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Quantifying the potential for mineral carbonation of processed kimberlite with the Rietveld-PONKCS method

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Abstract

Quantitative phase analysis (QPA) using the Rietveld method and X-ray diffraction (XRD) patterns is useful for predicting the reactivity of a rock to carbon dioxide (CO_2) and for quantifying mineral carbonation. Lizardite and smectites in kimberlite are reactive to CO_2, but they are structurally disordered and cannot be quantified using the standard Rietveld approach. In this study, the Partial Or No Known Crystal Structure (PONKCS) method was used to model the peak profiles of smectite and lizardite to account for turbostratic stacking disorder in synthetic samples of processed kimberlite. Lizardite and montmorillonite PONKCS models were made using XRD patterns collected with three X-ray diffractometers: two XRDs from the same manufacturer and of similar model (XRDs B1 and B2) and another XRD from a different manufacturer (XRD A1). Five synthetic samples of processed kimberlite of known compositions were prepared and used to test the results of these PONKCS models for data collected using all three instruments. The results provide a total bias ranging from 4.8–14.1 wt% using correctly calibrated, instrument-specific PONKCS models. We also tested the sensitivity of the PONKCS method to changes in instrument geometry: PONKCS models calibrated for one instrument (XRD B1) were used in refinements with XRD data collected on an instrument made by a different manufacturer (XRD A1), or on a similar instrument made by the same company but having a slightly different geometry (XRD B2). Results were highly inaccurate when PONKCS models calibrated to XRD B1 were used with patterns collected on XRD A1 (32.1–71.6 wt% total bias for our weighed mixtures). Our results show that the smaller differences in instrument parameters between XRD B1 and XRD B2 can also lead to inconsistent and less accurate QPA results using PONKCS (9.8–32.7 wt% total bias). Therefore, correct calibration of PONKCS models to a specific XRD instrument is required for accurate QPA and quantification of CO_2 mineralization in clay-rich rocks.

Keywords: Rietveld method, mineral carbonation, carbon mineralization, PONKCS, lizardite, smectites