

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

**EMIL MAKOVICKY<sup>1,\*</sup>**

<sup>1</sup>Institute of Geoscience and Natural Resource Management, University of Copenhagen, Østervoldgade 10, 1350 Copenhagen, Denmark

### **ABSTRACT**

The polytypic structures of vaterite,  $\text{CaCO}_3$ , 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  $\text{CO}_3$  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  $120^\circ$  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