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Equation of state of $Ca_3Cr_2Ge_3O_{12}$ garnet

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Materials of garnet-type structure are of general interest, as justified by their physicochemical properties [1]. The $Ca_3Cr_2Ge_3O_{12}$ (CCGO) germanate garnet attracts scientists' attention because of its magnetic [2,3] and dielectric [4] properties. A single crystal of $Ca^{II}_3Cr^{III}_2(GeO_4)_3$, was obtained by utilizing the flux growth method. Atoms of each of the four component elements occupy one crystallographically distinct position. In the present study, we combine the experimental in-situ high-pressure X-ray diffraction and *ab-initio* calculations for CCGO. The X-ray diffraction experiments were carried out using the angle-dispersive mode at ESRF ID15B beamline. The *ab-initio* total-energy simulations were carried out within the framework of density functional theory (DFT). in the studied pressures ranging to 9.5 GPa, the garnet crystal structure is conserved. The structure was refined using the Rietveld procedure. The experimental $V(p)$ variation was modelled through fitting the Birch-Murnaghan equation. The equation-of-state fitting result is shown in Fig. 1. The theoretical $V(p)$ variation obtained using the density functional theory is found to be in line with experimental data.

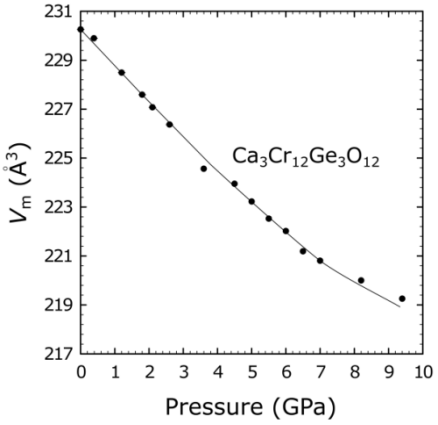

Figure 1. Unit cell volume as a function of pressure for $Ca_3Cr_2Ge_3O_{12}$. Experimental points are shown together with the result of Birch-Murnaghan equation of state fitting (solid line).

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