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LETTER

A new $(Mg_{0.5}Fe^{3+}_{0.5})(Si_{0.5}Al^{3+}_{0.5})O_3$ $LiNbO_3$-type phase synthesized at lower mantle conditions

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ABSTRACT

A new $(Mg_{0.5}Fe^{3+}_{0.5})(Si_{0.5}Al^{3+}_{0.5})O_3$ $LiNbO_3$-type phase was synthesized at 27 GPa and 2000 K under highly oxidized conditions using an advanced multi-anvil apparatus. Single crystals for this phase are 0.2–0.3 mm in dimension and maroon in color. They crystallize in a noncentrosymmetric structure with space group $R3c$ and lattice parameters of $a = b = 4.8720(6)$ Å, $c = 12.898(2)$ Å, and $V = 265.14(8)$ Å^3. Fe^{3+} and Al^{3+} cations substitute into A (Mg^{2+}) and B (Si^{4+}) sites through charge-coupled substitution mechanism, respectively. The distortion of BO_6 ($B = Si_{0.5}Al^{3+}_{0.5}$) octahedra is 1.6 times higher than that of AO_6 (A $= Mg_{0.5}Fe^{3+}_{0.5}$) octahedra. This phase is probably recovered from bridgmanite at lower-mantle conditions by a diffusionless transition because of the displacement of A cations and distortion of BO_6 octahedra on releasing pressure. Bridgmanite can thus contain the $FeAlO_3$ component (50 mol%) beyond previously reported solubility limit (37 mol%). The present study shows that the Earth's most abundant elements form a new Fe^{3+}- and Al^{3+}-rich $LiNbO_3$-type compound from bridgmanite at lower mantle conditions. This new compound provides a new insight into the complicated crystal chemistry of $LiNbO_3$-type phase/bridgmanite and constrains the pressure and temperature conditions for shocked meteorites.

Keywords: $LiNbO_3$-type, single crystals, bridgmanite, crystal chemistry, lower mantle