

Abstract Submitted
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Gas-phase infrared spectroscopy of ionic uranyl coordination complexes¹ DAVID MOORE, UC Berkeley, ANITA GIANOTTO, Idaho National Lab, NICK POLFER, FOM Institute for Plasma Physics, JOS OOMENS, FOM Institute for Plasma Physics, MIKE VAN STIPDONK, Wichita State University, GARY GROENEWOLD, Idaho National Lab — The uranyl dication (UO_2^{2+}) is the primary carrier of uranium in environmental and biological systems, yet relatively little is known about its chemical properties. Mass spectrometric studies have confirmed that the properties, and in particular the reactivity of the uranyl center is rather dependent on its coordination environment. The current study uses IRMPD spectroscopy of ionic uranyl complexes, recorded using a free-electron laser coupled to an FTICR mass spectrometer, to investigate the effects of cluster size and composition on the infrared spectra. The central observation from the current study is that the asymmetric uranyl stretch is quite sensitive to the coordination environment, showing clear, reproducible, incremental redshifts as the number and electron donating ability of the ligands is increased. These spectral trends are accurately reproduced by computed frequencies from DFT calculations. Results from complexes containing anionic ligands are also presented, and are consistent with the presence of a significant barrier to electron transfer within the complexes.

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