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Low-temperature behavior of $NaGaSi_2O_6$

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Abstract

Synthetic $NaGaSi_2O_6$-pyroxene, space group $C2/c$, was investigated at low temperature between 295 to 110 K by X-ray diffraction. The evolution of the unit-cell parameters as a function of temperature does not indicate any structural phase transition down to 110 K. Calculated values for the Debye temperature, θ_D, and the Grüneisen parameter, γ, are 653(39) and 0.84(8) K, respectively, close to those of other pyroxenes. Five complete intensity data collections were performed at 295, 235, 190, 145, and 110 K to investigate the temperature dependence of the crystal structure. The space group remains $C2/c$ down to 110 K, but anomalies were found between 235 and 190 K for the temperature dependencies of the volume and strain of the M1 polyhedron. This anomalous behavior could be related to variations of the Ga-O2(C1,D1) bond length and the O1(A1,B1)-Ga-O2(C1,D1) bond angle. The $C2/c$-$P\bar{1}$ phase transition observed in a previous work for $NaTiSi_2O_6$ at about 200 K did not occur for $NaGaSi_2O_6$ down to the minimum temperature investigated in this work. This is not due to the different ionic radius at M1 site or to a different tetrahedral chain extension between these two compositions but it is likely due to unfilled t_{2g} orbitals, which do not exist in $NaGaSi_2O_6$.

Keywords: Clinopyroxene, crystal structure, X-ray diffraction, low temperature