Energetics of the Microporous Oxides, $Na_{2-y}M_yNb_{2-x}Ti_xO_{6-x}(OH)_x \cdot H_2O$ (M = Li, Sr, Ca, Mg, Y, Cu, Ni)

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A system of microporous oxides, called SOMS (Sandia Octahedral Molecular Sieves), has shown excellent selectivity for ion exchange and removal of radioactive ions like Sr_2 from nuclear wastes and hard ions like Mg_2 and Ca_2 from industrial waste streams and ground water. These oxides have the general composition $Na_2Nb_{2-x}TixO_{6-x}(OH)_x \cdot H_2O$ [1]. On heating, they lose water to form the corresponding perovskite phase, $Na_2Nb_{2-x}Ti_xO_{6-0.5x}$. We have previously compared the stabilities of the microporous and the perovskite phases for different values of x [2].

Currently, we are investigating the energetics of $Na_2Nb_{2-x}TixO_{6-x}(OH)_x \cdot H_2O$ (x = 0.4) ion-exchanged with various monovalent, divalent and trivalent cations. Using high temperature oxide melt solution calorimetry to determine the enthalpies of formation, We show that the ion-exchanged SOMS is less stable, with respect to the enthalpy of formation from oxides, than the parent SOMS. The destabilization is least for SOMS substituted with divalent cations Sr, Ca and Mg. This suggests that the effectiveness of ion exchange may be kinetically controlled.

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[2] H. Xu, A. Navrotsky, M. Nyman, T.M. Nenoff, *J. Mater. Res.* **20**, 618 (2005).