

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 ($C_2H_4N_3$)Cl and its derivative with antimony trichloride - $(C_2H_4N_3)_2[SbCl_5] \cdot (C_2H_4N_3)Cl$ containing unsubstituted 1,2,4-triazolium cations were determined. $(C_2H_4N_3)Cl$ 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, $\beta = 95.87(3)^\circ$; $V = 895.2(3)$ Å³, $Z = 8$, $d_c = 1.566$, $d_m = 1.56(2)$ g·cm⁻³. At room temperature, crystals of $(C_2H_4N_3)_2[SbCl_5] \cdot (C_2H_4N_3)Cl$ are orthorhombic, space group $P2_12_12_1$, $a = 8.318(2)$, $b = 11.381(2)$, $c = 19.931(4)$ Å, $V = 1886.8(7)$ Å³, $Z = 4$, $d_c = 1.917$, $d_m = 1.91(2)$ g·cm⁻³. In both crystals the 1,2,4-triazole rings are planar. The anionic sublattice of $(C_2H_4N_3)_2[SbCl_5] \cdot (C_2H_4N_3)Cl$ consists of polymeric $[SbCl_5]_n^{2-}$ 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 $[SbCl_6]^{3-}$ polyhedra 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.