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The transformation of amorphous calcium carbonate, ACC, to crystalline phases as function of time and temperature.

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We present results from a structural study of the transformation of freeze dried amorphous calcium carbonate, ACC, in crystalline material using pair distribution function analysis, PDF analysis, of X-ray powder diffraction data, XPD data. PDF analysis allows for the analysis of local order of structural subunit in the range between molecular unit (1. and 2. coordination sphere) and long range periodicity as in crystalline materials.
ACC was precipitated from aqueous solutions at 298 K and 278 K using different amounts of Mg cations as stabilizer. The samples were immediately separated from the solution and freeze dried. For the transformation study, the samples were heated and analysed using XPD until they were crystallized. The radial distribution obtained from the XPD data were compared to simulated radial distributions of the calcium carbonate polymorphs and their hydrated phases.
An ACC precipitated from a solution with Ca:Mg:CO_3 = 1:5:4 at 298 K (ration in mmol, pH = 8.2) and freeze dried right after isolation from the solution revealed a close resemblance with ikaite in its local order. Another ACC with Ca:Mg:CO_3 = 1:10:1.4 (T = 298, pH = 8.7) showed distinctly different local order resembling monohydrocalcite. Both ACC, however, still had considerable amounts of water dominating the Ca-coordination sphere. During the transformation to calcite, the structural changes in the sample concerned the hydrate water coordinating Ca which was removed and replaced by the carbonate oxygens.
The study shows that ACC obtained from different starting solutions show specific local order. Freeze drying leads to solid ACC powder which still contain considerable amounts of hydrate water.
Structural subunits are distinct in ACC and different from the crystalline phase. The study supplements recent reports presented by Konrad et al., Purgstaller et al., and Tobler et al..

F. Konrad et al., Cryst. Growth Des. 16, 6310−6317(2016)
B. Purgstaller et al., Geochimica et Cosmochimica Acta 174, 180–195(2016)
DJ. Tobler et al., Cryst. Growth Des. 16, 4500−4508(2016)