

Single-crystal X-ray diffraction study of high-pressure phases of KHCO₃

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ABSTRACT

Monoclinic and triclinic high-pressure phases of KHCO₃ 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 $V = 260.9(2)$ Å³. The crystal structure of phase IV, excluding the hydrogen atoms, was successfully determined by direct methods and is isostructural with a cesium hydrogen carbonate CsHCO₃.

Keywords: KHCO₃, high pressure, single-crystal X-ray diffraction, hydrogen bond