

**o.m5.p1** Evidence for a structural phase transition in the quasi-2D spin dimer system  $\text{SrCu}_2(\text{BO}_3)_2$ . K. Sparta, G. Redhammer, P. Roussel, G. Roth, G. Heger, *Institut für Kristallographie, RWTH-Aachen, Jägerstraße 17-19, 52056 Aachen, Germany.*

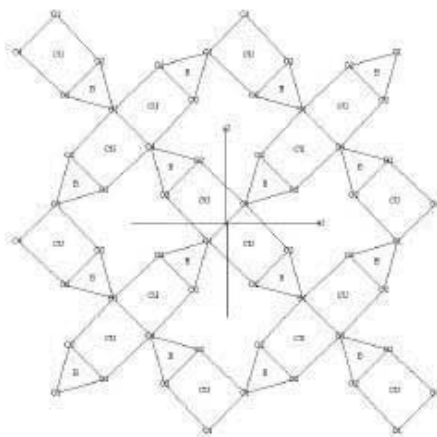
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The strontium copper orthoborate  $\text{SrCu}_2(\text{BO}_3)_2$  is a quasi two dimensional compound which crystallizes in the space group I42m at room temperature<sup>1</sup>, with cell parameters  $a = 8.9906(1) \text{ \AA}$  and  $c = 6.6480(1) \text{ \AA}$ .

The structure is formed by a succession of  $\text{Cu}(\text{BO}_3)$ - and Sr- layers alternating along the 4-fold axis. In the  $\text{Cu}(\text{BO}_3)$ - layers, the atoms are arranged in distorted  $\text{CuO}_4$  squares and  $\text{BO}_3$  triangles (see figure). The  $\text{Cu}^{2+}$  ions, interacting in an antiferromagnetic way, lie on a triangular lattice, which leads to a spin frustration at low temperatures<sup>2</sup>.

We have studied the temperature dependence of the structure of this compound by means of single crystal and powder X-ray diffraction, and single crystal neutron diffraction. As expected from Raman scattering measurements<sup>3</sup>,  $\text{SrCu}_2(\text{BO}_3)_2$  undergoes a structural phase transition, at  $T_S \approx 398 \text{ K}$ . The space group becomes I4/mcm at high temperature. This continuous second order phase transition is due to the movement of all the atoms in the  $\text{Cu}(\text{BO}_3)$ - layer into a common mirror plane.

In this work, we present our experimental results showing the phase transition in pure  $\text{SrCu}_2(\text{BO}_3)_2$ , and the influence of Zn doping on the temperature evolution of the structure. The origin of the phase transition and its possible implications for the low temperature magnetic behavior will be discussed.



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[2] Miyahara S., Ueda K. " Exact Dimer Ground State of the Two Dimensional Heisenberg Spin System  $\text{SrCu}_2(\text{BO}_3)_2$ .", *Phys. Rev. Lett.*, (1999), vol. 82: 3701 - 3704.

[3] Sparta K. et al. " Structural Phase Transition in the 2D Spin Dimer Compound  $\text{SrCu}_2(\text{BO}_3)_2$ .", submitted.