Dehydration and Formation Enthalpy of Mg, Ca, Sr, Ba-exchanged Zeolite Beta

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Zeolite beta (BEA) is a high silica zeolite with large pores and is important as a potential catalyst in the petrochemical industry due to its high acidity and peculiar pore system. Cationic variants of zeolite beta (Mg-BEA, Ca-BEA, Sr-BEA and Ba-BEA) were prepared via aqueous ion exchange. The hydrated samples were achieved by equilibrating with saturated Ca(NO3)2 solution which provides 50% humidity at room temperature. The dehydrated samples were achieved with a degassing process in a Micromeritics Surface Area Analyzer (ASAP 2020). High-temperature oxide melt solution calorimetry determined the dehydration enthalpy and the formation enthalpy from the constituent oxides. The total enthalpies of dehydration (per mole of water as well as per mole of framework tetrahedra) of the alkaline earth cation exchanged zeolites have similar values. This suggests the interplay of the effects related to alkali earth cation concentration and to size. The enthalpies of formation from oxides generally become more exothermic with decreasing average ionic potential as has been observed in several other zeolites. Materials Studio software (Accelrys Inc.) was used to investigate location of the alkaline earth cations and bonding of water molecules in BEA zeolites.