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Vibrational Spectroscopy of Hydrated MOH⁺ Clusters BRETT MARSH, JONATHAN VOSS, JIA ZHOU, ETIENNE GARAND, Univ of Wisconsin, Madison — Hydrated metal ions have importance in a number of fields of chemistry including environmental chemistry, biological chemistry, and catalysis. Although the aqua complexes of transition metals are well studied there is a dearth of information on hydroxide containing metal clusters which have been implicated in catalytic mechanisms of water oxidation. In this work we use cryogenic ion vibrational spectroscopy (CIVS) to interrogate clusters of the form $MOH(H_2O)_n^+(M=$ Fe, Co, Ni, Cu, Zn) in the hydride stretching region (2400-3800 cm⁻¹). Comparison of the spectral data to density functional theory calculations allow for unambiguous assignment of the observed spectral features. The resulting spectra show both a metal dependent and size dependent shift of the hydroxide stretching frequency in all clusters. The spectra also reveal that the first solvation shells of Fe, Co, Cu, and Zn containing clusters are composed of 4 ligands while the first solvation shell in Ni clusters is at least 6 ligands. This is markedly different from previous work on $Ni(H_2O)_n^+$, $Cu(H_2O)_n^+$, and $Zn(H_2O)_n^+$ cluster in which the first solvation shells are 4 ligands, 2 ligands, and 3 ligands respectively. Aspects of hydration in the second solvation shell of these clusters will also be discussed.

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