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Local structure determination of Zn-smectite

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Abstract

An aluminum-free zinc-bearing smectite (Zn-smectite) was synthesized under hydrothermal conditions, together with its magnesium substituted products. Its layer charge calculated by cation exchange capacity (CEC) is 117.4 mmol/100 g. Powder X-ray diffraction (XRD) revealed turbostratic stacking and showed that the d_{06l} value of the Zn-smectite was >1.525 Å, indicating that it is trioctahedral. Its d_{001} value increased from ca.12.8 Å to ca. 16.0 Å after ethylene glycol (EG) saturation. The Zn-smectite did not irreversibly collapse after heating the Li^+-saturated sample to 300 °C, suggesting that its layer charge was generated from octahedral-site vacancies (defects). The Zn-smectite resembles zincsilite-like minerals with interlayer Na^+ and Zn^{2+}. The intralayer structure of zincsilite was confirmed by pair distribution function (PDF) analysis, and the whole crystal structure was built and optimized by DFT calculation in the CASTEP module of the Materials Studio software. Synthetic zincsilite is triclinic, space group $P\bar{1}$, and its optimized unit-cell parameters are: a = 5.294 Å, b = 9.162 Å, c = 12.800 Å, α = 90.788°, β = 98.345°, and γ = 90.399°.

Keywords: Smectite, layer charge, local structure, turbostratic disorder, PDF