Crystal structure of (*R*)- α -methylphenylalanine methylester hydrochloride monohydrate, $C_{11}H_{15}NO_2 \cdot HCl \cdot H_2O$

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Source of material: The title compound was prepared by treatment of H-D-(α -Me)Phe-OH with $SOCl_2$ in anhydrous methanol. Crystallization was done from methanol, mp 369 K - 370 K.

The torsion angle $N1-C3-C2-O2$ is $-145.4(3)^\circ$. The N1 atom acts as the H-bond donor to the O1, Cl and O1W atoms within the same asymmetric unit, and to the symmetry equivalent $(-1-x, 1/2+y, -1-z)$ O1 and $(-1-x, -1/2+y, -1-z)$ Cl atoms. The O1W atom is H-bonded to two symmetry equivalent, $(x, y, -1+z)$ and $(-1-x, -1/2+y, -1-z)$, Cl atoms.

$C_{11}H_{15}ClNO_3$, monoclinic, $P2_1$ (No. 4), $a = 12.757(2) \text{ \AA}$, $b = 6.865(1) \text{ \AA}$, $c = 7.999(1) \text{ \AA}$, $\beta = 108.8(1)^\circ$, $V = 663.2 \text{ \AA}^3$, $Z = 2$, $\rho_m = 1.240 \text{ g cm}^{-3}$, $R(F) = 0.040$, $R_w(F) = 0.044$.

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

Crystal:	prism, size 0.8 x 0.4 x 0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	2.79 cm ⁻¹
Diffractometer:	Philips PW1100
Scan mode:	$\theta/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	56°
$N(hkl)_{\text{unique}}$:	1720
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	144
Program:	SHELX-76

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

Atom	Site	x	y	z	U_{iso}
H(1W)	2a	-0.4008	-0.2875	-0.8803	0.069
H(2W)	2a	-0.4182	-0.1168	-0.8053	0.050
H(1NA)	2a	-0.4050	-0.4250	-0.6227	0.041
H(1NB)	2a	-0.4515	-0.4427	-0.5205	0.065
H(1NC)	2a	-0.4262	-0.6445	-0.5946	0.141
H(1A)	2a	-0.2142	-0.7593	0.1122	0.119
H(1B)	2a	-0.3708	-0.7629	0.0536	0.161
H(1C)	2a	-0.2805	-0.9300	-0.0053	0.208
H(4A)	2a	-0.1621	-0.3707	-0.2588	0.039
H(4B)	2a	-0.2724	-0.2954	-0.2796	0.054
H(4C)	2a	-0.2224	-0.2922	-0.4229	0.064
H(5A)	2a	-0.2260	-0.5777	-0.6082	0.046
H(5B)	2a	-0.2716	-0.7762	-0.5630	0.040
H(7)	2a	-0.1621	-0.9528	-0.2702	0.186
H(8)	2a	0.0257	-1.0323	-0.0709	0.080
H(9)	2a	0.1812	-0.8417	-0.0872	0.050
H(10)	2a	0.1512	-0.5675	-0.2938	0.043
H(11)	2a	-0.0301	-0.4797	-0.4601	0.064

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	2a	-0.49109(7)	-0.35913	-0.2153(1)	0.0720(5)	0.0600(6)	0.0459(4)	0.0213(5)	0.0265(4)	0.0120(4)
O(1)	2a	-0.3875(2)	-0.8011(4)	-0.3229(3)	0.054(1)	0.053(2)	0.048(1)	-0.018(1)	0.015(1)	0.002(1)
O(2)	2a	-0.2535(2)	-0.6447(4)	-0.1151(2)	0.051(1)	0.051(1)	0.0314(9)	-0.001(1)	0.0108(9)	0.003(1)
N(1)	2a	-0.4035(2)	-0.4966(5)	-0.5473(3)	0.038(1)	0.040(1)	0.038(1)	0.004(1)	0.011(1)	0.003(1)
C(1)	2a	-0.2742(4)	-0.7755(8)	0.0145(5)	0.104(3)	0.077(3)	0.037(2)	-0.008(3)	0.018(2)	0.015(2)
C(2)	2a	-0.3194(2)	-0.6748(5)	-0.2789(3)	0.035(1)	0.040(2)	0.034(1)	0.002(1)	0.012(1)	-0.002(1)
C(3)	2a	-0.2931(2)	-0.5383(5)	-0.4118(3)	0.032(1)	0.037(2)	0.030(1)	-0.001(1)	0.006(1)	-0.001(1)
C(4)	2a	-0.2395(2)	-0.3461(6)	-0.3376(4)	0.054(2)	0.042(2)	0.043(1)	-0.011(2)	0.018(1)	-0.007(2)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(5)	2a	−0.2245(2)	−0.6535(5)	−0.5063(3)	0.038(1)	0.044(2)	0.033(1)	−0.001(1)	0.012(1)	−0.004(1)
C(6)	2a	−0.1099(2)	−0.7091(5)	−0.3886(4)	0.039(1)	0.036(2)	0.033(1)	0.002(1)	0.013(1)	−0.002(1)
C(7)	2a	−0.0925(3)	−0.8653(7)	−0.2739(4)	0.052(2)	0.039(2)	0.055(2)	0.003(2)	0.025(1)	0.007(2)
C(8)	2a	0.0139(3)	−0.9131(6)	−0.1630(5)	0.062(2)	0.057(3)	0.050(2)	0.018(2)	0.019(1)	0.013(2)
C(9)	2a	0.1028(3)	−0.8079(7)	−0.1703(4)	0.047(2)	0.072(3)	0.044(2)	0.013(2)	0.007(1)	−0.000(2)
C(10)	2a	0.0877(3)	−0.6540(7)	−0.2861(4)	0.042(2)	0.059(2)	0.056(2)	−0.006(2)	0.015(1)	−0.007(2)
C(11)	2a	−0.0176(3)	−0.6034(5)	−0.3936(4)	0.042(2)	0.042(2)	0.049(2)	−0.001(1)	0.017(1)	0.006(1)
O(1W)	2a	−0.3758(2)	−0.2412(5)	−0.8034(3)	0.059(1)	0.077(2)	0.052(1)	0.005(1)	0.014(1)	0.014(1)

Reference

1. Sheldrick, G. M.: SHELX -76, Program for Crystal Structure Determination, Cambridge, UK 1996.