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Unraveling complex <2 µm clay mineralogy from soils using X-ray diffraction profile modeling on particle-size sub-fractions: Implications for soil pedogenesis and reactivity

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Abstract

A specific methodology was developed to refine the complex clay mineralogy commonly encountered in soil environments. The soil examined was a Cambisol developed into a ferralitic paleosol. The sample was split into four sub-fractions of different particle sizes (<0.05, 0.05–0.1, 0.1–0.2, and 0.2–2 µm), and their respective mass contributions to the overall <2 µm clay fraction were determined. For each sub-fraction, X-ray diffraction (XRD) patterns were modeled using a trial-and-error approach based on the direct comparison of experimental and calculated profiles. Quantitative information derived from the fitting procedure for the different sub-fractions allowed for the determination of the complex mineralogy of the <2 µm clay fraction through the identification and quantification of eight clay phases. The results show that the finest and most reactive clay fraction (<0.05 µm) was totally hidden in the XRD pattern of the <2 µm fraction, the fraction commonly considered in soil mineralogical analyses. Similarly, this procedure revealed the presence of illite-smectite-chlorite and kaolinite-illite mixed-layer minerals seldom described in soil literature using classical methods. The use of this methodology improved our understanding of the pedogenesis of this soil through the identification and quantification of clay phases structural properties. The analysis of the evolution of structural parameters with particle size allowed for the detection of local modifications in the interlayer composition of expandable and hydroxy-interlayered vermiculite layers. Following this approach, key information can be derived to determine subtle changes in clay mineralogical composition that are related to microorganism and/or plant activity.

Keywords: Clay minerals, XRD data, crystal structure, smectite, hydroxy-interlayered vermiculite, illite, kaolinite, order-disorder, mixed-layer minerals, interstratification