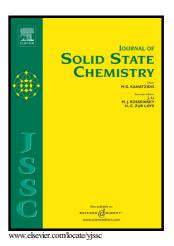
### Author's Accepted Manuscript

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#### **ACCEPTED MANUSCRIPT**

# Structure of Li<sub>5</sub>AlS<sub>4</sub> and comparison with other lithium-containing metal sulfides

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#### Abstract

Lithium aluminum sulfide (Li<sub>5</sub>AlS<sub>4</sub>) 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<sub>5</sub>AlS<sub>4</sub> 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<sup>+</sup> and T<sup>-</sup> sites) are filled with lithium and aluminum atoms. All octahedral interstices between the second pair of sulfur layers are

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