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Elastic behavior and pressure-induced structural evolution of nepheline: Implications for the nature of the modulated superstructure

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ABSTRACT

The elastic behavior and the pressure-induced structural evolution of a natural nepheline ($K_{0.54}Na_{3.24}Ca_{0.03}Al_4Si_4O_{16}$) were investigated by in-situ single-crystal X-ray diffraction up to 7.5 GPa with a diamond anvil cell under hydrostatic conditions. As observed in previous studies, at room conditions the diffraction pattern of nepheline includes satellite reflections, whereas the structure refinement to the Bragg reflections confirms that the O1 site is displaced from the triad at (2/3, 1/3, *z*). The reflection conditions confirm that the space group of the average structure of nepheline remains as $P6_3$ throughout the pressure range investigated, and no significant compression of the T-O bonds was measured up to 7.5 GPa. As pressure was increased to around 1 GPa the integrated intensities of the satellites decreased slightly, and at 1.8 GPa no significant intensity of the satellites was detected. Over the same pressure range the O1 site moved toward the triad and thus the tilts of the T1 and T2 tetrahedra decreased. The presence of the subsidiary non-Bragg reflections is therefore related to the split of the O1 site. When the satellites disappear at pressures above 2 GPa, the O1 site is on the triad at (2/3, 1/3, *z*), corresponding to a straight T1-O1-T2 bond. Below 2 GPa the structure responds to increased pressure by tilting of all four tetrahedra and above 2 GPa by tilting of the T3 and T4 tetrahedra alone. The change in compression mechanism arising from the changes in the O1 position is associated with changes in the compression of the unit-cell axes and the unit-cell volume. The volume can be described by fourth-order Birch-Murnaghan equation-of-state with parameters V_0 = 723.57(4) Å^3, K_{T0} = 47.32(26) GPa, K' = 2.77(24), and K'' = 0.758(79) GPa^{-1}. The elastic behavior along the **a-** and **c**-axis can be described with a "linearized" fourth-order Birch-Murnaghan equations-of-state, with the following refined parameters: a_0 = 9.9911(2) Å, $K_{T0}(a)$ = 43.1(3) GPa, $K'(a)$ = 2.5(3), and $K''(a)$ = 0.68(8) GPa^{-1} for the **a**-axis and c_0 = 8.3700(1) Å, $K_{T0}(c)$ = 58.6(3) GPa, $K'(c)$ = 4.0(3), and $K''(c)$ = 0.85(11) GPa^{-1} for the **c**-axis. The pressure-induced structural evolution in nepheline up to 7.5 GPa appears to be completely reversible. The recovery of the modulation upon complete pressure release points to the framework of nepheline having an instability corresponding to a rigid-unit mode with a wave vector corresponding to the observed positions of the satellite reflections.

Keywords: Crystal structure, nepheline, modulated structure, XRD data, single crystal, high pressure, compressibility, structural evolution