

Heat capacity and thermodynamic functions of partially dehydrated sodium and zinc zeolite A (LTA)

**MATTHEW S. DICKSON¹, PETER F. ROSEN¹, GRACE NEILSEN^{1,†}, JASON J. CALVIN¹,
ALEXANDRA NAVROTSKY², AND BRIAN F. WOODFIELD^{1,*}**

¹Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602, U.S.A.

²School of Molecular Sciences and Center for Materials of the Universe, Arizona State University, Tempe, Arizona 85281, U.S.A.

ABSTRACT

Zeolite A (LTA) is an industrially important zeolite that exhibits sorption-induced framework flexibility, the thermodynamics of which are poorly understood. In this work, we report heat capacity measurements on zinc and sodium zeolite A from 1.8 to 300 K and compare the heat capacity of water in sodium zeolite A with that of water in other zeolites. The heat capacity of zeolitic water varies significantly depending on the hydration level and identity of the host zeolite, and more tightly bound water exhibits strong inflections in its heat capacity curve. This suggests a combination of effects, including differences in water-framework binding strength and hydration-dependent flexibility transitions. We also report fits of the heat capacity data using theoretical functions, and we report values for $C_{p,m}^{\circ}$, $\Delta_0^{\dagger}S_m^{\circ}$, $\Delta_0^{\dagger}H_m^{\circ}$, and Φ_m° from 0 to 300 K. These results contribute to a systematic thermodynamic understanding of the effects of cation exchange, guest molecule confinement, and sorbate-dependent flexibility transitions in zeolites.

Keywords: Zeolite, framework flexibility, gate opening, zeolitic water, heat capacity