

## **Orientation of channel carbonate ions in apatite: Effect of pressure and composition**

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### **ABSTRACT**

X-ray structure and FTIR spectroscopy evidence is reviewed for two separate orientations of carbonate ions in the *c*-axis channel of carbonate apatite (CHAP) synthesized at high pressure and temperature: A1 carbonate has two O atoms close to the *c*-axis, whereas A2 carbonate has only one. The A2 orientation is reevaluated and its local structure refined using a rigid body model. A2 is the high-pressure configuration, but the A1 → A2 transformation is also dependent on bulk composition, especially the presence of type B carbonate. In the dry CaO-P<sub>2</sub>O<sub>5</sub>-CO<sub>2</sub> system, the A1 → A2 transformation is initiated beyond about 4 GPa in type A CHAP compared with 1–2 GPa in A-B CHAP. Also, A2 carbonate is only weakly present in Na-bearing A-B CHAP synthesized at 0.5–1 GPa, which is assumed to be close to the threshold pressure for the transformation. The pressure stability of A2 is believed to be related to its central location in the channel and equitable distribution of bond distances to Ca<sub>2</sub> cations in the channel wall (2.25 to 2.54 Å).

**Keywords:** Apatite structure, high-pressure phase transformation, biomineralization, CO<sub>2</sub> sequestration