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Cancrinite: Crystal structure, phase transitions, and dehydration behavior with temperature

ISHMAEL HASSAN,[1,*] SYTLE M. ANTAO,[2] AND JOHN B. PARISE[2]

[1]Department of Chemistry, University of the West Indies, Mona, Kingston 7, Jamaica
[2]Mineral Physics Institute and Department of Geosciences, State University of New York, Stony Brook, New York 11794-2100, U.S.A.

ABSTRACT

The structural behavior of a cancrinite, $Na_{5.96}Ca_{1.52}[Al_6Si_6O_{24}](CO_3)_{1.57}\cdot 1.75H_2O$, was determined by using in situ synchrotron X-ray powder diffraction data [$\lambda = 0.91806(5)$ Å] at room pressure and from 25 to 982 °C. The sample was heated at a rate of about 9.5 °C/min, and X-ray traces were collected at about 15 °C intervals. The satellite reflections in cancrinite were lost at about 504 °C, where a phase transition occurs. All the unit-cell parameters for cancrinite also show a discontinuity at 504 °C. Initially, the [$Ca\cdot CO_3$] clusters and their vacancies are ordered in the channels, and this ordering is destroyed on heating to give rise to the phase transition. Cancrinite loses water continuously until about 625 °C; thereafter an anhydrous cancrinite phase exists. From 25 to 952 °C, a minimal amount of CO_2 is lost from the structure. Over this temperature range, the average <Al-O-Si> bridging angle, which is an indication of the degree of rotation of the tetrahedra, increases from 143.7(4) to 147.7(5)°. Rotations of the tetrahedra are caused by expansion of the Na1-O2 bond lengths.

Keywords: Cancrinite, high-temperature structure, phase transitions, dehydration, Rietveld refinements, synchrotron radiation