High-pressure topotactic transition of layered $CsCoO_2$ to stuffed cristobalite form

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$CsCoO_2$, featuring a two-dimensional layered architecture of edge- and vertex-linked CoO_4 tetrahedra, is known to exhibit a temperature-driven reversible second-order phase transformation ($\alpha \rightarrow \beta$) at 100K, corresponding to a small structural relaxation with concurrent tilting and breathing modes of the edge-shared CoO_4 tetrahedra [1-2]. In the present investigation, we find that pressure induces another phase transition ($\beta \rightarrow \gamma$) that dramatically changes the tetrahedral connectivity to that of a three-dimensional cristobalite [3]. This new transition is strongly first order, topotactic, reversible, diffusionless, and quenchable. Using the ISODISTORT software package [4], the simplest displacive transformation pathway connecting the two phases was found to employ a common subgroup of the β-phase and γ-phase space groups.

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