

Slabs from Cubic Sb_2O_3 interspersed between puckered BN-Type $\text{CuCl}_x\text{Br}_{1-x}$ Layers

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New compounds, $\text{CuSb}_2\text{O}_3\text{X}$ ($\text{X} = \text{Cl}, \text{Br}$), were obtained from chemical reactions taking place in sealed evacuated silica tubes. The structure consists of slabs of cubic antimony(III) oxide and hexagonal puckered CuX layers.

The compounds crystallize in the monoclinic space group Cc, but pseudo merohedral mimetic twinning produces the Laue symmetry 6/mmm. Unphysical short distances precludes the solution in any hexagonal (or trigonal) space group, and this is fully resolved by considering a twinned solution.

The antimony atoms have tetrahedral $[\text{SbO}_3\text{E}]$ coordination, E being the stereochemically active $5s^2$ lone pair electrons. The antimony oxide cages, Sb_4O_6 , are slightly distorted but of the same type as found in cubic Sb_2O_3 .

The Sb_2O_3 slabs are interspersed between hexagonally packed CuX ($\text{X} = \text{Cl}, \text{Br}$) layers resembling the boron nitride hexagonal structure. The Cu atoms have distorted $[\text{CuX}_3\text{O}]$ tetrahedral coordination. The oxygen atom in each tetrahedron belongs to the nearest Sb_4O_6 cage. The CuX network is regularly distorted at the nodes in between the $[\text{CuX}_3\text{O}]$ tetrahedra.

Keywords: stereochemically active lone pair, Sb_4O_6 cages, puckered CuX network