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Evidence for monazite-, barite-, and $AgMnO_4$ (distorted barite)-type structures of $CaSO_4$ at high pressure and temperature

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ABSTRACT

Using laser-heated diamond-anvil cells, we have observed $CaSO_4$ undergoing phase transitions from its ambient anhydrite structure to the monazite type, and at highest pressure and temperature to crystallize in the barite-type structure. On cooling, the barite structure distorts from an orthorhombic to a monoclinic lattice to produce the $AgMnO_4$-type structure. The barite-structured form of $CaSO_4$ that we encounter at high pressure and temperature has been, in particular, long expected as a high-pressure phase of $CaSO_4$-anhydrite from systematic trends of similar $A^{II}B^{VI}O_4$-type sulfates, selenates, and tellurates, but has not been observed before. Similarly, the monoclinic distortion of the barite structure has itself been proposed as an intermediate phase between anhydrite and barite types through comparison with the phase diagrams of $NaBF_4$ and $NaClO_4$. This result has important consequences for identifying structural trends between different ABO_4-type phases of Group II sulfates, selenates, tellurates, chromates, molybdates and tungstates that crystallize in anhydrite, zircon, monazite, barite and scheelite-type structures at ambient and high pressures.