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Thermal behavior of afghanite, an ABABACAC member of the cancrinite group

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Abstract

Thermal behavior of afghanite, $(Na_{15}K_5Ca_{11})_{\Sigma 31}[Si_{24}Al_{24}O_{96}](SO_4)_6Cl_6$, *P*31*c*, *a* = 12.7961(7) Å, *c* = 21.4094(13) Å, an eight-layer member of the cancrinite group, has been investigated by combined electron microprobe analysis, X-ray single-crystal diffraction, and high-temperature X-ray powder diffraction. Non-ambient X-ray powder diffraction data were collected in the 323–1223 K thermal range on a specimen from Case Collina, Latium, Italy. Structural refinement and site assignment based on the bond-valence analysis, performed on room-temperature single-crystal X-ray diffraction data, provided more accurate site allocation of cations than the available model in the literature. The results show that the cancrinite cages alternating with the liottite cages are more compressed along the **c**-axis than the remaining ones. As a result the chlorine atom, located at the center of the cages, is driven off-axis to release the steric strain due to the cage compression. Thermal expansion shows a discontinuity at 448 K for both *a* and *c* unit-cell parameters, a feature previously reported for other cancrinite-like minerals. Up to 448 K, the *c*-parameter expands significantly and more than the *a*-parameter. A further discontinuity has been detected at 1073 K for the *c*-parameter. Mean linear and volume thermal expansion coefficients ($\times 10^{-6}$ K^{-1}) in the $323 < T < 448$ K thermal range are $\overline{\alpha_a}$ = 12.9(4), $\overline{\alpha_c}$ = 17.9(9), and $\overline{\alpha_V}$ = 43.7(18). Above this discontinuity temperature, the thermal expansion is reverted becoming greater for the *a*-parameter. Mean linear and volume thermal expansion coefficients in the $448 < T < 1073$ K thermal range are $\overline{\alpha_c}$ = 8.22(3), $\overline{\alpha_c}$ = 3.52(4), and $\overline{\alpha_V}$ = 19.68(8). In the $1073 < T < 1223$ K thermal range the values are $\overline{\alpha_a}$ = 6.35(9), $\overline{\alpha_c}$ = 5.02(14), and $\overline{\alpha_V}$ = 17.74(9). Afghanite shows a significant microstrain at RT that increases up to ca. 700 K and subsequently decreases as a function of *T*. Cooling to RT allows a significantly release of ε_0 microstrain, which is coupled with a significant expansion of the *c*-parameter as compared to the starting RT data. The expansion of the *c*-parameter has been mainly attributed to the full expansion of the cancrinite cages alternating with the liottite cages. Upon reheating at 1173 K, the microstrain increases back to approximately the same value calculated for the first heating process. Repeated heating-RT-cooling cycles led to the partial afghanite structure disruption and the partial conversion, via an intermediate disordered phase, to haüyne. As repeated heating/cooling cycles did not modify the ε_0 values both at RT and at HT, it can therefore be concluded that the strain release occurs prevalently during the first heating/cooling cycle.

Keywords: Afghanite, cancrinite group, X-ray single-crystal diffraction, high-temperature X-ray powder diffraction, Rietveld method