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Vibrational Characterization of the Hydrogen Bonding Network of a Microsolvated Ruthenium Polypyridyl Electrocatalytic Water Oxidation Intermediate ERIN DUFFY, JONATHAN VOSS, ETIENNE GARAND, Univ of Wisconsin, Madison — Detailed molecular-level understanding of the electrocatalytic mechanism of homogeneous water oxidation remains elusive due to the difficulty of studying reaction intermediates by traditional analytical methods. Our experimental apparatus combines an electrospray ionization source, two cryogenic ion traps, and a time-of-flight photofragmentation infrared spectrometer for the controlled formation and vibrational interrogation of solvated ionic clusters. We have utilized this approach to acquire infrared spectra of stepwise-solvated $[Ru(tpy)(bpy)(OH)]^{2+}$ (tpy = 2,2′;6′,2”-terpyridine, bpy = 2,2′-bipyridine), an electrochemical intermediate of the well-known molecular catalyst, $[Ru(tpy)(bpy)(OH_2)]^{2+}$. Through comparison with the spectra of microsolvated $[Ru(tpy)(bpy)(OH_2)]^{2+}$, insights into the role of the hydrogen bonding network on catalytic structure and activity, specifically proton-coupled electron transfer (PCET), will be discussed.

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