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Investigation of dioctahedral smectite hydration properties by modeling of X-ray diffraction profiles: Influence of layer charge and charge location

Eric Ferrage,[1,2,*] Bruno Lanson,[1] Boris A. Sakharov,[3] Nicolas Geoffroy,[1] Emmanuel Jacquot,[2] and Victor A. Drits[3]

[1]Environmental Geochemistry Group, LGIT—Maison des Géosciences, Joseph Fourier University—CNRS, BP53, 38041 Grenoble cedex 9, France
[2]ANDRA, Parc de la Croix Blanche, 1-7 rue Jean Monnet, 92298 Châtenay-Malabry cedex, France
[3]Geological Institute, Russian Academy of Sciences, 7 Pyzhevsky Street, 109017 Moscow, Russia

Abstract

Hydration of the <1 μm size fraction of a high-charge montmorillonite (Clay Minerals Society Source Clay SAz-1), and of low- and high-charge beidellites (Source Clays SbId-1 and SbCa-1, respectively) was studied by modeling of X-ray diffraction patterns recorded under controlled relative humidity (RH) for Sr- and/or Ca-saturated specimens. The influence of layer charge and charge location on smectite hydration was studied. Distribution of layers with different hydration states (dehydrated–0W, monohydrated–1W, bihydrated–2W, or tri-hydrated–3W) within smectite crystals often leads to two distinct contributions to the X-ray diffraction pattern, each contribution having different layer types randomly interstratified. Structure models are more heterogeneous for beidellite than for montmorillonite. For beidellite, two distinct populations of particles with different coherent scattering domain sizes account for the heterogeneity. Increased hydration heterogeneity in beidellite originates also from the presence of 0W (non-expandable) and of 1W layers under high relative humidity (RH) conditions. Similarly, after ethylene-glycol (EG) solvation, some beidellite layers incorporate only one plane of EG molecules whereas homogeneous swelling was observed for montmorillonite with the systematic presence of two planes of EG molecules.

For montmorillonite and beidellite, the increase of layer charge shifts the 2W-to-1W and the 1W-to-0W transitions toward lower RH values. For all samples, layer thickness of 0, 1, and 2W layer types was similar to that determined for low-charge SWy-1 montmorillonite (Source Clay SWy-1), and no change of layer thickness was observed as a function of the amount or of the location of layer charge. However, layer thickness increased with increasing RH conditions.

Keywords: XRD data, Smectite, hydration, phyllosilicate, interstratification, montmorillonite, beidellite, layer charge