

DOI: 10.1002/zaac.200670032

Electronic and magnetic properties of the spin $1/2$ compound $\text{Na}_3\text{Cu}_2\text{SbO}_6$

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Keywords: cuprate; low-dimensional magnetism

Due to their versatile crystal chemistry and the related unusual low-temperature magnetic properties, Cu(II) compounds with complex oxo-anions of non-metals have attracted growing interest during the last years. Recently, the structure of a new sodium copper antimonate $\text{Na}_3\text{Cu}_2\text{SbO}_6$ has been reported [1]. This compound contains Cu_2O_6 sub-units built from edge-sharing CuO_2 plaquettes. The Cu_2O_6 sub-units are arranged in chains along the y direction, interrupted by SbO_6 octahedra (see Figure). The Cu–O–Cu bond angle in the Cu_2O_6 units is about 95° , therefore a competition of ferromagnetic and antiferromagnetic interactions can be expected [2]. Here, we present a combined experimental and theoretical study of the structural, thermodynamic and electronic properties of this compound. The micro-crystalline powder sample was prepared by a solid-state reaction. As starting materials Na_2CO_3 , $\text{Cu}_2(\text{OH})_2\text{CO}_3$ and Sb_2O_5 were used. A homogeneous powder mixture was pressed into pellets and calcined for 24 h at 873 K and for 240 h at 1273 K in a platinum crucible. X-ray diffraction data of the resulting $\text{Na}_3\text{Cu}_2\text{SbO}_6$ powder gave no indication of additional phases. The thermodynamic properties of the system have been characterised by magnetic susceptibility and specific heat measurements. The electronic and magnetic structure has been analysed starting from DFT band structure calculations that are mapped to an effective tight-binding model and subsequently to a Heisenberg model. A variety of possible magnetic ground states is compared with respect to their total energy and with the experimental data.

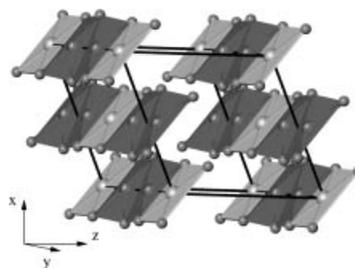


Fig. 1 The monoclinic structure of $\text{Na}_3\text{Cu}_2\text{SbO}_6$. Cu_2O_6 sub-units are printed in dark grey. From the SbO_6 octahedra only the middle plane is shown (light grey). The O atoms are presented by small spheres, the Na ions between the layers are not shown.

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