ABSTRACT

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The Crystal Structure of $Cs_6In_2S_6$

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Dark red single crystals of moderately air sensitive $Cs_6In_2S_6$ were obtained by using the ***Azide-route***[1-3]. $Cs_6In_2S_6$ crystallizes in the $K_6Al_2Se_6$ structure type[4] (space group $P2_1/c$ (no. 14)) with the unit cell dimensions a = 8.3616(9) Å, b = 13.5847(9) Å, c = 10.872(1) Å, β = 126.70(1)°, and V = 990.1(1)Å^3 (Z = 2).

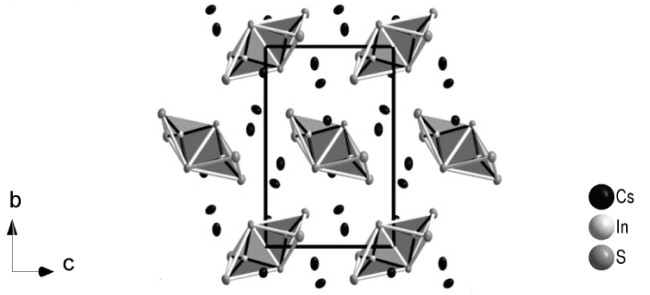

Figure 1. Section of the crystal structure of $Cs_6In_2S_6$ with trans corner-sharing $[In_2S_6]$ double tetrahedra embedded between cesium atoms. (95% probability ellipsoids)

The crystal structure consists of *trans* corner-sharing $[In_2S_6]^{6-}$ double tetrahedra which are located in an alkali metal surrounding of cesium. The three crystallographic independent cesium atoms have a six (Cs1 and Cs3) and seven fold coordination (Cs2).

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