MS6 – P2: Intermediate scapolite: behavior at non-ambient conditions and unusual symmetry

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The scapolite series of minerals represents a complex non-binary solid solution, which end members are: marialite [$Na_4Al_3Si_9O_{24}Cl$], meionite [$Ca_4Al_6Si_6O_{24}CO_3$] and silvialite [$Ca_4Al_6Si_6O_{24}SO_4$]. The members which composition falls on the marialite-meionite joint appears to be the most common in natural occurrences [1,2]. The members close to marialite on one side and to meionite on the other side, are usually reported to crystallize in the tetragonal *I*4/*m* space group, whereas intermediate scapolites are usually found in the primitive space group $P4_2/n$. In this study, we report a scapolite of intermediate composition $(Na_{1.86}Ca_{1.86}K_{0.23}Fe_{0.01})(Al_{4.36}Si_{7.64})O_{24}[Cl_{0.48}(CO_3)_{0.48}(SO_4)_{0.01}]$, which, based on both X-ray and neutron single-crystal diffraction data, shows an anomalous *I*-centered lattice (Figure 1), possibly due to anti-phase domains too small to be detected by diffraction techniques. The behavior at non-ambient conditions of the same sample has been investigated at high-*P* (ambient-*T*) by single-crystal XRD at the former ID09 beamline of ESRF (Grenoble) and at high-*T* (ambient-*P*) by powder XRD at the MCX beamline of the Elettra synchrotron (Trieste), providing the following thermodynamic parameters: β_{V0} = 0.0143(4) GPa^{-1} and α_{V0} = $1.87(4)\cdot10^{-5}$ K^{-1}, respectively, which confirm that compressibility and thermal expansivity increase, along the solid solution series, from meionite to marialite [3-6]. A *P*-induced phase transition towards a triclinic polymorph has been observed at 9.87 GPa at ambient-*T*. An *in situ* single-crystal XRD experiment at combined high *P* and *T* (using a resistive-heated DAC), performed at the P02.2 beamline of the Petra-III synchrotron (Hamburg), allowed to detect the occurrence of the same phase transition at 10.51 GPa at 650 °C.

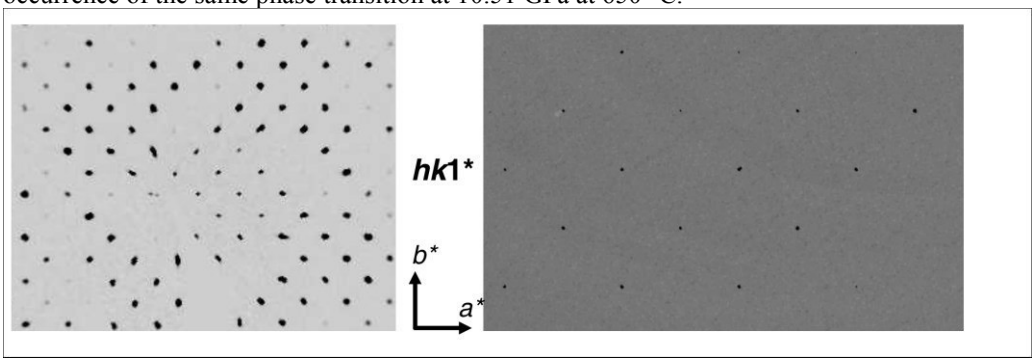

Figure 1. Reconstructions of the *hk*1* reciprocal lattice plane, based on conventional diffractometer (*left*) and synchrotron (*right*) XRD data. No violations of the systematic absences expected for an *I*-centered lattice are shown.

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