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Structure of Li_5AlS_4 and comparison with other lithium-containing metal sulfides

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Abstract

Lithium aluminum sulfide (Li_5AlS_4) was synthesized by solid state reaction, and its crystal structure was characterized by *ab initio* structure determination on the basis of powder neutron diffraction (ND) data. Li_5AlS_4 was found to have monoclinic unit cell (space group, $P2_1/m$) with the lattice parameters: $a = 6.8583(4)$ Å, $b = 7.8369(4)$ Å, $c = 6.2488(4)$ Å, and $\beta = 90.333(4)^\circ$. This structure is built from a hexagonal close-packed (*hcp*) arrangement of sulfur atoms with a stacking sequence of ...ABAB.... The *hcp* sulfide lattice consists of two different double-sulfide layers alternately stacked along the *c*-axis. Between the first pair of sulfur layers all the tetrahedral interstices (T^+ and T^- sites) are filled with lithium and aluminum atoms. All octahedral interstices between the second pair of sulfur layers are

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