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Synthesis and crystal structure of $LiNbO_3$-type $Mg_3Al_2Si_3O_{12}$: A possible indicator of shock conditions of meteorites

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Abstract

$LiNbO_3$-type $Mg_{2.98(2)}Al_{1.99(2)}Si_{3.02(2)}O_{12}$ (py-LN) was synthesized by recovering a run product from 2000 K and 45 GPa to ambient conditions using a large volume press. Rietveld structural refinements were carried out using the one-dimensional synchrotron XRD pattern collected at ambient conditions. The unit-cell lattice parameters were determined to be $a = 4.8194(3)$ Å, $c = 12.6885(8)$ Å, $V = 255.23(3)$ Å^3, with $Z = 6$ (hexagonal, $R3c$). The average A-O and B-O distances of the AO_6 and BO_6 octahedra have values similar to those that can be obtained from the sum of the ionic radii of the averaged A- and B-site cations and oxygen (2.073 and 1.833 Å, respectively). The present compound has the B-site cations at the octahedral site largely shifted along the c axis compared with other $LiNbO_3$-type phases formed by back-transition from perovskite (Pv)-structure, and as a result, the coordination number of this site is better described as 3+3. It appears therefore that the B-site cation in the octahedral position cannot be completely preserved during the back-transition because of the small size of Si and Al, which occupy usually a tetrahedral site at ambient conditions. The formation of py-LN can be explained by the tilting of BO_6 octahedra of the perovskite structure having the pyrope composition and formed at high P-T conditions. The tilting is driven by the decrease in ionic radius ratio between the A-site cation and oxygen during decompression. This also explains why there is no back-transition from the Pv-structure to the ilmenite-structure during decompression, since this is a reconstructive phase transition whose activation energy cannot be overcome at room temperature. Py-LN may be formed in shocked meteorites by the back-transformation after the garnet-bridgmanite transition, and will indicate shock conditions around 45 GPa and 2000 K.

Keywords: Bridgmanite, large volume press, Rietveld analysis, $LiNbO_3$, high pressure