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Multi-modal, micro-spectroscopic speciation of legacy phosphorus in two U.S. mid-Atlantic agricultural soils

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To understand phosphorus (P) mobility in agricultural soils and its potential environmental risk, it is essential to directly measure solid phase P speciation. Often, bulk P K-edge X-ray absorption near edge structure (XANES) spectroscopy followed by linear combination fitting (LCF) is utilized to determine the solid P phases in soil. However, this method may limit results to only a few major phases. Additionally, XANES spectra for different P species may have very similar features, leading to an over or underestimate of their contribution to LCF. Here, an improved P speciation by pairing multi-modal micro-focused X-ray fluorescence (μ-XRF) mapping coupled with μ-XANES analysis to directly speciate major and minor P phases on the micron scale is provided. We combined maps of both tender (P, S, Al, Si) and hard energy (Ca, Fe, Mn) elements to evaluate the elemental co-locations with P. To better account for uncertainty assigning XANES peaks to individual compounds, a more quantitative fingerprinting by "spectral feature analysis" was completed. With this analysis, an R-factor is reported for the fit. These results were compared to traditional LCF. Pre-edge fitting results revealed the presence of a two-component pre-edge feature for phosphate adsorbed to ferrihydrite. Additionally, phytate co-precipitated with ferrihydrite (Phytate-Fe-Cop) had a pre-edge feature, indicating direct association with Fe. Lastly, a unique P species associated with manganese oxide was identified in the soil via multi-modal mapping and μ-XANES. These results allow for better prediction of P dissolution and mobility.