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Improved structural model of green rust sulfate, GR_{SO_4}

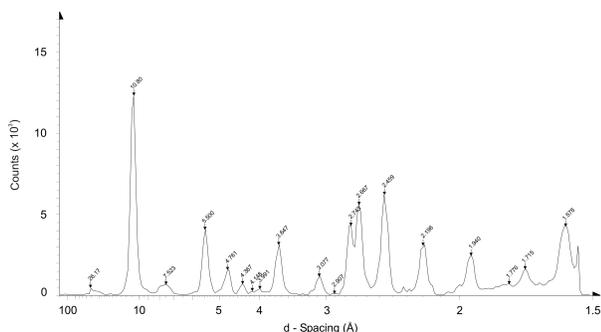
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Mobility and contaminants in groundwater and their uptake by minerals depends on surface reactivity. Transformation of a mineral to a new, often more stable phase, can alter the contaminant's behaviour. Solutions moving from reducing environments bear substantial quantities of Fe(II) and when it oxidises, a suite of very fine-grained minerals can form. A better understanding of the transformation processes of these phases will improve our ability to model the fate of reactive contaminants in nature.

Green Rust, built of brucite-type layers of Fe(II)Fe(III)-hydroxide, has anions such as sulphate, chloride and carbonate filling the interlayers to balance the charge. It also includes a number of structure water molecules. They are most commonly found in environments where redox conditions are near the Fe(II)/Fe(III) boundary, such as on corroding metal and soil. Recently developed waste management methods that use Fe(0) in reactive barriers are also certain to contain GR as one of the transition phases between the metallic iron and ferric-(hydr)oxides. GR is also believed to be an important intermediate in the oxidative transformation of Fe(II) phases, important in settings where Fe(II) concentrations are very high. It oxidises readily and can take up and immobilise (heavy metals and radioactive elements) and break down (organic) compounds.

Accurate parameters to describe solubility and structural behaviour are critical for predictive modelling. Structural models exist for GR, but recent studies suggest they are not complete or correct. Current work in an atmosphere-controlled glove box examines the role of composition on structure using capillary-tube X-ray diffraction and atomic force microscopy. It proves the role of substituting ions on structural and chemical properties.



CT-XRD trace of GR_{SO_4} made in an inert environment, showing details in the structure not observed previously.