

ELECTRONIC SPECTRA OF BARE AND SOLVATED RUTHENIUM POLYPYRIDINE COMPLEXES

SHUANG XU, *JILA and Department of Physics, University of Colorado at Boulder, Boulder, CO, USA*;
JAMES E. T. SMITH, J. MATHIAS WEBER, *JILA and the Department of Chemistry and Biochemistry,*
University of Colorado-Boulder, Boulder, CO, USA.

We present work on a prototypical water oxidation catalyst, namely the aqua-complex $[(\text{bpy})(\text{tpy})\text{Ru}-\text{OH}_2]^{2+}$ (2,2'-bpy = bipyridine, tpy = 2,2':6',2''-terpyridine), and its hydrated clusters $[(\text{bpy})(\text{tpy})\text{Ru}-\text{OH}_2]^{2+} \cdot (\text{H}_2\text{O})_n$, with $n = 1 - 4$. This complex is the starting species in a catalytic cycle for water oxidation. We couple electrospray ionization mass spectrometry with laser spectroscopy to circumvent challenges that arise in reactive solutions from speciation. Here, we report the electronic spectrum of $[(\text{bpy})(\text{tpy})\text{Ru}-\text{OH}_2]^{2+}$ by photodissociation spectroscopy of mass selected, cryogenically prepared ions, and we examine effects of its microhydration environment on its electronic structure. In particular, we investigate the solvatochromic shift of the spectral envelope upon sequential addition of water molecules up to the tetrahydrate.