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Chabazite: Energetics of hydration, enthalpy of formation, and effect of cations on stability

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ABSTRACT

The stability of synthetic cation-exchanged zeolites having the chabazite framework (CHA) and their cation-water interaction were studied using high-temperature reaction calorimetry. Four cations (K, Na, Li, and Ca) were exchanged into CHA. The enthalpies of formation were determined for all samples, and the partial molar enthalpy of hydration was measured by varying the water content of one Ca-CHA.

The enthalpy of formation depends strongly on the exchanged cation, becoming more exothermic in the order Ca, Li, Na, K. The integral hydration enthalpy does not depend strongly on the nature of the cation, but becomes slightly less exothermic with increasing aluminum content. For the one Ca-CHA studied in detail, the average enthalpy of hydration is –34.6 ± 1.2 kJ/mol relative to liquid water. A quadratic fit to the transposed temperature drop data gives $\Delta \bar{h}_{H_2O} = -52.97 (\pm 4.74) + 2.94 (\pm 0.68)$ n (kJ/mol), where $\Delta \bar{h}_{H_2O}$ is the partial molar enthalpy of hydration and n is the number of water molecules per 24 oxygen formula.