American Mineralogist, Volume 96, pages 447–450, 2011

LETTER

Crystal chemistry of sodium in the Earth's interior: The structure of $Na_2MgSi_5O_{12}$ synthesized at 17.5 GPa and 1700 °C

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ABSTRACT

The crystal structure and chemical composition of a crystal of $Na_2MgSi_5O_{12}$ garnet synthesized in the model system $Mg_3Al_2Si_3O_{12}$–$Na_2MgSi_5O_{12}$ at 17.5 GPa and 1700 °C have been investigated. Quantitative analysis leads to the following formula: $Na_{1.98}Mg_{1.00}Si_{5.01}O_{12}$. $Na_2MgSi_5O_{12}$ garnet was found to be tetragonal, space group $I4_1/acd$, with lattice parameters a = 11.3966(6), c = 11.3369(5) Å, V = 1472.5(1) Å^3. The structure was refined to R = 5.13% using 771 independent reflections. Sodium and Mg are disordered at the X sites (with a mean bond distance of 2.308 Å for both the sites), whereas Si is ordered at both the Y (mean: 1.793 Å) and Z sites (means: 1.630 and 1.624 Å). Na-bearing majoritic garnet may be an important potential sodium concentrator in the lower parts of the upper mantle and transition zone. The successful synthesis of the $Na_2MgSi_5O_{12}$ end-member and its structural characterization is of key importance because the study of its thermodynamic constants combined with the data of computer modeling provides new constraints on thermobarometry of majorite garnet assemblages.

Keywords: Garnets, sodium, majorite, crystal structure, microprobe analysis, synthesis