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Stability, themal expansion and bulk modulus of Na-Dawsonite up to 2.9 GPa

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Dawsonite ($NaAlCO_3[OH]2$), an uncommon mineral that occurs naturally in e.g. alkaline shales and coal bearing rocks, is one of the potential candiates for mineral trapping of CO_2 in the framework of carbon capture and storage (CCS). It is assumed to precipitate from dissolution of minerals typical for deep seated saline aquifers, namely alkali feldsspar and clay minerals in the presence of Na-rich brines and elevated CO_2-concentrations.

Little is known about the thermal stability of Dawsonite at high pressure high temperature conditions comparable to the earth crust and currently no data for the thermal expansion and bulk modulus of Dawsonite are available. These data might be helpful for further thermodynamic model calculations to predict the formation and/or dissolution in a certain environment.

Na-Dawsonite was synthesized from an aqueous solution of $NaHCO_3$ and Al(OH)3 in a stainless steel autoclave at a temperature of 175 °C. X-Ray Powder diffraction revealed a single phase Dawsonite after removing excess $NaHCO_3$ with distilled water.

The thermal decomposition of the orthorhombic Dawsonite crystal structure was studied by means of in situ energy dispersive X-ray diffraction in a high pressure Multi-anvil device (MAX 80) at the Beamline F2.1 of HASYLAB, DESY, Germany in the pressure range 0.075 to 1.9 GPa. The onset temperature of the crystal structure break down showed a strong increase from 390 °C at 0.075 GPa to 540 °C at 1 GPa and remained nearly unchanged up to a pressure of 1.9. GPa.

The thermal expansion was measured at a pressure of 1.6 GPa from room temperature up to 550 °C. Although the diffraction spectra apparently remained unchanged at elevated temperatures, a detailed analysis of the lattice parameters a, b and c revealed a striking discontinuity in the temperature dependance of b and c. Between 200 °C and 250 °C the slope of both parameters change significantly, while the lattice constant a is nearly constant over the whole temperature range. This behaviour might be attributed to a so far unknown phase transition thus the calculated volumetric thermal expansion alpha = 4,07 . 10-5 K-1 is based only on data sets collected above 250 °C.

The isothermal bulk modulus K of Na-Dawsonite was calculated from the volume change of the unit cell in the pressure range 0.5 to 2.9 GPa. With K = 61 GPa the bulk modulus of Na-Dawsonite is comparable to $CaCO_3$.