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The structure of monohydrocalcite and the phase composition of the beachrock deposits of Lake Butler and Lake Fellmongery, South Australia

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Abstract

Samples of beachrock from Lakes Butler and Fellmongery, near Robe, South Australia, were examined by neutron and X-ray powder diffraction. Considerable variation in phase composition was observed, although all samples possessed monohydrocalcite, calcite, aragonite, and magnesian-calcite. The Rietveld refinement of the structure of monohydrocalcite showed significant changes in the orientation of water molecules and a major change in the orientation of a carbonate group with respect to the currently accepted structure. The current refinement shows that the hydrogen-bonding structure consists of three distinct networks, with each of the three carbonate groups being bonded to a single water molecule via one linear and one bifurcated hydrogen bond.

Keywords: Monohydrocalcite, carbonate minerals, magnesian-calcite, powder diffraction