American Mineralogist, Volume 89, pages 492–497, 2004

Tugtupite: High-temperature structures obtained from in situ synchrotron diffraction and Rietveld refinements

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ABSTRACT

The structural behavior of tugtupite, (ideally $Na_8[Al_2Be_2Si_8O_{24}]Cl_2$), a member of the sodalite-group minerals, at room pressure and from 33 to 982 °C on heating, was determined by using in situ synchrotron X-ray powder diffraction data [$\lambda = 0.91997(4)$ Å] and Rietveld refinement. The sample was heated at a rate of 9.5 °C/min and X-ray traces were collected at intervals of 16 °C. The unit-cell parameters for tugtupite increase smoothly and non-linearly to 982 °C. The percent volume change between 33 and 982 °C is 2.97(3)%. In tugtupite, large displacement parameters occur for the Na and Cl atoms, and the Na-Cl bond expands with temperature. The $[Na_4{\cdot}Cl]^{3+}$ clusters expand with increases of the Na-Cl bond length by 0.073(3) Å between 33 and 982 °C. This forces the Na atoms toward the plane of the framework six-membered rings, and causes the framework tetrahedra to rotate. The framework TO_4 ($T = Al^{3+}$, Be^{2+}, or Si^{4+}) tetrahedra distort slightly with temperature, but the T-O distances remain nearly constant. This mechanism causes a fairly high-rate of expansion in tugtupite. If the Na atom reaches approximately the plane of the six-membered ring, because of the increase in bonding to the Na atom, the expansion will be retarded, but tugtupite melts before this occurs. Tugtupite melts at 1029 °C. The NaCl component in tugtupite is lost in two main stages; 1.8 wt% NaCl is first lost at about 1007 °C, and 8.2 wt% NaCl is lost in several steps between 1019 and 1442 °C.