Crystal and Molecular Structure of 1,2,4-Triazolium Chloride and its Salt with Antimony Trichloride - Bis(1,2,4-triazolium) pentachloroantimonate(III)-1,2,4-triazolium Chloride

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1,2,4-Triazolium Cation, Chloroantimonates(III), Hydrogen Bonds

The structures of 1,2,4-triazolium chloride (C$_2$H$_4$N$_3$)Cl and its derivative with antimony trichloride - (C$_2$H$_4$N$_3$)$_2$[SbCl$_5$] - (C$_2$H$_4$N$_3$)Cl containing unsubstituted 1,2,4-triazolium cations were determined. (C$_2$H$_4$N$_3$)Cl crystallizes in the monoclinic system, space group P2$_1$/n with the unit cell dimensions at 86 K: $a = 9.425(2)$, $b = 8.557(2)$, $c = 11.158(2)$ Å, $\alpha = 95.87(3)^\circ$; $V = 895.2(3)$ Å$^3$, $Z = 8$, $d_c = 1.566$, $d_m = 1.56(2)$ g·cm$^{-3}$. At room temperature, crystals of (C$_2$H$_4$N$_3$)$_2$-[SbCl$_5$] - (C$_2$H$_4$N$_3$)Cl are orthorhombic, space group P2$_1$2$_1$2$_1$, $a = 8.318(2)$, $b = 11.381(2)$, $c = 19.931(4)$ Å, $V = 1886.8(7)$ Å$^3$, $Z = 4$, $d_c = 1.917$, $d_m = 1.91(2)$ g·cm$^{-3}$. In both crystals the 1,2,4-triazole rings are planar. The anionic sublattice of (C$_2$H$_4$N$_3$)$_2$[SbCl$_5$] - (C$_2$H$_4$N$_3$)Cl consists of polymeric [SbCl$_5$]$_n$ zig-zag chains composed of distorted [SbCl$_6$]$_3$ octahedra connected via their vertices and the single Cl$^-$ anions. The cavities between the inorganic chains are filled by 1,2,4-triazolium cations. The nature of the distortion of the [SbCl$_6$]$_3$ octahedra has been studied by examining correlations between the Sb-Cl bond lengths and the strength of hydrogen bonds, which join the anionic sublattice and the organic cations. This study confirms that the deformation of the [SbCl$_6$]$_3$ octahedra is caused by hydrogen bonds.