Interlayer water structure in Na-, K- and Cs-birnessite

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Birnessite (Bi) is a major oxide mineral of manganese nodules found on the ocean floor. It is a layer-type mineral composed of Mn octahedral sheets with monovalent cations (Na^+, K^+ and Cs^+) intercalated. However, the low crystallinity and fine-grained size of natural birnessite limit full characterization of the structure, particularly water structure in the interlayer which greatly impacts the mineral reactivity for metal sorption. In this study, we investigated the interlayer structures of Na-, K- and Cs-Bi using classical molecular dynamics (MD) simulations. While the *d*-spacing of Na-Bi was greater than that of K-Bi in experiments, our MD simulations calculated the *d*-spacing of K-Bi greater than that of Na-Bi. MD simulations with variations in the water content suggest that a much greater water content in Na-Bi is required to be consistent with experimental results, indicating large uncertainties in the interlayer water content. When the water content increased up to a buserite type mineral, MD simulations found an abrupt expansion of the *d*-spacing along with increased disorder in the orientations of the water molecules. We discuss the effects of the interlayer water structure on the *d*-spacing of birnessite.

Keywords: Birnessite, Molecular dynamics simulation, Manganese, Interlayer, water content

