

Stoichiometry effects on BaSO₄ crystallisation: Experiments and theory

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Minerals are formed by a reaction through oppositely charged ions. The crystallisation process is traditionally understood by assuming an ideal 1:1 ratio for both ions. For barite (BaSO₄) crystallisation it is often the case in natural conditions that either Ba²⁺ or SO₄²⁻ is in large surplus and many other minerals are also often formed in a non-ideal ratio. The effect of having either ion in surplus is not well understood. Besides explaining the natural crystal formation, understanding the crystallisation process is also of great interest in geothermal energy, gas, and oil industry due its undesirable scale formation enhanced by its low solubility. We studied the crystallisation process by measuring the light absorbance of solutions (UVVIS) where BaSO₄ is forming under non-ideal ratios and linking this to theory on different crystallisation steps: nucleation and growth.

The absorbance was fitted to a two-step crystallisation model, combining aspects of scattering, nucleation, and growth theory. For most cases, the fits are quite accurate and the observations are in reasonable agreement with similar experiments and modelling in literature. Stoichiometry has a large effect on both crystallisation steps. Nucleation is always inhibited by a surplus of either ion, while growth can be promoted by a small surplus of Ba²⁺. Growth does however also become inhibited for a larger surplus of Ba²⁺ or a surplus of SO₄²⁻. Overall, our methodology provides greater insight on how both nucleation and growth impact crystallisation and could be useful for examining the formation of other minerals as well.