Crystal structure of benzyl-(2-hydroxyethyl)-dimethylammonium iodide, $[C_{11}H_{18}NO]^+ I^-$

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

Crystal:	white needle, size 0.08 x 0.12 x 0.50 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	25.07 cm ⁻¹
Diffractometer:	Stoe STAD14
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	298 K
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{unique}}$:	2176
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	200
Programs:	SHELXS-86, SHELXL-93

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	0.203(4)	-0.145(4)	0.234(3)	0.05(1)
H(1B)	4e	0.315(4)	-0.249(5)	0.225(4)	0.06(1)
H(3)	4e	0.457(4)	-0.299(5)	0.383(4)	0.06(1)
H(4)	4e	0.491(5)	-0.305(5)	0.571(4)	0.09(2)
H(5)	4e	0.347(5)	-0.171(5)	0.667(4)	0.08(2)
H(6)	4e	0.203(5)	-0.033(5)	0.587(4)	0.08(2)
H(7)	4e	0.187(5)	-0.034(5)	0.407(4)	0.06(2)
H(8B)	4e	0.560(4)	-0.025(4)	0.170(3)	0.05(1)
H(8C)	4e	0.542(4)	-0.073(5)	0.287(4)	0.07(2)
H(8A)	4e	0.533(4)	-0.187(5)	0.194(3)	0.05(1)
H(9B)	4e	0.376(4)	0.076(4)	0.307(4)	0.05(1)
H(9A)	4e	0.255(5)	0.090(5)	0.225(3)	0.06(1)
H(9C)	4e	0.389(5)	0.134(5)	0.190(4)	0.06(1)
H(10A)	4e	0.232(4)	-0.050(3)	0.071(3)	0.027(9)
H(10B)	4e	0.372(5)	0.007(5)	0.043(4)	0.06(1)
H(11B)	4e	0.290(4)	-0.200(4)	-0.051(3)	0.05(1)
H(11A)	4e	0.332(4)	-0.275(5)	0.058(4)	0.07(2)
H(12)	4e	0.498(8)	-0.264(8)	-0.042(6)	0.14(3)

Source of material: The compound was synthesized by reaction of benzyl iodide with an ice-cooled solution of 2-(dimethylamino)-ethanol in methanol. After refluxing, the solvent was removed under reduced pressure, and the residue was taken up in ether, filtered and evaporated to a solid.

The title compound is the anchoring group of a strongly basic anion-exchanger of type II.

$C_{11}H_{18}NO$, monoclinic, $P12_1/a1$ (No. 14), $a = 10.144(9)$ Å, $b = 9.994(3)$ Å, $c = 12.511(7)$ Å, $\beta = 94.88(9)^\circ$, $V = 1263.8$ Å³, $Z = 4$, $R(F) = 0.027$, $R_w(F^2) = 0.062$.

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}
C(1)	4e	0.2894(5)	-0.1640(4)	0.2533(3)	0.051(3)	0.035(2)	0.052(2)	-0.005(2)	0.004(2)	0.000(2)
C(2)	4e	0.3142(4)	-0.1614(4)	0.3730(3)	0.052(2)	0.043(2)	0.044(2)	-0.005(2)	0.005(2)	0.002(2)
C(3)	4e	0.4061(5)	-0.2449(5)	0.4254(4)	0.081(3)	0.050(3)	0.052(3)	0.011(3)	0.005(2)	0.003(2)
C(4)	4e	0.4231(6)	-0.2500(6)	0.5366(4)	0.086(4)	0.066(3)	0.055(3)	0.002(3)	-0.005(3)	0.011(3)
C(5)	4e	0.3453(6)	-0.1701(6)	0.5949(4)	0.091(4)	0.074(4)	0.045(3)	-0.023(3)	0.005(3)	-0.005(3)
C(6)	4e	0.2542(6)	-0.0857(6)	0.5446(4)	0.083(4)	0.076(4)	0.057(3)	0.000(3)	0.019(3)	-0.009(3)
C(7)	4e	0.2381(5)	-0.0818(6)	0.4342(4)	0.056(3)	0.064(3)	0.064(3)	0.008(3)	0.015(2)	0.002(3)
C(8)	4e	0.5155(4)	-0.0936(6)	0.2119(4)	0.045(3)	0.057(3)	0.062(3)	0.001(2)	0.003(2)	-0.003(3)
C(9)	4e	0.3448(6)	0.0759(5)	0.2298(5)	0.064(3)	0.033(2)	0.066(3)	0.002(2)	0.012(3)	-0.002(2)

Table 3. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(10)	4e	0.3246(5)	−0.0692(4)	0.0739(3)	0.056(3)	0.043(2)	0.046(2)	0.006(2)	0.006(2)	0.005(2)
C(11)	4e	0.3512(5)	−0.1982(5)	0.0162(4)	0.066(3)	0.045(3)	0.043(2)	−0.005(2)	0.004(2)	−0.006(2)
N(1)	4e	0.3700(3)	−0.0640(3)	0.1931(3)	0.043(2)	0.032(2)	0.045(2)	0.001(1)	0.005(1)	−0.001(1)
O(1)	4e	0.4835(4)	−0.2009(4)	−0.0090(3)	0.085(3)	0.051(2)	0.086(3)	−0.009(2)	0.039(2)	−0.024(2)
I(1)	4e	0.93956(3)	0.03492(3)	0.18400(2)	0.0602(2)	0.0418(2)	0.0456(2)	0.0002(2)	0.0054(1)	0.0051(1)

References

1. Sheldrick, G. M.: SHELXS-86. Program for the solution of crystal structures. University of Göttingen, Germany 1986.
2. Sheldrick, G. M.: SHELXL-93. Program for refining crystal structures. University of Göttingen, Germany 1993.