

## **Single-crystal X-ray diffraction study of high-pressure phases of KHCO<sub>3</sub>**

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### **ABSTRACT**

Monoclinic and triclinic high-pressure phases of KHCO<sub>3</sub> were identified using in situ high-pressure single-crystal X-ray analysis. These monoclinic and triclinic phases, designated as phases IV and V, respectively, differ from three previously identified phases: I–III. The lattices of the two phases are superimposed along  $\mathbf{a}_V^* = 2 \times \mathbf{a}_I^*$  and  $hk0$  and  $h0l$  nets of both phases lie on the same plane, i.e., the (100) plane is common in both lattices in real space. The space group of phase IV is  $P2_1/b11$  with lattice constants of  $a = 10.024(3)$  Å,  $b = 6.912(5)$  Å,  $c = 4.1868(11)$  Å,  $\alpha = 115.92(4)^\circ$ , and  $V = 260.9(2)$  Å<sup>3</sup>. The crystal structure of phase IV, excluding the hydrogen atoms, was successfully determined by direct methods and is isostructural with a cesium hydrogen carbonate CsHCO<sub>3</sub>.

**Keywords:** KHCO<sub>3</sub>, high pressure, single-crystal X-ray diffraction, hydrogen bond