American Mineralogist, Volume 94, pages 616–621, 2009

High-pressure phase transformation in $LiFeGe_2O_6$ pyroxene

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ABSTRACT

A synthetic pyroxene with composition $LiFeGe_2O_6$ and space group $P2_1/c$ at ambient conditions was investigated by single-crystal X-ray diffraction using a diamond anvil cell. The unit-cell parameters and crystal structure were determined at eight different pressures up to 8.7 GPa. Between 4.16 and 4.83 GPa, the sample shows a strongly first-order phase transition as indicated by a drastic drop in a, c, β, and unit-cell volume. The transition is marked by the disappearance of b-type reflections ($h + k$ = odd) forbidden in a C-centered lattice. The volume bulk modulus of the $P2_1/c$ phase is estimated to be 110 GPa as compared to 147 GPa of the $C2/c$ one. The crystal structure evolution as a function of pressure is mainly influenced by the kinking of tetrahedral chains; the A and B non-symmetry equivalent chains of the $P2_1/c$ phase undergo strong deformations up to 4.16 GPa (A chain ~2%, B chain ~5.3%). At the transition, the two chains become symmetry equivalent and the single tetrahedral chain of the $C2/c$ phase shows only minor deformations with pressure (~1.9%) due to its already strong kinking (~130°). Such behavior is the main reason for the strong difference in compressibility between the low- and high-symmetry forms.

Keywords: Single-crystal structure analysis, germanates, high-pressure phase transformations, X-ray diffraction