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LETTER

Crystal structure and Raman spectrum of a high-pressure Li-rich majoritic garnet, $(Li_2Mg)Si_2(SiO_4)_3$

HEXIONG YANG,[1,*] JÜRGEN KONZETT,[2] ROBERT T. DOWNS,[1] AND DANIEL J. FROST[3]

[1]Department of Geosciences, University of Arizona, 1040 E. 4th Street, Tucson, Arizona 85721-0077, U.S.A.
[2]Institut für Mineralogie und Petrographie, Universität Innsbruck, Innrain 52, A-6020 Innsbruck, Austria
[3]Bayerisches Geoinstitut, Universität Bayreuth, Universitätsstrasse 30, D-95447 Bayreuth, Germany

ABSTRACT

A Li-rich majoritic garnet (LiMGt), $(Li_2Mg)Si_2(SiO_4)_3$, 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^3. The 8-, 6-, and 4-coordinated cation sites in LiMGt are occupied by $(Li^+ + Mg^{2+})$, Si^{4+}, and Si^{4+}, respectively. Whereas the SiO_6 octahedron is nearly regular, the XO_8 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^+ for Mg^{2+} at the dodecahedral site. Furthermore, both Si-O symmetric stretching (A_{1g}-ν_1) and O-Si-O symmetric bending (A_{1g}-ν_2) modes of LiMGt shift significantly to higher frequencies relative to the corresponding ones of pyrope. In contrast, the A_{1g}-(SiO_4) 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 $(Li^+ + Si^{4+})$ for $(Mg^{2+} + Al^{3+})$ 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