

Raman Spectroscopic Investigations of Aluminate Sodalites

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The sodalite structure can be described as a borderline-case between dense frameworks like quartz or feldspars and open frameworks like zeolites (Weller, 2000). The aim of this study is to understand the temperature-induced phase transitions in aluminate sodalites, $[M_8X_2][Al_{12}O_{24}]$ -SOD, in particular the system $[Ca_8(MoO_4)_2][Al_{12}O_{24}]$ -SOD (CAM)- $[Ca_8(WO_4)_2][Al_{12}O_{24}]$ -SOD (CAW) (henceforth referred to as CAMW), using Raman spectroscopy. Between the endmembers CAM and CAW, at room temperature an isostructural solid solution series exists throughout the whole composition range. All solid solution members undergo temperature induced phase transitions. DTA measurements show that CAMW with $x(W) \leq 0.35$ undergoes three phase transitions and CAMW with higher tungsten content two (Peters et al., 2009). The phases are called *C* (cubic), T^2 , T^1 (not observed for $x(W) > 0.35$) and *RT* (room temperature), according to the nomenclature of van Smaalen et al. (1997). The cubic phase is observed for temperatures $T > \sim 640 - \sim 660$ K. At room temperature up to 625K, an orthorhombic phase with known structure exists which was described by Depmeier (1992) as a commensurately modulated variant of the cubic parent phase. To understand the phase transitions, it is necessary to obtain more information about the competitive interactions of the three partial structures: *i*) the sodalite framework, *ii*) the cage cations, and *iii*) the cage anions. It could be shown that the $RT \rightarrow T^2$ phase transition is correlated with an initiating movement of the XO_4 tetrahedra. The tetrahedra become perfectly dynamically disordered in the cubic phase. Furthermore, two additional interactions between the sodalite framework and the tetrahedrally shaped oxyanions could be found. They seem to be related with a difference in the temperature dependent behaviour of molybdate and tungstate. The nature of these interactions remains disputable and needs additional research.

References:

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