Alternative method for interlayer water determination via cross-validated computational model

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Clay and clayey materials are commonly analyzed with XRD to determine the layer basal spacing or hydration and intercalation processes. Through the investigation of these parameters and the effect of the interlayer particles, a deeper knowledge of the long- and short-term effects of water exposure can be attained. However there are several occasions where XRD measurements are not practical or possible, hence alternatives are necessary.

In this study we examine the swelling and water uptake as a function of relative humidity (0-98% RH) and interlayer cation (Li, Na, K Cs, Mg, Ca, Cu, Sr) for homoionic montmorillonite from purified Wyoming Bentonite MX-80. This is done using FTIR-ATR, gravimetric measurements and XRD as a means to confirm the models produced.

The resulting data is used to construct numerical models to estimate water layer distribution as a function of relative humidity, with FTIR data being deconstructed using MCR-ALS calculations and the gravimetric data being fitted to a multicomponent composition of the Dubinin-Astakhov equation for micro pore adsorption of vapors.

The combination and cross-validation of these methods allow for the determination of hydration states from the individual methods, as well as open up the possibility to measure other variables otherwise undetectable such as total pore/interlayer water distribution.
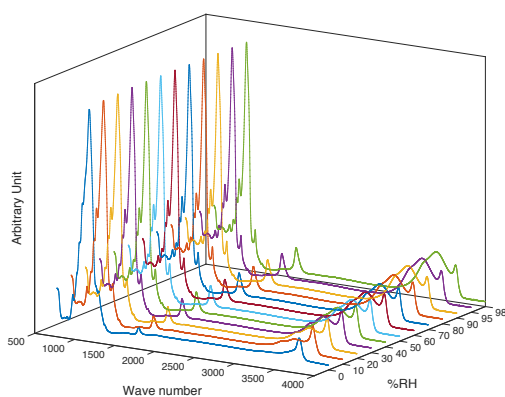
Figure 1: FTIR spectra of an adsorption series as function of %RH for homoionic Ca-montmorillonite.