

Combined Synchrotron X-ray Diffraction Studies to Synthetic Gallogermanate Cancrinite: 1. Synchrotron X-ray Single Crystal Diffraction Studies

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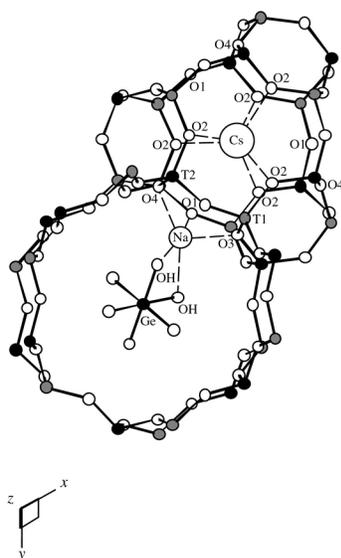
Beamline(s): X3A1

A synthetic aluminogermanate and a gallogermanate with the CAN framework topology have been synthesized under hydrothermal conditions and characterized by single crystal synchrotron X-ray diffraction [1]. AlGe-CAN, $\text{Na}_6\text{Cs}_2\text{Al}_6\text{Ge}_6\text{O}_{24}\cdot\text{Ge}(\text{OH})_6$, is hexagonal, space group P6_3 with $a = 12.968(1)$, $c = 5.132(1)$ Å, $V = 747.4(1)$ Å³. The T-sites exhibit complete ordering of Al and Ge atoms, similar to the framework models of aluminosilicate analogues. GaGe-CAN, $\text{Na}_6\text{Cs}_2\text{Ga}_6\text{Ge}_6\text{O}_{24}\cdot\text{Ge}(\text{OH})_6$, is hexagonal, apparently space group P6_3mc with $a = 12.950(2)$, $c = 5.117(1)$ Å, $V = 743.2(2)$ Å³. Although the observed data are consistent with the presence of the c -glide and consequent disordering of Ga and Ge atoms at the T-sites, calculation using a DLS-optimized framework in space group P6_3 reveals that the intensities of the $hh\bar{2}hl$ reflections with $l = 2n + 1$ are less than 0.07% of the strongest (0002) reflection, suggesting that P6_3 is probably the true space group (see X7A section). Inspection of the framework T-O-T bond angles demonstrates greater relative cell contraction for GaGe-CAN compared to AlGe-CAN and aluminosilicate counterparts. In both structural models, $\text{Ge}(\text{OH})_6$ -octahedra are occluded in the 12-ring channels running along the 6_3 -axes. The sodium cations fully occupy the sites above the 6-ring windows in the 12-ring channels. The cesium cations fully occupy the sites in the middle of the cancrinite cages.

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References: [1] Y. Lee, J.B. Parise, A. Tripathi, S.J. Kim, and T. Vogt. (2000) *Microporous Mesoporous Mater.*, 39, 445.

(a) AlGe-CAN



(b) GaGe-CAN

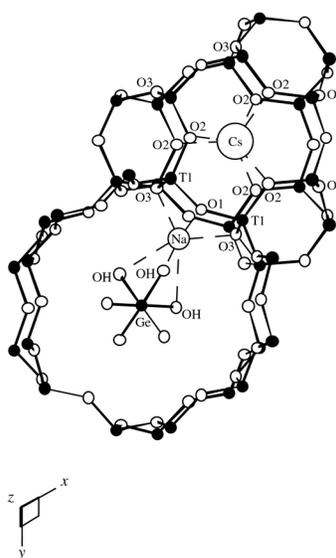


Figure. Ball and stick representations of the structural models for (a) AlGe-CAN and (b) GaGe-CAN viewed sub-parallel to [001]. A 12-ring channel and a cancrinite cage are shown to illustrate the coordinations of the extra-framework cations and the $\text{Ge}(\text{OH})_6$ -octahedra. Only one sodium cation is shown for clarity