*American Mineralogist, Volume 99, pages 2416–2423, 2014*

# High-pressure elasticity of sodium majorite garnet, $Na_2MgSi_5O_{12}$

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## Abstract

Garnet is the second most abundant mineral phase in the upper mantle and transition zone settings. The crystal structure of garnet is quite flexible and hence it is able to accommodate various cations, including large incompatible cation such as sodium. We used first-principles simulation based on density functional theory and two widely used approximations—local density approximation (LDA) and generalized gradient approximation (GGA)—to explore the crystal structure, equation of state, and elasticity of sodium bearing majorite garnet with $Na_2MgSi_5O_{12}$ stoichiometry at pressures relevant to the upper mantle and transition zone. We find that the pressure-volume results based on LDA can be explained by a Birch Murnaghan finite strain equation of state with $V_0$ = 1447.6 (± 0.1) Å$^3$, $K_0$ = 177.4 (± 0.4) GPa, and $K'_0$ = 3.93 (± 0.02). The results based on GGA can be explained by a Birch Murnaghan finite strain equation of state with $V_0$ = 1525.8 (± 0.2) Å$^3$, $K_0$ = 160.2 (± 0.4) GPa, and $K'_0$ = 3.96 (± 0.02). The full elastic moduli tensor for Na-majorite with tetragonal symmetry exhibits slight deviation from the cubic symmetry with $C_{11} < C_{33}$, $C_{12} \sim C_{13}$, and $C_{44} \sim C_{66}$. The magnitude of the tetragonal strain also captures the slight deviation from the cubic symmetry. At pressures corresponding to the upper mantle and mantle transition zone, the compressional wave velocity, $v_P$, and shear wave velocity, $v_S$, for the Na-majorite garnet are fast compared to a wide variety of garnets such as pyrope, grossular, almandine, and majorite garnet. Although single-crystal anisotropy of Na-majorite is greater than pyrope, it is still low compared to the major mantle phases.

**Keywords:** Elasticity, equation of state, sodium majorite, mantle transition region