American Mineralogist, Volume 89, pages 102–109, 2004

Dehydration dynamics of bikitaite: Part II. Ab initio molecular dynamics study

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Abstract

High-temperature behavior and the process of thermal dehydration in the natural zeolite bikitaite have been studied by ab initio molecular dynamics simulations, and favorably compared with the X-ray powder diffraction data presented in Part I of this work (Ferro et al. 2003). The microscopic dynamical behavior of the extraframework species (water molecules and Li cations) has been characterized as a function of temperature. Two regimes have been detected, and the transition is characterized by the breaking of the one-dimensional water chain typical of bikitaite at room temperature. The elementary steps for the diffusion of water inside the bikitaite channels have been studied by means of a rare-events-sampling technique (Bluemoon Ensemble). The activation free-energy for a site-to-site water jump has been calculated and a mechanism for the dehydration process is proposed.