

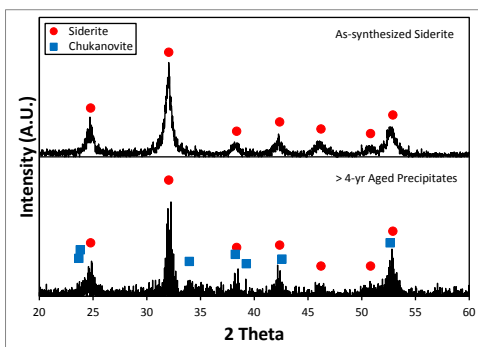
# Thermodynamic Modeling of Siderite and Chukanovite in the WIPP Relevant Brines

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## Experimental Discovery

Under anoxic conditions experimentally synthesized siderite ( $\text{FeCO}_3$ ) has been aged in brine solutions consisting of (0.15 and 1.5m) NaCl and (0.01, 0.1, 0.5, 1.0, 1.5 and 2.0m)  $\text{Na}_2\text{CO}_3$ . During the aging process we have observed decreases of pH values over the aging times, indicating precipitation of an hydroxyl-bearing phase consistent with chukanovite [1]. X-ray Diffraction (XRD) analyses of as-synthesized siderite and > 4-year-aged precipitates in sample reactors show the co-existence of chukanovite [ $\text{Fe}_2(\text{OH})_2\text{CO}_3$ ] and siderite. The analyzed XRD spectra are shown in the figure below. Our results indicate that chukanovite and siderite are in equilibrium.



## Discussion of Results

Based on this observation, we have implemented the Pitzer thermodynamic model to optimize the thermodynamic interaction factors for activity coefficient determination, and subsequently estimated the formation energy of chukanovite.

[1] from technical exchange discussion with Dr. Helge Moog at GRS in Germany.

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