0.0467
H31	0.0109	0.5623	0.6196	0.0280*
H41	0.0984	0.4686	0.6938	0.0307*
H51	−0.0314	0.3608	0.6321	0.0348*
H61	0.3830	0.2993	0.6134	0.0373*
H62	0.1859	0.2942	0.5738	0.0373*
H71	0.5381	0.7103	0.6072	0.0358*
H72	0.3813	0.6642	0.5634	0.0358*
H91	0.3281	0.9100	0.6830	0.0446*
H92	0.3318	0.8319	0.7322	0.0446*
H93	0.5014	0.8204	0.6855	0.0446*
H101	−0.0446	0.8617	0.6614	0.0420*
H102	−0.0489	0.7846	0.7110	0.0420*
H103	−0.1000	0.7424	0.6527	0.0420*
H111	−0.2767	0.4231	0.4974	0.0440*
H112	−0.2551	0.4283	0.5606	0.0440*
H113	−0.1215	0.3454	0.5276	0.0440*
H121	−0.1700	0.6470	0.4897	0.0393*
H122	−0.1497	0.6526	0.5529	0.0393*

H123	0.0416	0.6899	0.5162	0.0393*
H141	0.1512	0.4869	0.3806	0.0478*
H142	0.0183	0.5729	0.4116	0.0478*
H143	−0.0569	0.4550	0.4125	0.0478*
H151	0.4693	0.5383	0.4281	0.0426*
H152	0.4714	0.5420	0.4916	0.0426*
H153	0.3377	0.6251	0.4588	0.0426*
H161	0.3561	0.3584	0.4302	0.0425*
H162	0.3559	0.3595	0.4937	0.0425*
H163	0.1486	0.3255	0.4620	0.0425*
H181	0.4273	0.0961	0.6993	0.0579*
H182	0.3670	0.1741	0.7462	0.0579*
H183	0.4826	0.2162	0.6940	0.0579*
H191	0.0561	0.0405	0.6904	0.0560*
H192	−0.0143	0.1166	0.7371	0.0560*
H193	−0.1211	0.1259	0.6798	0.0560*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0317 (11)	0.0293 (9)	0.0272 (9)	0.0020 (8)	0.0007 (8)	−0.0052 (8)
C2	0.0298 (9)	0.0214 (8)	0.0237 (9)	−0.0011 (8)	0.0033 (7)	−0.0026 (7)
C3	0.0266 (9)	0.0199 (8)	0.0235 (8)	0.0010 (7)	0.0019 (7)	−0.0005 (7)
C4	0.0306 (9)	0.0208 (8)	0.0253 (9)	0.0016 (8)	0.0041 (8)	−0.0001 (7)
C5	0.0405 (11)	0.0215 (9)	0.0251 (9)	−0.0017 (8)	0.0040 (8)	0.0035 (7)
C6	0.0458 (12)	0.0213 (9)	0.0261 (10)	0.0013 (9)	0.0033 (8)	0.0001 (7)
C7	0.0355 (10)	0.0250 (9)	0.0289 (10)	−0.0054 (8)	0.0058 (8)	−0.0020 (8)
O1	0.0284 (7)	0.0454 (9)	0.0473 (9)	0.0007 (7)	−0.0019 (7)	−0.0021 (7)
O2	0.0406 (8)	0.0185 (6)	0.0236 (6)	0.0008 (6)	0.0042 (6)	−0.0005 (5)
O3	0.0286 (6)	0.0205 (6)	0.0217 (6)	0.0018 (6)	0.0004 (5)	−0.0011 (5)
O4	0.0341 (7)	0.0263 (7)	0.0318 (7)	0.0039 (6)	−0.0048 (6)	0.0017 (6)
O5	0.0715 (11)	0.0194 (6)	0.0262 (7)	0.0048 (7)	0.0107 (7)	0.0014 (5)
O6	0.0517 (9)	0.0191 (6)	0.0259 (7)	0.0006 (6)	−0.0004 (7)	−0.0019 (5)
O7	0.0447 (8)	0.0226 (6)	0.0235 (7)	−0.0015 (6)	0.0034 (6)	0.0005 (5)
C8	0.0382 (11)	0.0195 (9)	0.0263 (10)	−0.0002 (8)	0.0015 (8)	0.0014 (7)
C9	0.0497 (14)	0.0251 (10)	0.0366 (11)	−0.0050 (9)	−0.0017 (10)	−0.0059 (8)
C10	0.0399 (12)	0.0317 (10)	0.0332 (10)	0.0044 (9)	0.0025 (9)	0.0031 (8)
Si1	0.0258 (2)	0.0192 (2)	0.0259 (2)	0.00095 (18)	−0.0020 (2)	0.0000 (2)
C11	0.0308 (10)	0.0310 (10)	0.0481 (13)	−0.0052 (8)	−0.0045 (10)	0.0043 (9)
C12	0.0349 (11)	0.0268 (9)	0.0366 (10)	0.0078 (8)	−0.0036 (9)	0.0001 (8)
C13	0.0314 (9)	0.0221 (9)	0.0242 (8)	0.0028 (7)	−0.0037 (7)	−0.0010 (7)
C14	0.0500 (12)	0.0421 (11)	0.0275 (9)	0.0076 (11)	−0.0094 (9)	−0.0020 (9)
C15	0.0397 (11)	0.0351 (11)	0.0318 (10)	−0.0026 (9)	0.0053 (9)	0.0015 (8)
C16	0.0430 (12)	0.0268 (10)	0.0363 (11)	0.0064 (9)	0.0028 (9)	−0.0021 (8)
C17	0.0492 (12)	0.0188 (8)	0.0249 (9)	−0.0006 (8)	0.0019 (9)	−0.0018 (7)
C18	0.0597 (17)	0.0468 (13)	0.0383 (12)	0.0057 (12)	−0.0106 (12)	−0.0037 (11)
C19	0.0662 (17)	0.0282 (10)	0.0457 (13)	−0.0093 (11)	0.0102 (12)	−0.0026 (10)

Geometric parameters (Å, º)

C1—C2	1.528 (3)	C10—H102	1.000
C1—O1	1.196 (3)	C10—H103	1.000
C1—O4	1.346 (2)	Si1—C11	1.867 (2)
C2—C3	1.538 (3)	Si1—C12	1.8695 (19)
C2—C7	1.518 (3)	Si1—C13	1.879 (2)
C2—O2	1.434 (2)	C11—H111	1.000
C3—C4	1.537 (3)	C11—H112	1.000
C3—O3	1.422 (2)	C11—H113	1.000
C3—H31	1.000	C12—H121	1.000
C4—C5	1.514 (3)	C12—H122	1.000
C4—O4	1.460 (2)	C12—H123	1.000
C4—H41	1.000	C13—C14	1.539 (3)
C5—C6	1.530 (3)	C13—C15	1.540 (3)
C5—O5	1.428 (2)	C13—C16	1.541 (3)
C5—H51	1.000	C14—H141	1.000
C6—O6	1.427 (2)	C14—H142	1.000
C6—H61	1.000	C14—H143	1.000
C6—H62	1.000	C15—H151	1.000
C7—O7	1.421 (2)	C15—H152	1.000
C7—H71	1.000	C15—H153	1.000
C7—H72	1.000	C16—H161	1.000
O2—C8	1.465 (2)	C16—H162	1.000
O3—Si1	1.6745 (13)	C16—H163	1.000
O5—C17	1.440 (2)	C17—C18	1.501 (3)
O6—C17	1.429 (2)	C17—C19	1.504 (3)
O7—C8	1.427 (2)	C18—H181	1.000
C8—C9	1.514 (3)	C18—H182	1.000
C8—C10	1.503 (3)	C18—H183	1.000
C9—H91	1.000	C19—H191	1.000
C9—H92	1.000	C19—H192	1.000
C9—H93	1.000	C19—H193	1.000
C10—H101	1.000		

C2—C1—O1	128.22 (19)	H102—C10—H103	109.476
C2—C1—O4	109.10 (16)	O3—Si1—C11	109.26 (9)
O1—C1—O4	122.68 (19)	O3—Si1—C12	109.91 (8)
C1—C2—C3	102.43 (15)	C11—Si1—C12	109.35 (10)
C1—C2—C7	116.29 (17)	O3—Si1—C13	105.02 (7)
C3—C2—C7	118.43 (16)	C11—Si1—C13	111.41 (9)
C1—C2—O2	106.60 (15)	C12—Si1—C13	111.79 (9)
C3—C2—O2	109.64 (15)	Si1—C11—H111	109.467
C7—C2—O2	102.97 (14)	Si1—C11—H112	109.467
C2—C3—C4	99.66 (15)	H111—C11—H112	109.475
C2—C3—O3	109.51 (14)	Si1—C11—H113	109.467
C4—C3—O3	110.77 (14)	H111—C11—H113	109.476
C2—C3—H31	116.048	H112—C11—H113	109.476

C4—C3—H31	114.899	Si1—C12—H121	109.467
O3—C3—H31	105.931	Si1—C12—H122	109.467
C3—C4—C5	116.37 (16)	H121—C12—H122	109.476
C3—C4—O4	105.02 (15)	Si1—C12—H123	109.466
C5—C4—O4	110.24 (16)	H121—C12—H123	109.476
C3—C4—H41	108.208	H122—C12—H123	109.476
C5—C4—H41	102.775	Si1—C13—C14	109.38 (14)
O4—C4—H41	114.577	Si1—C13—C15	110.36 (13)
C4—C5—C6	117.96 (17)	C14—C13—C15	108.62 (17)
C4—C5—O5	107.94 (15)	Si1—C13—C16	110.05 (13)
C6—C5—O5	102.90 (15)	C14—C13—C16	109.25 (16)
C4—C5—H51	102.898	C15—C13—C16	109.15 (17)
C6—C5—H51	107.931	C13—C14—H141	109.467
O5—C5—H51	117.957	C13—C14—H142	109.467
C5—C6—O6	102.35 (15)	H141—C14—H142	109.476
C5—C6—H61	111.222	C13—C14—H143	109.467
O6—C6—H61	111.222	H141—C14—H143	109.475
C5—C6—H62	111.222	H142—C14—H143	109.476
O6—C6—H62	111.222	C13—C15—H151	109.467
H61—C6—H62	109.467	C13—C15—H152	109.466
C2—C7—O7	102.18 (15)	H151—C15—H152	109.476
C2—C7—H71	111.263	C13—C15—H153	109.466
O7—C7—H71	111.263	H151—C15—H153	109.476
C2—C7—H72	111.263	H152—C15—H153	109.476
O7—C7—H72	111.263	C13—C16—H161	109.467
H71—C7—H72	109.467	C13—C16—H162	109.467
C2—O2—C8	108.63 (14)	H161—C16—H162	109.475
C3—O3—Si1	122.88 (11)	C13—C16—H163	109.467
C1—O4—C4	110.13 (15)	H161—C16—H163	109.476
C5—O5—C17	109.89 (14)	H162—C16—H163	109.476
C6—O6—C17	106.97 (14)	O5—C17—O6	105.17 (14)
C7—O7—C8	107.80 (14)	O5—C17—C18	108.98 (18)
O2—C8—O7	104.78 (14)	O6—C17—C18	110.88 (19)
O2—C8—C9	107.40 (16)	O5—C17—C19	109.42 (18)
O7—C8—C9	111.84 (17)	O6—C17—C19	108.32 (17)
O2—C8—C10	109.88 (16)	C18—C17—C19	113.72 (19)
O7—C8—C10	108.37 (17)	C17—C18—H181	109.467
C9—C8—C10	114.16 (18)	C17—C18—H182	109.467
C8—C9—H91	109.467	H181—C18—H182	109.476
C8—C9—H92	109.467	C17—C18—H183	109.467
H91—C9—H92	109.476	H181—C18—H183	109.476
C8—C9—H93	109.467	H182—C18—H183	109.476
H91—C9—H93	109.475	C17—C19—H191	109.467
H92—C9—H93	109.476	C17—C19—H192	109.467
C8—C10—H101	109.467	H191—C19—H192	109.476
C8—C10—H102	109.467	C17—C19—H193	109.466
H101—C10—H102	109.476	H191—C19—H193	109.476
C8—C10—H103	109.466	H192—C19—H193	109.476

H101—C10—H103	109.475