

Synergistic incorporation of lead and selenate into barite[†]

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Barite is a common mineral phase in both natural and engineered environments and can act as a major sorbent for toxic ions in natural water due to its low solubility. The interactions of common toxic ions such as lead (Pb^{2+}) and selenate (SeO_4^{2-}) with barite are not fully understood at the molecular scale. In this work, the sorption of lead (100 μM) and selenate (0–300 μM) at water-barite (001) interface was studied at pH \sim 5.5 using *in situ* specular crystal truncation rod and element-specific resonant anomalous X-ray reflectivity. In 100 μM $\text{Pb}(\text{NO}_3)_2$ solution without selenate, lead exclusively incorporates into the outermost atomic layer of barite. In 100 μM Na_2SeO_4 solution without lead, almost no selenate sorbs at the interface. In solution containing both 100 μM $\text{Pb}(\text{NO}_3)_2$ and 30–300 μM Na_2SeO_4 , lead incorporates even deeper, i.e., down to the third atomic layer, as well as adsorbs on the surface, while selenate incorporates and adsorbs at the same depth and height as lead does, revealing a strong positional correlation between lead and selenate at the interface. As a result, we observe enhanced sorption of both lead and selenate in the binary solutions compared to solutions with only lead or selenate. We propose that this synergistic sorption may be due to the coupled exchange of lead and selenate for barium and sulfate, respectively, in the crystal structure or by a ligand (selenate) assisted dissolution and subsequent healing process at the interface. This work provides basic understanding for the behavior of barite in terms of affecting the transport of toxic ions in natural and engineered settings.

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