Spectroscopy and Structure of the Simplest Actinide Bonds

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Understanding the influence of electrons in partially filled f- and d- orbitals on bonding and reactivity is a key issue for actinide chemistry. This subtle question can be investigated using a combination of well-defined experimental measurements and high-level theoretical calculations. Gas phase spectroscopic data are particularly valuable for the evaluation of theoretical models. Consequently, the primary objectives of our research program are to obtain gas phase spectra for small actinide and lanthanide compounds. Development of the tools for recording such spectra is also a component of this endeavor. To complement the experimental effort we are investigating the potential for using relativistic ab initio calculations and semi-empirical models to predict and interpret the electronic energy level patterns for f-element compounds.

Multiple resonance spectroscopy and jet cooling techniques are being used to unravel the complex electronic spectra of Th and U compounds. Recent results for the oxides, sulfide and halides will be discussed. Systematic errors in the accepted values for the ionization energies have been discovered, and the patterns of electronic states for these molecules provide information concerning the occupation of the 5f orbitals and their participation in bond formation.

Date: Friday, December 8, 2017
Time: 11:00 a.m. to 12:00 p.m.
Location: AHC3–205, MMC (Live)
Marine Sciences Building Room 105 (MSB-105) – BBC (via Polycom)