

Ruthenium and Osmium Complexes with Ligands Capable of Proton Coupled Electron Transfer

Jared J. Paul, Department of Chemistry, Villanova University

In many reactions of biological and chemical interest, electron transfer events are accompanied by changes in proton content. Our lab is interested in synthesizing metal complexes with ligands that have proton transfer capabilities, enabling us to study how the protonation state affects the electronic structure of these complexes. We have synthesized a series of metal complexes containing hydroxy-substituted-polypyridyl ligands, most notably $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)]^{2+}$ ($\text{bpy} = 2,2'$ -bipyridine, $\text{bpy}(\text{OH})_2 = 4,4'$ -dihydroxy-2,2'-bipyridine), illustrated below. These complexes have been studied by x-ray crystallography, UV/Visible spectroscopy, electrochemistry and computational methods. Upon deprotonation, the Metal to Ligand Charge Transfer transition of $[\text{Ru}(\text{bpy})_2(\text{bpy}(\text{OH})_2)]^{2+}$ red shifts as the deprotonated ligand mixes with the metal center, resulting in new mixed Metal-Ligand to Ligand Charge Transfer transitions. The absorbance spectrum of the complex varies as a function of polarity and hydrogen-bonding ability of the solvent.

