

## **High-pressure behavior of åkermanite and gehlenite and phase stability of the normal structure in melilites**

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### **ABSTRACT**

Åkermanite ( $\text{Ca}_2\text{MgSi}_2\text{O}_7$ ) and gehlenite ( $\text{Ca}_2\text{Al}_2\text{SiO}_7$ ) have been studied at high pressure by synchrotron radiation powder and single-crystal diffraction up to 30 GPa. At about 2 GPa, the incommensurately modulated structure (IC) transforms to a normal structure (N). The bulk modulus for the N structure, fitted with a Birch Murnaghan EoS on powder data, is 93.5(5) GPa. The compressibility is anisotropic, and it is greater along the  $c$  axis, in the direction perpendicular to the tetrahedral layers of the structure. Above 15 GPa, a phase transition is observed, marked by a discontinuity in the elastic behavior and a small change in intensity and in the full-width at half maximum (FWHM) of the powder diffraction peaks. The diffraction patterns are indexed with respect to tetragonal cell of the N-melilite structure up to 30 GPa. A hysteresis in the elastic behavior is observed during decompression. In contrast, single-crystal data show a new monoclinic phase appearing above 15 GPa. The unit-cell parameters are  $a = 8.82(1) \text{ \AA}$ ,  $b = 7.34(1) \text{ \AA}$ ,  $c = 9.13(1) \text{ \AA}$ ,  $\beta = 115.1(2)^\circ$ . This unit cell is similar to that of  $\text{Ca}_2\text{ZnGe}_{1.25}\text{Si}_{0.75}\text{O}_7$  reported in the literature. A refinement using the corresponding model in space group  $P2_1/n$  fits the single-crystal data with a reasonable  $R_{\text{Bragg}} = 15\%$ , considering that the crystal is twinned and the mosaicity is large. Gehlenite has a higher bulk modulus, 106.1(4) GPa, than does åkermanite. The compressibility is anisotropic, and the behavior is similar to that of åkermanite, but the presence of Al in tetrahedral sites decreases the compressibility parallel to the (001) plane. The structure of gehlenite is stable up to 25 GPa, when a phase transition occurs.

**Keywords:** Melilite, high pressure, single crystal, compressibility, phase transition