

## Phase transition of partially-hydrated CePO<sub>4</sub> under high-pressure conditions

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CePO<sub>4</sub> is a dimorphic material with multiple potential applications, among which energy storage devices [1] and sensors for O<sub>2</sub>, Fe<sup>2+</sup>, Co<sup>2+</sup> and glucose.[2–6] At ambient conditions it crystallizes in both a monoclinic monazite (S.G. *P*2<sub>1</sub>/*n*) and an hexagonal structure (S.G. *P*6<sub>2</sub>22).[7] The latter polymorph mainly exist in the hydrated CePO<sub>4</sub>·*x*H<sub>2</sub>O form, being water necessary for its stabilization. The stability of the hexagonal polymorph has thus been mainly the concern of high-temperature studies, which have shown that upon annealing and water removal, hexagonal CePO<sub>4</sub> indeed collapses to the monazite structure.[8,9] Monazite CePO<sub>4</sub> has also been shown to be stable in high-pressure conditions up to at least 20 GPa [10,11] while there is a complete lack of high-pressure studies on hexagonal CePO<sub>4</sub>.

The behavior of the hexagonal polymorph under high-pressure conditions, up to 21 GPa, is presented here. A second-order phase transition to a novel polymorph is detected at a pressure of 10 GPa for hexagonal, partially-hydrated CePO<sub>4</sub>. This previously unreported high-pressure phase has a monoclinic structure with an atomic arrangement similar to that of the low-pressure phase, but with reduced symmetry, and belongs to monoclinic *C*2 space group. There is no detectable volume discontinuity at the phase transition.

Here we provide structural information on the new phase and determine the axial compressibility and bulk modulus for both phases. The compressibility is found to be anisotropic for both polymorphs and their bulk moduli is about 2/3 of that of the denser monazite phase.

In addition, the isothermal compressibility tensor for the high-pressure structure is reported at 10 GPa and the direction of maximum compressibility is calculated. The possible role of water and of the pressure medium in the high-pressure behavior is also discussed

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