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Finding the lost child of the norsethite family: $BaFe[CO_3]_2$, a new double carbonate - synthesis, structural characterisation, and geostability implications for high and low PT

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The norsethite-family is often used as a geochemical and crystl chemical analogue for the rhombohedral double carbonate system: dolomite-ankerite-kutnahorite. $BaFe(CO_3)_2$, a new ordered double carbonate is synthesized for the first time by high PT (700°C, 6 GPa) solid-state reaction [1]. The formation of $BaFe(CO_3)_2$ through solid-state reaction is apparently slower than that of $BaMg(CO_3)_2$ and $BaMn(CO_3)_2$ under the same experimental conditions. Solid products are characterized by single crystal XRD, thermogravimetric analysis, differential scanning calorimetry, electron microprobe, and Raman and FT infrared spectroscopy. The charge and spin states of Fe in the new phases is determined using Nuclear forward scattering of synchrotron radiation. The reaction from polycrystalline powders in the presence of CO_2-bearing solution in contrast to water as a flux medium indicates the $BaFe(CO_3)_2$ instability at high PT conditions. The experimentally derived phases belong to crystal structures of the R-3m and R-3C space groups, respectively. The thermodynamic properties of the double carbonate at standard conditions are estimated and a phase diagram is constructed depicting the stability field in low-temperature aqueous environments with these results being compared to natural aqueous solutions.

[1] Liang W., Peters C., Li L., Leupold O., Li H., Boettcher, M.E. (2021) $BaFe(CO_3)_2$, a new double carbonate: Synthesis, structural characterization, and geostability implications for high and low PT. Geochemistry - Chemie der Erde, on-line 1.2021