

Barite surface reactivity in NaCl media: A CD-MUSIC model interpretation

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Barite, the most common barium-containing mineral, has been studied extensively because of industrial implications. Specifically, barite is the predominant scale-forming mineral in gas and petroleum pipelines, and thus restricts flow and adversely impacts oil production. Conversely, it is used widely in industry because of its high specific gravity, for its X-ray attenuation properties, and elements such as ²²⁶Ra may be sequestered in its structure. Consequently, numerous studies have focused on understanding barite crystal growth mechanisms, or utilizing chelating agents to inhibit scale formation. Collectively, the studies have shown that barite crystal growth is controlled by solution composition; including, ionic strength, ionic media, and the presence of competing divalent cations (i.e., Ca²⁺, Sr²⁺, and Mg²⁺). Despite these crystal growth and ion adsorption/exchange studies, the surface charging behavior of barite in aqueous solutions has not been evaluated fully. Zeta potential and isoelectric point measurements suggest an iep value for barite above pH 7.2.

The work presented here focuses on the surface charging behavior of barite in NaCl media at 0.03 and 0.3 *m* ionic strength, from 15 to 50 °C. Additionally, the adsorption of Ca²⁺ is discussed. The studies were performed using detailed potentiometric titrations, and the results were described by the CD-MUSIC model. Potentiometric titrations coupled with surface complexation models are routinely used to evaluate and describe the surface charging behavior of metal-oxide phases. The surface oxygen atoms of such phases hydroxylate readily and impart pH-dependent surface charge. However, such an approach has rarely been applied to sulfate phases. This work shows that the charging behavior of barite is minimal, the surface is slightly positively charged below pH 8, and charging increases with increasing ionic strength and temperature. Barite surface charge is also influenced by the presence of Ca²⁺ in solution.

Since the (001) surface dominates on natural and synthetic barite crystals, we constrained the CD-MUSIC model fits with molecular information for the (001) surface^[1].

^[1] Bracco, *et al.* (2017) J. Phys. Chem. C, 121, 12236.