

LETTER

**Crystal structure and Raman spectrum of a high-pressure Li-rich majoritic garnet,  
(Li<sub>2</sub>Mg)Si<sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>**

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ABSTRACT

A Li-rich majoritic garnet (LiMGt), (Li<sub>2</sub>Mg)Si<sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>, was synthesized at 15 GPa and 1500 °C and its structure studied with single-crystal X-ray diffraction and Raman spectroscopy. It is cubic with space group *Ia* $\bar{3}d$  and unit-cell parameters  $a = 11.2660(2)$  Å and  $V = 1429.91(1)$  Å<sup>3</sup>. The 8-, 6-, and 4-coordinated cation sites in LiMGt are occupied by (Li<sup>+</sup> + Mg<sup>2+</sup>), Si<sup>4+</sup>, and Si<sup>4+</sup>, respectively. Whereas the SiO<sub>6</sub> octahedron is nearly regular, the XO<sub>8</sub> dodecahedron is the most distorted of all known silicate garnets in terms of the bond-length distortion index. All Raman peaks of LiMGt are broader than those of pyrope, due to the substitution of Li<sup>+</sup> for Mg<sup>2+</sup> at the dodecahedral site. Furthermore, both Si-O symmetric stretching ( $A_{1g}$ - $\nu_1$ ) and O-Si-O symmetric bending ( $A_{1g}$ - $\nu_2$ ) modes of LiMGt shift significantly to higher frequencies relative to the corresponding ones of pyrope. In contrast, the  $A_{1g}$ -(SiO<sub>4</sub>) rotational mode of LiMGt displays a much lower frequency than that of pyrope. This study represents the first structural report on a garnet with an all-silicate framework and suggests that, like Na incorporation in garnets, the pressure-dependent coupled substitution of (Li<sup>+</sup> + Si<sup>4+</sup>) for (Mg<sup>2+</sup> + Al<sup>3+</sup>) is likely one of the primary mechanisms for Li enrichment in garnets in the mantle and the transition zone.

**Keywords:** Majoritic garnet, crystal structure, Raman spectroscopy, high pressure