Crystal structure of 1-butyl-3-cyclododecyloxymethylimidazolium chloride monohydrate, (C\textsubscript{20}H\textsubscript{37}N\textsubscript{2}O)Cl \cdot H\textsubscript{2}O

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Abstract

C\textsubscript{20}H\textsubscript{39}ClN\textsubscript{2}O\textsubscript{2}, triclinic, P\textsubscript{1} (no. 2), a = 8.078(2) Å, b = 8.517(2) Å, c = 16.743(3) Å, α = 81.62(3)°, β = 77.27(3)°, γ = 78.94(3)°, V = 1096.3 Å\textsuperscript{3}, Z = 2, R\textsubscript{gt}(F) = 0.055, wR\textsubscript{ref}(F\textsuperscript{2}) = 0.205, T = 293 K.

Source of material

The 1-butyl-3-cyclododecyloxymethylimidazolium chloride was prepared by the reaction of 1-butylimidazole and chloromethylcyclododecylether in anhydrous benzene according to the procedure described in [1]. Chloromethylcyclododecylether was prepared by passing HCl gas through a mixture of formaldehyde and cyclododecanol [2]. Colorless plate-like crystals of the title compound were obtained by slow evaporation from a solution in ethyl acetate/methanol (10:1, v/v) at room temperature.

Experimental details

The hydrogen atoms participating in D–H···A hydrogen interactions were refined (D = O, C; A = Cl, O).

Discussion

The aim of the X-ray analysis of 1-butyl-3-cyclododecyloxymethylimidazolium chloride was defining the influence of quaternization of imidazol ring and anion-cation interaction on the molecule conformation. The title compound crystallizes with one molecule of water. Strong hydrogen bonds were formed between chloride anions and water molecules. These interactions lead to closed planar Cl···H1W–O–H2W···Cl(−x,−y+1,−z+1)···H2W–O–H1W···Cl systems bonded with the cation part by hydrogen bond between chloride anion and H2 atom located at the acid carbon atom in imidazol ring (d(C2···Cl) = 3.396(3) Å and d(C2–H2A···Cl) = 159.9(3)°). Formation of this hydrogen bond results in averaged N1—C2 and C2—N2 bond lengths of 1.318(4) Å and 1.317(4) Å, respectively.

Table 1. Data collection and handling.

| Crystal: | colorless plate, size 0.05 × 0.25 × 0.35 mm |
| Wavelength: | Cu K\textsubscript{α} radiation (1.54178 Å) |
| μ: | 16.45 cm\textsuperscript{-1} |
| Diffractometer, scan mode: | Kuma KM-4, 2θ/θ |
| 2θ\textsubscript{max}: | 161.7° |
| N(hkl)\textsubscript{measured}, N(hkl)\textsubscript{unique}: | 4834, 4614 |
| Criterion for I\textsubscript{obs}, I\textsubscript{obs}/σ(I\textsubscript{obs}): | I\textsubscript{obs} > 2σ(I\textsubscript{obs}), 2466 |
| N(param)\textsubscript{refined}: | 247 |
| Programs: | SHELXS-97 [6], SHELXL-97 [7] |

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References