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LETTER

The crystal structure of gypsum-II determined by single-crystal synchrotron X-ray diffraction data

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ABSTRACT

The crystal structure of gypsum-II, a polymorph of $CaSO_4 \cdot 2H_2O$ stable above 4 GPa, has been solved using single-crystal synchrotron X-ray diffraction data collected at 5.35 and 6.74 GPa. Gypsum-II is monoclinic, space group $P2_1/n$, with lattice parameters a = 5.865(12), b = 15.045(14), c = 5.478(12) Å, β = 115.3(2)°, and V = 437.0(14) Å^3 at 5.35 GPa, and a = 5.776(2), b = 15.017(2), c = 5.473(2) Å, β = 114.98(4)°, and V = 430.3(2) Å^3 at 6.74 GPa. The crystal structure has been refined to R_1 = 3.7 (5.35 GPa) and 3.9% (6.74 GPa). It closely resembles that of gypsum at room pressure with a stacking of CaO_8 and SO_4 polyhedra along the **b**-axis to form layers. With increasing pressure, a continuous increase in distortion of the SO_4 tetrahedron and a strong change in the bonding style of the water molecules are observed. The mechanism of phase transformations previously hypothesized in gypsum, on the basis of high-pressure spectroscopic data, is here clarified for the polymorph stable between 4–8 GPa.

Keywords: Gypsum, high pressure, crystal structure, phase transition, Ca-sulfate