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

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Received August 23, 1996, CSD-No. 402609

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

Crystal:	yellow needle, size 0.2 x 0.35 x 1.5 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	4.04 cm ⁻¹
Diffractometer:	Nicolet P3
Scan mode:	Wyckoff
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	58°
$N(hkl)_{\text{unique}}$:	1384
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	134
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1)	4a	-0.0044(4)	1.5513(1)	0.4029(1)	0.032
H(2)	4a	0.1982(4)	1.4552(2)	0.2828(1)	0.034
H(21)	4a	0.61(1)	1.445(3)	0.306(3)	0.07(1)
H(3)	4a	-0.0405(5)	1.3530(2)	0.3936(2)	0.037
H(31)	4a	0.174(9)	1.239(3)	0.320(3)	0.07(1)
H(4A)	4a	0.0990(6)	1.3398(2)	0.5503(1)	0.041
H(4B)	4a	0.3998(6)	1.3481(2)	0.5212(1)	0.041
H(5A)	4a	0.060(7)	1.509(2)	0.553(2)	0.037(7)
H(5B)	4a	0.343(6)	1.512(2)	0.547(2)	0.025(6)
H(6)	4a	0.5295(4)	1.6182(2)	0.4134(2)	0.038
H(61)	4a	0.403(8)	1.732(3)	0.504(3)	0.06(1)
H(7A)	4a	0.4197(7)	1.7461(2)	0.3043(2)	0.058
H(7B)	4a	0.3305(7)	1.6405(2)	0.2579(2)	0.058
H(8)	4a	0.04(1)	1.781(3)	0.325(3)	0.09(2)

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

$C_6H_{14}ClNO_4$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 5.066(1)$ Å, $b = 12.899(2)$ Å, $c = 13.734(2)$ Å, $V = 897.5$ Å³, $Z = 4$, $R(F) = 0.034$, $R_w(F^2) = 0.091$.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	4a	0.2116(1)	0.96021(5)	0.35928(4)	0.0335(3)	0.0587(3)	0.0308(2)	-0.0029(2)	0.0012(2)	-0.0106(2)
C(1)	4a	0.1819(4)	1.5357(1)	0.4153(1)	0.0246(9)	0.0280(8)	0.0268(8)	0.0026(8)	-0.0018(7)	0.0017(7)
C(2)	4a	0.2689(4)	1.4475(2)	0.3488(1)	0.029(1)	0.0352(9)	0.0214(7)	0.0051(8)	-0.0051(7)	-0.0021(7)
O(21)	4a	0.5487(3)	1.4408(2)	0.3490(1)	0.0306(8)	0.055(1)	0.0297(7)	0.0067(7)	0.0056(7)	-0.0029(7)
C(3)	4a	0.1519(5)	1.3532(2)	0.4010(2)	0.032(1)	0.0271(9)	0.0342(9)	0.0019(8)	-0.0063(8)	-0.0050(7)
O(31)	4a	0.2552(4)	1.2563(1)	0.3723(1)	0.056(1)	0.0307(7)	0.0451(8)	0.0106(8)	-0.0140(9)	-0.0116(6)
C(4)	4a	0.2236(6)	1.3732(2)	0.5068(1)	0.046(1)	0.0270(8)	0.0282(8)	-0.0017(9)	0.001(1)	0.0013(7)
N(5)	4a	0.2094(4)	1.4893(1)	0.5160(1)	0.0303(9)	0.0281(7)	0.0246(7)	0.0001(7)	0.0009(7)	-0.0027(6)
C(6)	4a	0.3416(4)	1.6350(2)	0.4072(2)	0.027(1)	0.0293(8)	0.037(1)	0.0009(8)	0.0030(8)	-0.0005(8)
O(61)	4a	0.2655(4)	1.7005(1)	0.4867(1)	0.0367(9)	0.0314(7)	0.0383(8)	-0.0003(7)	-0.0017(7)	-0.0064(6)
C(7)	4a	0.2965(7)	1.6889(2)	0.3106(2)	0.067(2)	0.038(1)	0.039(1)	0.002(1)	0.013(1)	0.0086(9)
O(8)	4a	0.0344(6)	1.7271(2)	0.3024(2)	0.078(2)	0.0413(9)	0.046(1)	0.002(1)	-0.022(1)	0.0065(8)

Acknowledgments. We are grateful to the Fonds der Chemischen Industrie for financial support, and to the Landesgraduiertenförderung Baden-Württemberg awarding a doctoral fellowship to F.-M. Kieß.

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