Water organization in Na-saponite: An experimental validation of numerical data

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The crystal-structure and stepwise hydration behaviour of smectite as a function of relative humidity (RH) have been extensively studied by X-ray diffraction (XRD). Although powerful, XRD accounts poorly for the actual statistical positional disorder of interlayer water. Computational simulations provide relevant information by supplying detailed molecular pictures of the system. Still, relatively few studies have confronted simulation results with experimental data and existing comparisons do not allow assessing the validity of the semi-empirical atomic interaction parameters used in theoretical simulations.

Hydration behaviour of two synthetic Na-saponites with different layer charges (0.4 and $0.7/O_{10}(OH)_2$) was studied by XRD from 92% RH down to ~ 0% RH. Calculated XRD patterns were then fitted to experimental profiles to determine for each sample the RH conditions to obtain almost homogeneous mono-hydrated and bi-hydrated state. Additional neutron diffraction (ND) patterns on both H_2O and D_2O saturated specimens were used to increase the contrast of sensitivity of the modelling approach towards water. Layer thickness derived from XRD was used to constrain a simulation box for Grand Canonical Monte-Carlo simulations (GCMC-μ, V, T). The obtained density profiles of interlayer species were then introduced for calculation of XRD and ND patterns whereas water content was compared to that determined from gravimetric water sorption measurements. The proposed collation procedure between GCMC and XRD/ND methods provides a quantitative critical assessment of the numerous potentials and different models used for microscopic simulations of interlayer water.

Contrasting sources of magmatic epidote-bearing monzodiorites and tonalites, NE Brazil

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The 618 Ma Curral de Cima tonalite and the 577 Ma Lourenço monzodiorite in the eastern Alto Pajeú terrane, northeastern Brazil, are examples of magmatic epidote-bearing plutons. Both plutons carry ferrohornblende, biotite, titanite and epidote. Amphibole-rich clots (ARC) are only present in the Curral de Cima tonalite; co-magmatic dioritic enclaves are present in the Lourenço pluton. Major, trace and isotope chemistry suggest that the major rocks of the two plutons probably followed similar differentiation trends but formed from protoliths derived from age and compositionally different source rocks. Whole-rock and mineral chemistries of the two plutons have similar yet very distinct evolution trends in variation diagrams, with almost no overlap. The mineral phases and the predominantly metaluminous nature of the Curral de Cima tonalite, the presence of ARC, and obvious juvenile component (average $\varepsilon Nd = -3.55$; average $^{87}Sr/^{86}Sr = 0.7083$; $T_{DM} = 1.36$ Ga), all point to an I-type source for these rocks. These data together with high calculated $\delta^{18}O$ (whole rock) (10.0‰) for the tonalite and high $\delta^{18}O$ value for an ARC (9.3‰) are compatible with the hypothesis that ARC represent fragments of an hydrothermally altered metabasaltic source rock. On the other hand, average $\delta^{18}O$ (whole rock) for the Lourenço monzodiorite is 7.8‰, average $^{87}Sr/^{86}Sr = 0.7083$, εNd (0.57Ga) values are strongly negative (average -14.6), and $T_{DM} = 1.92$ Ga. These data are compatible with long residence time and probably reflect a mixture of igneous sources (Neoproterozoic juvenile magma) and ancient radiogenic Mesoproterozoic crust as source rock.