SNBL	**Experiment title:** Low-temperature structural transition in theoparacelsite $Cu_3(OH)_2As_2O_7$, a potentially low-deimensional quantum spin mineral system.	**Experiment number**: 01-02-705
Beamline: BM01A	**Date of experiment**: from: 26-Nov-05 to: 29-Nov-05	**Date of report**: 28-Feb-07
Shifts: 9	**Local contact(s)**: Dmitry CHERNYSHOV	*Received:*

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Single crystals of the mineral theoparacelsite [1], $Cu_3(OH)_2As_2O_7$, (RT structure: *Pmma*, *a*=8.3212(8), *b*=2.9377(3), *c*=4.6644(5) Å, Z=2/3), and of its hydrated version $Cu_3(OH)_2$ $As_2O_7 \cdot 3/2H \cdot 3/4(H_2O)$, (RT structure: *C2/m*, *a* = 19.158(3), *b* = 2.9361(6), *c* = 9.193(2) Å, β=103.26(1)°, Z=8/3) were studied at 100 K and 15 K using the MAR345 image plate detector (λ=0.71 Å), cryostreamer and Helijet.
Theoparacelsite is isotypic to $CuGeO_3$ and $CuSiO_3$, low-dimensional quantum spin systems, which undergo structural phase transitions at low temperatures. The As tetrahedral site was found at RT in theoparacelsite to be partially occupied (occ. = 2/3) and affected by disorder, which is indicated by very high displacement factors and by diffuse intensity in planes perpendicluar to the *b*-axis. The same disorder on As sites, and very similar diffuse intensity, in planes perpendicular to the *b*-axis, were found in the hydrated theoparacelsite (the mineral is currently being submitted to the IMA for the approval). A possible structural phase transitions in both compounds were expected at low temperature.
From the analysis of the diffraction data it can be concluded that both compounds conserve their average RT crystal structures down to 15 K. The thermal dilatation shows an anomaly along the *b*-axis in both compounds as shown in the Figure 1.

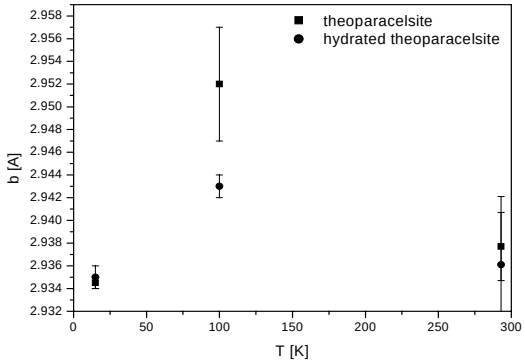
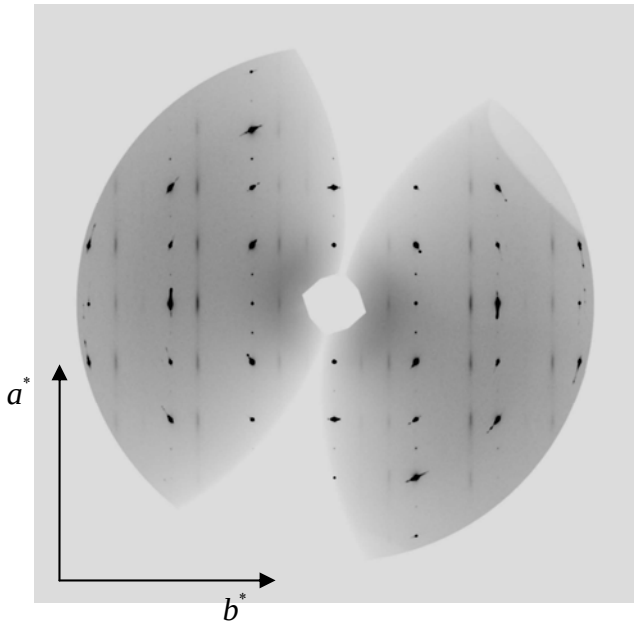


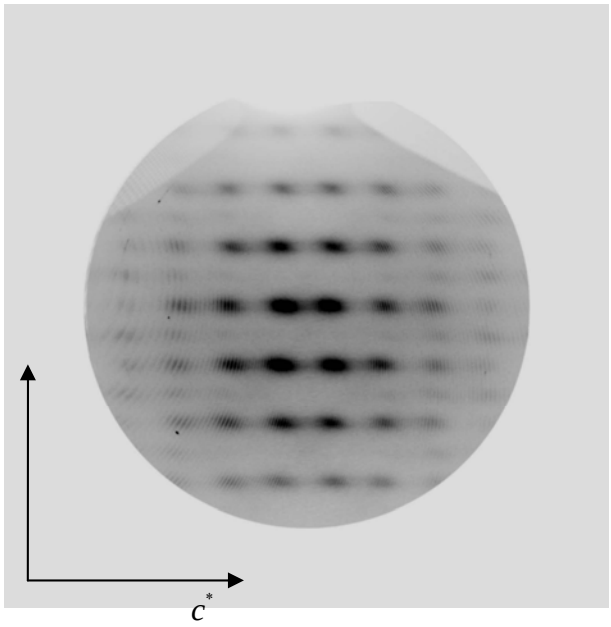
Figure 1 : The lattice parameter *b* in both compounds as a function of temperature showing the non-linear behavior. Other lattice parameters as well as the cell volume increase linearly with the temperature.

Figure 2 shows the sections in the reciprocal space of both compounds measured at 15 K. The planes of the diffuse intensity are in both compounds perpendicular to the b^*-axis and occur with the periodicity 3-times shorter then the reciprocal lattice of both crystals. The diffuse intensity shows better developed maxima at low temperatures. The maxima follows the periodicidy of the lattice in a^* and c^* directions in both compounds. This observations show that the diffuse intensity is related to the disordered As site, which is probably ordered in individual chains of AsO_4 tetrahedra running along the *b*-axis in both compounds. The average correlation length as determined from the halfwidth of the diffuse intensity maxima is about 62 Å in both compounds. Detailed analysis of the diffuse intensity is currently being performed.

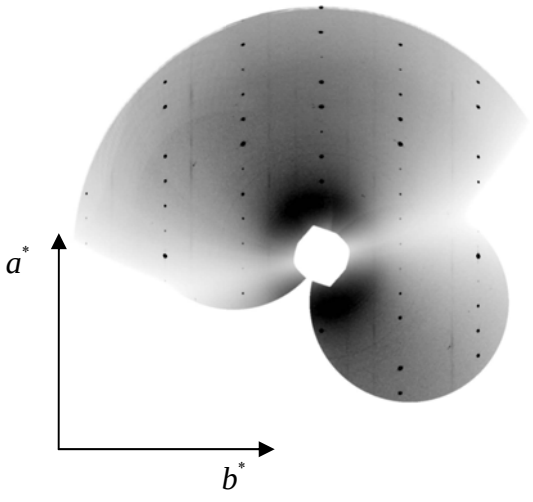
Theoparacelsite, *hk*0, 15 K



Theoparacelsite, *h*5/3*l*, 15 K



Hydrated theoparacelsite, *hk*0, 15 K



Hydrated theoparacelsite, *h*5/3*l*, 15 K

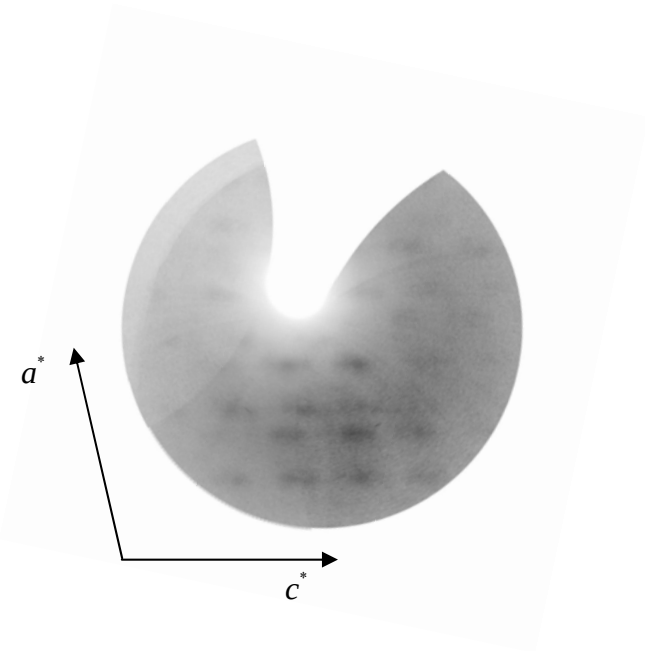


Figure 2: Sections in the reciprocal space of theoparacelsite (upper) and hydrated theoparacelsite (lower) showing the diffuse intensity measured at 15 K (λ=0.71 Å).

[1] Sarp, H. & Cerny, R.; *Archs. Sci. Genève* **54** (2001) 7-14