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Vaterite: Interpretation in terms of OD theory and its next of kin

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Abstract

The polytypic structures of vaterite, $CaCO_3$, described in recent literature, have been reinterpreted in terms of the order-disorder (OD) theory, which allows us to explain and systematize all the observed and predicted polytypes of the mineral in a unified fashion. In terms of this theory, the structure consists of OD layers that comprise a layer of calcium coordination polyhedra and the attached halves of the standing CO_3 groups. The two-sided layer group of symmetry of the OD layer is $c2/m$, whereas the interlayer symmetry operations are three twofold rotation axes at 120° to one another, as well as a mirror plane in the common layer boundaries and partial *c* glide planes perpendicular to the boundary. Depending on the orientation of the active twofold rotation axis with respect to the above-defined layer mesh, performed independently in each stacking step, maximally ordered simple stacking sequences $P6_122$, $P6_522$, $C2/c$, $C2/c2/m2_1/m$, and a more complicated sequence $P3_12$ or $P3_22$, as well as several complicated or disordered sequences is obtained (before eventual relaxation to a subgroup of a particular space group). A perfect copy of the vaterite OD layer occurs in the structures of the bastnäsite-synchysite polysomatic series of fluorocarbonates. In these structures, the REE layers, configurationally analogous to the Ca-based OD layer, have layer symmetry $p32$ and their stacking does not lead to polytypism and OD phenomena; these are generated on the Ca-based OD layers.

Keywords: Vaterite, calcium carbonate, polytypes, OD theory