American Mineralogist, Volume 93, pages 1191–1194, 2008

LETTER

A P_{H_2O}-dependent structural phase transition in the zeolite natrolite

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ABSTRACT

The crystal structures of natrolite and its dehydrated high-temperature phases (α1- and α2-metanatrolite) have been determined from powder X-ray diffraction measurements as a function of temperature and partial pressure of water (P_{H_2O}) to characterize the phase transition behavior. The evolution of crystal structure as a function of temperature shows two different phase transitions, depending on the P_{H_2O}, with α1-metanatrolite occurring at elevated P_{H_2O} and α2-metanatrolite occurring at low P_{H_2O}. Our discovery of α2-metanatrolite implies the existence of more than one transition mechanism, which we correlate with the migration of Na^+ ions and the *rate* of evolution of H_2O molecules. The transition behavior is rationalized in terms of two cooperating mechanisms: (1) dehydration-induced processes, which determine the phase transition temperature; and (2) thermally induced processes, which determine how the framework and its extraframework cations are modified.

Keywords: Phase transition, natrolite, crystal structure, Rietveld refinement, TGA