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High-Temperature Crystal Chemistry of aluminate sodalites $Ca_8[Al_{12}O_{24}]((Mo_{1-x},W_x)O_4)_2$ (x = 0.0, 0.25, 0.5)

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Solid solutions of aluminate sodalites, $Ca_8[Al_{12}O_{24}]((Mo_{1-x},W_x)O_4)_2$, x = 0, 0.25, 0.5 have been studied by powder high-temperature X-ray diffraction (25–1100 ˚C, temperature step = 6–25 ˚C). Isotypical compounds $Ca_8[Al_{12}O_{24}](MoO_4)_2$ and $Ca_8[Al_{12}O_{24}](WO_4)_2$ are characterized by series of thermal reversible polymorphic transitions (Smaalen, Dinnebier, Katzke et al., 1997; Depmeier, Vogt, Buhrer, 1991).

We present new HTXRD data on a special thermal effect at 700–750 ºC, at which the curve of the temperature dependence of the parameter a cubic cell has an inflection and dramatically reduced the half-width of all reflections for the compositions x = 0 and 0.25. It is not associated with a change in symmetry or the existence of two-phase region. Perhaps, it occurs due to the effect of increasing the dynamic disorder of the tetrahedra MoO_4 (WO_4) to their full rotation.

Bulk expansion of low-temperature orthorhombic modification of α_V = (16–17) $\times$ 10^{-6} ˚C^{-1} for the compositions x = 0, 0.25 and 0.5. Along the [100] and [010] expansion increases while along the [001] it decreases. The polymorphic transition is characterized by sharp convergence parameters in the HTXRD study, two-phase region was observed during the transition from to tetragonal to cubic modification. The bulk expansion of the latter is α_V = 26 $\times$ 10^{-6} ˚C^{-1} for these phases, it is weakly decreases to 700-750 ˚C which takes the value of α_V equal to 22, 21, 24 $\times$ 10^{-6} ˚C^{-1} for x = 0, 0.25, 0.5, respectively. Above this temperature, the expansion increases up to values of α_V equal to 36, 32, 32 $\times$ 10^{-6} ˚C^{-1}.

A few superstructure reflections during the polymorphic transition do not disappear completely, but above the transition temperature of the position does not coincide with the calculated values for the respective superstructures. Most of them (21 reflections) corresponds to the composition x =0.5, least of them (5 reflections) - the composition of x = 0.

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