Prototype Sandia Octahedral Molecular Sieve (SOMS)
Na$_2$Nb$_2$O$_6$$\cdot$H$_2$O: Synthesis, Structure and
Thermodynamic Stability

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A new microporous phase Na$_2$Nb$_2$O$_6$$\cdot$H$_2$O, which transforms to NaNbO$_3$ perovskite on
heating, has been synthesized by the hydrothermal method. Rietveld analysis of powder
synchrotron X-ray diffraction data reveals that the structure comprises a framework of [NbO$_6$]
and [NaO$_6$] octahedra with other Na$^+$ being located in the channels (space group C2/c, a =
17.0511(9) Å, b = 5.0293(2) Å, c = 16.4921(6) Å, β = 113.9422(2)). This phase belongs to the
recently synthesized Sandia octahedral molecular sieves (SOMS) family, Na$_2$Nb$_{2-x}$M$_{x}$O$_6$$\cdot$H$_2$O
(M = Ti, Zr) and is the archetype for the substituted structures. Using drop-
solution calorimetry into molten 3Na$_2$O-4MoO$_3$ at 974 K, the enthalpies of formation of Na$_2$
Nb$_2$O$_6$$\cdot$H$_2$O from the constituent oxides and from the elements have been determined to be
$-295.4$ ± $4.8$ and $-2895.5$ ± $6.4$ kJ/mol, respectively. From the drop-solution calorimetric
data for Na$_2$Nb$_2$O$_6$$\cdot$H$_2$O and its dehydrated perovskite phase, the enthalpy of the dehydration
reaction, Na$_2$Nb$_2$O$_6$$\cdot$H$_2$O $\rightarrow$ 2NaNbO$_3$ + H$_2$O, has been derived, and its implications for phase
stability are discussed.