μ(MoKα) = 13.124 mm^{-1}, F_{000} = 736, $2\theta_{max}$ = 70°, 24673 reflection collected, 1243 unique reflections, R_{int} = 0.0298, multi-scan absorption correction, T_{min} = 0.3161, T_{max} = 0.3718, completeness 100%, 35 parameters refined, absolute structure parameter = 0.04(5), R_1 [$I > 2\sigma(I)$] = 0.0149, R_1 [all data = 0.0289], wR_2 [$I > 2\sigma(I)$] = 0.0157, wR_2 [all data = 0.0291], Δe_{max} = 0.775 eÅ^{-3}, Δe_{min} = -0.748 eÅ^{-3}.

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Keywords: tin oxide compounds, mineral, precise crystal structure analysis

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Structure and magnetic properties of new triple molybdates $CsMZr_{0.5}(MoO_4)_3$ (M = Al, Ga, In, Sc, Cr, V, Fe).

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Isostructural complex molybdates $CsMZr_{0.5}(MoO_4)_3$ (M = Al, Ga, In, 3d-elements) demonstrate a variety of physical–chemical, electrophysical and optical properties depending on the trivalent cation. The crystal structures of $CsAlZr_{0.5}(MoO_4)_3$ and $CsFeZr_{0.5}(MoO_4)_3$ phases were refined from single-crystal X-ray diffraction [1, 2]. The structure represents a three-dimensional framework of corner-shared MoO_4-tetrahedra and $(M,Zr)O_6$-octahedra (S.G. *R*-3); the channels along the c- axis are filled by Cs-ions, which should provide high ionic conductivity at elevated temperatures.

In our work, the compounds with M = Al, Ga, In, Sc, Cr, V, Fe were synthesized by solid state reaction in air or in a sealed silica tube (for M = V) and investigated by X-ray powder diffraction with a STOE STADI P diffractometer (Mo-$K\alpha_1$-radiation). All diffraction patterns were analyzed by full-profile Rietveld refinements, using the software package WinPLOTR [3]. Magnetic properties have been studied with a superconducting quantum interference device (SQUID) from Quantum Design.

The lattice parameters of $CsMZr_{0.5}(MoO_4)_3$ increase nonlinearily with increasing radius of the trivalent element M. The same correlation is observed for the melting point of these phases. Investigation of magnetic properties of the compounds with 3d transition metals Cr, Fe and V showed a paramagnetic behaviour below room temperature and a deviation between field-cooled and zero-field cooled data below ca. 10 K, indicating a ferro- or ferrimagnetic ordering. However, since this is rather unusual for such magnetic diluted frameworks, because the interatomic distances M-M for M=V, Cr and Fe in $CsMZr_{0.5}(MoO_4)_3$ are about 5.5 Å, and the 9*e*-site in the structure is occupied statistically with a magnetic cation only by 2/3 and with Zr by 1/3, the presence of a spin-glass type behavior is discussed.

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High-temperature elastic properties of sanidine.

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Sanidine crystals from the Eifel, Germany, are well-known for irreversible changes of their optical properties at moderately high annealing temperatures (starting from about 750°C), which are probably related to changes in the Al/Si order [1]. Polarised infrared spectra and NMR studies indicate a relatively high amount of water in the Eifel sanidines (~ 200 wt-ppm), compared to low-sanidine crystals from Madagascar (~ 1 wt-ppm) [2,3]. The sanidine megacrystals from the Eifel are further characterised by very low concentrations of dislocations indicating hydrothermal growth conditions [4]. However, the reason for the rapid changes of their optical properties is still not understood.

We studied the elastic behaviour of sanidines from various eruptive centres of the Eifel and from Madagascar (served as a reference) between room temperature and 1100°C using resonant ultrasound spectroscopy. All samples were of gem-quality without visible inclusions or cracks.

The elastic properties of our 'dry' Madagascar sanidine agree well with literature values obtained by the plate-resonance technique close to room temperature [5]. The temperature evolution of the elastic constants is fully reversible without any discontinuity. Remarkable is the positive temperature coefficient of the shear stiffness c_{44} which is related to the structural instability driving the ferroelastic phase transition in Na-rich alkalifeldspars due to framework shearing. Additionally, a small ultrasound dissipation peak appears at about 890°C.

On the other hand, 'hydrous' sanidines from the Eifel show reversible exponential increase of ultrasound dissipation above 800°C, followed by rapid irreversible softening of all resonance frequencies by about 8 % above 970°C. The latter phenomenon is most likely related to the development and propagation of micro-cracks in the sample. Both effects are probably caused by the increasing mobility and eventually the loss of water dissolved in the crystal structure of these nominally anhydrous minerals. The high mobility of the water molecules allows for a new, less ordered Al/Si equilibrium state to be reached on the time scale of the experiment. The associated increase of the configurational entropy leads to elastic softening of the macroscopic crystals.

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