

Is ettringite a suitable host phase for the sequestration of Se(VI) and other harmful ions?

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Ettringite, $\text{Ca}_6\text{Al}_2\text{O}_6(\text{SO}_4)_3 \cdot 26\text{H}_2\text{O}$, forms in alkaline environments during the early hydration of Portland cements in presence of sulfate ions. Natural occurrences are rare, but ettringite crystals have been described in some geological settings such as banded weathering crusts, associated with porlandite, $\text{Ca}(\text{OH})_2$, and overgrown on thaumasite, $\text{Ca}_3\text{Si}(\text{SO}_4)(\text{CO}_3)(\text{OH})_6 \cdot 12\text{H}_2\text{O}$, or gypsum. The fact that the crystal structure of ettringite can accommodate different substituting oxyanions, some of them radioactive or toxic, explains the environmental interest of this mineral. For instance Se(VI) incorporates into ettringite substituting for sulfate in structural positions [1]. However, the extent and mixing properties of this substitution remains poorly understood. Moreover, the incorporation of substituting ions has been typically studied by performing co-crystallization experiments in which defective and low crystallinity phases are frequently obtained.

In this work we have crystallized different members of the $\text{Ca}_6\text{Al}_2\text{O}_6(\text{SO}_4, \text{SeO}_4)_3 \cdot 26\text{H}_2\text{O}$ solid solution by mixing CaO (24 mmol) and stoichiometric amounts of $\text{Al}_2(\text{SO}_4)_3$, Al_2O_3 , Na_2SeO_4 in ultrapure water in a nitrogen glove-box to minimise the CO_2 contamination. Our results indicate the presence of a wide, asymmetric miscibility gap. Moreover, the dehydration behavior is demonstrated to depend dramatically on the degree of crystallinity of the ettringite host phase. A comparison between the thermal behavior (studied by X-ray diffraction) of natural and synthetic ettringite confirms the different evolution of their crystal structures. Well crystallized natural samples were found to be stable up to 100°C , while synthetic samples lose the short-range order at about 50°C . Therefore, the thermal behavior is proved to be sensitive to the crystallization conditions and must be considered when this phase is envisioned as a potential host phase for the uptake of harmful ions.

[1] Baur & Johnson (2003) *Cement Concret Res.* **33**, 1741-1748