American Mineralogist, Volume 102, pages 851–859, 2017

Thermo-elastic behavior of grossular garnet at high pressures and temperatures

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Abstract

The thermo-elastic behavior of synthetic single crystals of grossular garnet ($Ca_3Al_2Si_3O_{12}$) has been studied in situ as a function of pressure and temperature separately. The same data collection protocol has been adopted to collect both the pressure-volume (*P-V*) and temperature-volume (*T-V*) data sets to make the measurements consistent with one another. The consistency between the two data sets allows simultaneous fitting to a single pressure-volume-temperature Equation of State (EoS), which was performed with a new fitting utility implemented in the latest version of the program EoSFit7c. The new utility performs fully weighted simultaneous fits of the *P-V-T* and *P-K-T* data using a thermal pressure EoS combined with any *P-V* EoS. Simultaneous refinement of our *P-V-T* data combined with that of K^T as a function of *T* allowed us to produce a single *P-V-T-K*^{T} equation of state with the following coefficients:

V_0 = 1664.46(5) Å^3, K_{T0} = 166.57(17) GPa and K'= 4.96(7) $\alpha_{(300\ K,\ 1bar)} = 2.09(2)\times10^{-5}\ K^{-1}$

with a refined Einstein temperature (θ_E) of 512 K for a Holland-Powell-type thermal pressure model and a Tait third-order EoS. Additionally, thermodynamic properties of grossular have been calculated for the first time from crystal Helmholtz and Gibbs energies, including the contribution from phonons, using density functional theory within the framework of the quasi-harmonic approximation.

Keywords: Grossular, high-pressure, high-temperature, diffraction, bulk modulus, *P-V-T-K* fit, EosFit