

# Li<sub>2</sub>Ag<sub>7</sub>Sb<sub>3</sub>S<sub>9</sub> – a compound in the quasi-binary system Li<sub>3</sub>SbS<sub>3</sub> – Ag<sub>3</sub>SbS<sub>3</sub>

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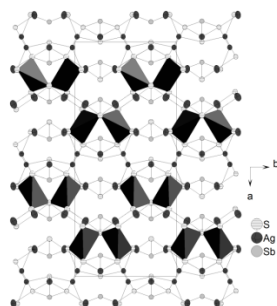
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In literature there are many compounds known with the composition  $M_3\text{SbS}_3$  ( $M=\text{Ag}^{[1]}$ ,  $\text{Cu}^{[2,3]}$ ,  $\text{Li}^{[4]}$ ,  $\text{Na}^{[5]}$ ,  $\text{K}^{[6]}$ ,  $\text{Rb}^{[6]}$ ,  $\text{Cs}^{[6]}$ ). We investigated the quasi-binary section  $\text{Li}_3\text{SbS}_3$  –  $\text{Ag}_3\text{SbS}_3$  for new quaternary materials.  $\text{Li}_2\text{Ag}_7\text{Sb}_3\text{S}_9$  has been synthesized by high temperature reaction of  $\text{Li}_2\text{S}$ ,  $\text{Ag}_2\text{S}$  and  $\text{Sb}_2\text{S}_3$ . The crystal structure of  $\text{Li}_2\text{Ag}_7\text{Sb}_3\text{S}_9$  was determined by single-crystal X-ray diffraction. The title compound crystallizes in the orthorhombic space group  $Pnma$  (No. 62) with  $a = 24.411(3)$  Å,  $b = 10.620(1)$  Å,  $c = 6.939(1)$  Å,  $V = 1798.9(5)$  Å<sup>3</sup>, and  $Z = 4$ . The anionic substructure of  $\text{Li}_2\text{Ag}_7\text{Sb}_3\text{S}_9$  consists of trigonal-pyramidal  $\text{SbS}_3$ , tetrahedral  $\text{LiS}_4$  and trigonal-planar  $\text{AgS}_3$  units. (Figure 1).

Thermal analysis revealed a reversible phase transition at 235°C and a melting point of 480°C.

The compound was further characterized by Raman spectroscopy. The Sb-S vibrations at 320 cm<sup>-1</sup> and 287 cm<sup>-1</sup> are in good agreement with data in literature<sup>[7]</sup>.

Impedance spectroscopy shows an ionic conductivity of 10<sup>-7</sup> S/cm at room temperature and 10<sup>-3</sup> S/cm at 300°C.



**Figure 1.** Section of the crystal structure of  $\text{Li}_2\text{Ag}_7\text{Sb}_3\text{S}_9$ . Lithium is located in the distorted tetrahedra.

- [1] F. Laufek, J. Sejkora, M. Dusek, *J. Geosci.*, **2010**, *23*, 21-26.  
[2] E. Makovicky, T. Balic-Zunic, *Can. Mineral.*, **1995**, *33*, 655-663.  
[3] A. Pfitzner, *Z. Anorg. Allg. Chem.*, **1994**, *620*, 1992-1997.  
[4] S. Huber, C. Preitschaft, R. Wehrich, A. Pfitzner, *Z. Anorg. Allg. Chem.*, **2012**, *638*, 2542-2548.  
[5] C. Pompe, A. Pfitzner, *Z. Anorg. Allg. Chem.*, **2013**, *639*, 296-300.  
[6] L. Schindler, M. Schwarz, C. Röhr, *Z. Naturforsch. B.*, **2013**, *68(12)*, 1295-1309.  
[7] A. Pfitzner, *Chem. Eur. J.*, **1997**, *3*, 2032-2038.