Crystal structure of 1,4-dideoxy-1,4-imino-D-mannitol hydrochloride, $C_6H_{14}ClNO_4$

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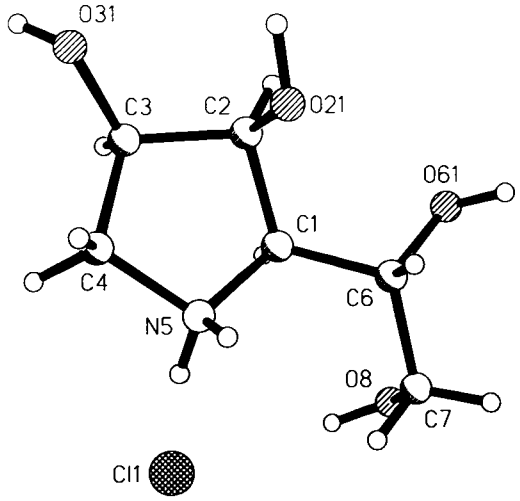

Source of material: The title compound (see refs. 1, 2) was prepared by nitroaldol addition of 2-*O*-benzyl-D-glyceraldehyde with (2*S*)-1,2-*O*-isopropylidene-3-nitro-1,2-butanediol (see refs. 3, 4), followed by catalytic hydrogenation, cyclization, deprotection (see refs. 5, 6).

$C_6H_{14}ClNO_4$, monoclinic, $P12_11$ (No. 4), a =5.283(1) Å, b =12.746(2) Å, c =6.772(1) Å, β =93.31(1)°, V =455.3 Å^3, Z =2, $R(F)$ =0.026, $R_w(F^2)$ =0.066.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow needle, size 0.15 x 0.35 x 0.8 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.98 cm^{-1}
Diffractometer:	Nicolet P3
Scan mode:	Wyckoff
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
N(hkl)$_{unique}$:	1084
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
N($param$)$_{refined}$:	106
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{iso}
H(1)	2*a*	1.0003(3)	0.1207(2)	0.1550(3)	0.029
H(2)	2*a*	1.1997(3)	0.1326(2)	–0.1384(3)	0.031
H(21)	2*a*	1.5943	0.1890	–0.1414	0.057
H(3)	2*a*	0.9871(4)	0.2858(2)	–0.0590(3)	0.035
H(31)	2*a*	1.1768	0.3872	–0.2392	0.063
H(4A)	2*a*	1.3957(5)	0.3583(2)	0.1931(4)	0.049
H(4B)	2*a*	1.1035(5)	0.3731(2)	0.2216(4)	0.049
H(5A)	2*a*	1.108(5)	0.233(2)	0.397(5)	0.041
H(5B)	2*a*	1.381(6)	0.220(2)	0.366(4)	0.041
H(6)	2*a*	1.4994(3)	0.0463(1)	0.2559(3)	0.033
H(61)	2*a*	1.3894	–0.0826	0.1013	0.056
H(7A)	2*a*	1.3262(4)	–0.0635(2)	0.4882(3)	0.042
H(7B)	2*a*	1.2750(4)	0.0535(2)	0.5451(3)	0.042
H(8)	2*a*	0.9047	0.0365	0.4799	0.061

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	2*a*	0.75457(8)	0.19967(5)	0.55513(7)	0.0256(2)	0.0491(3)	0.0289(2)	–0.0015(2)	0.0046(2)	–0.0070(2)
C(1)	2*a*	1.1832(3)	0.1338(2)	0.1689(3)	0.0188(8)	0.0240(9)	0.028(1)	–0.0010(7)	0.0008(7)	–0.0020(8)
C(2)	2*a*	1.2709(3)	0.1738(2)	–0.0263(3)	0.0243(9)	0.029(1)	0.0243(9)	0.0023(7)	0.0011(6)	0.0008(7)
O(21)	2*a*	1.5407(3)	0.1735(2)	–0.0165(2)	0.0258(7)	0.056(1)	0.0326(7)	0.0077(7)	0.0096(6)	0.0098(7)
C(3)	2*a*	1.1710(4)	0.2861(2)	–0.0301(3)	0.0224(8)	0.028(1)	0.038(1)	–0.0006(8)	0.0024(8)	0.0063(8)
O(31)	2*a*	1.2886(3)	0.3484(2)	–0.1697(3)	0.0349(8)	0.0434(9)	0.0479(9)	–0.0016(8)	0.0036(7)	0.0212(9)
C(4)	2*a*	1.2314(5)	0.3241(2)	0.1816(4)	0.056(2)	0.026(1)	0.042(1)	–0.002(1)	0.012(1)	–0.0024(9)
N(5)	2*a*	1.2318(3)	0.2265(1)	0.3060(3)	0.0230(8)	0.0293(9)	0.0294(8)	–0.0004(6)	0.0050(6)	–0.0041(7)
C(6)	2*a*	1.3148(4)	0.0347(2)	0.2476(3)	0.0258(9)	0.0240(9)	0.031(1)	0.0007(8)	0.0006(7)	–0.0011(8)
O(61)	2*a*	1.2550(3)	–0.0439(1)	0.1032(3)	0.0386(8)	0.0273(8)	0.0455(9)	0.0017(7)	–0.0041(7)	–0.0098(7)
C(7)	2*a*	1.2328(4)	–0.0007(2)	0.4482(3)	0.038(1)	0.032(1)	0.034(1)	–0.0029(9)	–0.0015(9)	0.0077(9)
O(8)	2*a*	0.9682(3)	–0.0221(1)	0.4476(3)	0.0422(9)	0.0355(9)	0.0453(9)	–0.0076(7)	0.0119(7)	0.0028(7)

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