Crystal structure of (2*S*,5*R*)-1-chloromethyl-2-hydroxymethyl-5-vinyl-1-azoniabicyclo[2.2.2]octane chloride, $(C_{11}H_{19}ClNO)Cl$

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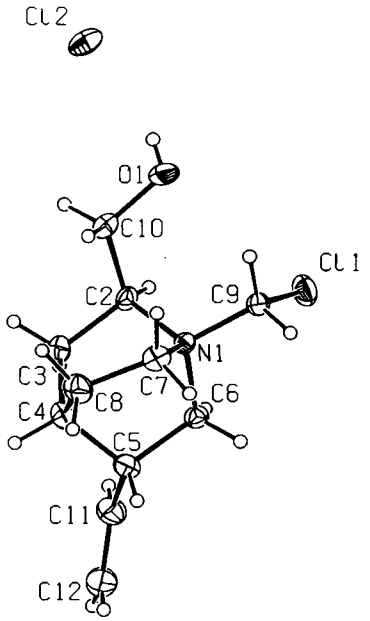

Source of material: 2-Hydroxymethyl-5-vinyl-quinuclidine (150 mg, see ref. 1) was dissolved in methylene chloride (5 ml). After 2-3 days at room temperature crystals of the title compound precipitated. Recrystallization from ethanol.
The atom numbering is systematic and does not correspond to the *Cinchona* alkaloid convention. Flack x parameter =–0.04(5).

$C_{11}H_{19}Cl_2NO$, orthorhombic, $P2_12_12_1$ (No. 19), a =8.796(2) Å, b =9.270(2) Å, c =15.184(3) Å, V =1238.1 Å^3, Z =4, $R(F)$ =0.024, $R_w(F^2)$ =0.057.

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

Crystal:	colorless, size 0.41 x 2.2 x 0.63 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.00 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	180 exposures, $\Delta\varphi$ = 1.5°
$T_{measurement}$:	300 K
$2\theta_{max}$:	56.34°
$N(hkl)_{unique}$:	2935
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	141
Programs:	SHELXS-86, SHELXL-93, PLATON

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*a*	0.0817(2)	0.7390(1)	0.2087(1)	0.045(1)
H(2)	4*a*	0.0589(2)	0.7561(2)	0.0671(1)	0.045(1)
H(3)	4*a*	0.2187(2)	0.6817(2)	0.0593(1)	0.045(1)
H(4)	4*a*	0.2377(2)	0.8941(2)	–0.0213(1)	0.045(1)
H(5)	4*a*	0.1855(2)	1.1201(2)	0.0571(1)	0.045(1)
H(6)	4*a*	0.1052(2)	1.1155(2)	0.1941(1)	0.045(1)
H(7)	4*a*	–0.0021(2)	0.9826(2)	0.1781(1)	0.045(1)
H(8)	4*a*	0.4499(2)	0.9176(2)	0.2129(1)	0.045(1)
H(9)	4*a*	0.3850(2)	1.0699(2)	0.1872(1)	0.045(1)
H(10)	4*a*	0.4505(2)	0.8434(2)	0.0758(1)	0.045(1)
H(11)	4*a*	0.4382(2)	1.0078(2)	0.0513(1)	0.045(1)
H(12)	4*a*	0.2488(2)	1.0402(1)	0.32155(9)	0.045(1)
H(13)	4*a*	0.2890(2)	0.8769(1)	0.33475(9)	0.045(1)
H(14)	4*a*	0.2763(2)	0.5637(1)	0.1891(1)	0.045(1)
H(15)	4*a*	0.3977(2)	0.6869(1)	0.1956(1)	0.045(1)
H(16)	4*a*	–0.0891(2)	0.9673(2)	0.0295(1)	0.045(1)
H(17)	4*a*	0.0186(3)	1.2064(2)	–0.0544(1)	0.045(1)
H(18)	4*a*	–0.1441(3)	1.1305(2)	–0.0692(1)	0.045(1)
H(19)	4*a*	0.296(2)	0.568(2)	0.320(1)	0.045(1)

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)	4*a*	0.03579(6)	0.91299(4)	0.35607(3)	0.0578(3)	0.0560(2)	0.0336(2)	–0.0011(2)	0.0128(2)	–0.0037(2)
Cl(2)	4*a*	0.26036(5)	0.31066(3)	0.31760(3)	0.0411(2)	0.0265(1)	0.0761(3)	–0.0019(2)	–0.0065(2)	0.0023(2)
O(1)	4*a*	0.3010(2)	0.6410(1)	0.30735(8)	0.0730(9)	0.0255(4)	0.0483(8)	0.0038(5)	–0.0074(7)	0.0066(5)
N(1)	4*a*	0.2160(1)	0.9214(1)	0.21102(7)	0.0252(6)	0.0214(4)	0.0270(6)	–0.0011(4)	–0.0010(5)	–0.0025(4)
C(2)	4*a*	0.1804(2)	0.7655(1)	0.1835(1)	0.0350(8)	0.0211(5)	0.0327(8)	–0.0040(5)	0.0025(7)	–0.0047(6)
C(3)	4*a*	0.1653(2)	0.7646(2)	0.0830(1)	0.056(1)	0.0335(7)	0.0326(9)	0.0002(7)	0.0001(9)	–0.0100(6)
C(4)	4*a*	0.2310(2)	0.9029(2)	0.0429(1)	0.050(1)	0.0444(7)	0.0262(8)	–0.0000(8)	0.0051(8)	–0.0017(6)
C(5)	4*a*	0.1288(2)	1.0310(2)	0.0682(1)	0.042(1)	0.0357(7)	0.0315(9)	–0.0053(7)	–0.0039(7)	0.0044(6)
C(6)	4*a*	0.0993(2)	1.0202(2)	0.1679(1)	0.0301(8)	0.0294(6)	0.0328(9)	0.0031(6)	–0.0033(7)	–0.0006(6)
C(7)	4*a*	0.3721(2)	0.9668(2)	0.1790(1)	0.0257(8)	0.0355(7)	0.046(1)	–0.0041(6)	0.0012(7)	0.0018(7)
C(8)	4*a*	0.3885(2)	0.9293(2)	0.0822(1)	0.040(1)	0.057(1)	0.043(1)	0.0011(8)	0.0134(8)	0.0066(8)
C(9)	4*a*	0.2162(2)	0.9426(1)	0.30842(9)	0.0409(9)	0.0279(6)	0.0286(8)	0.0001(5)	–0.0072(7)	–0.0030(5)
C(10)	4*a*	0.2979(2)	0.6567(1)	0.2156(1)	0.053(1)	0.0265(7)	0.045(1)	0.0045(6)	0.0028(9)	–0.0019(6)
C(11)	4*a*	–0.0167(2)	1.0380(2)	0.0178(1)	0.055(1)	0.0522(9)	0.039(1)	0.0026(9)	–0.0141(9)	0.0006(8)
C(12)	4*a*	–0.0506(3)	1.1339(2)	–0.0407(1)	0.078(2)	0.065(1)	0.051(1)	0.024(1)	–0.016(1)	–0.0016(9)

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