Glenn T. Seaborg Center Seminar

Wednesday, August 11, 2010
4:00 - 5:00 pm
Building 70A, Room 3377

Part I. Evaluating Covalency in a Series of Organometallic Lanthanide and Actinide Coordination Complexes with Unsupported Metal-Metal Bonds

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For generations, synthetic inorganic chemists have developed theories of chemical bonding through the study of molecular metal-metal bonds. Yet among the abundance of known bonds between metals spanning most of the Periodic Table, relatively few have been reported involving the actinide elements. In our work, reactions of $(CpSiMe_3)_3M$ (M = Ce, Nd, U) with $(Cp^*Al)_4$ or Cp^*Ga ($Cp^* = C_5Me_5$) afforded the isoelectronic, isostructural complexes $(CpSiMe_3)_3M–ECp^*$ (M = Ce, Nd, U; E = Al, Ga) The U complexes were isolated as crystalline solids and were characterized by multiple solution and solid-state physical methods. The lanthanide complexes were observed by variable-temperature ^1H NMR spectroscopy but were not isolated. Results from a comprehensive thermodynamic analysis indicate that Cp*E ligands are excellent actinide/lanthanide discriminators, particularly for single donor-atom ligands.

Part II. DFT Investigation of Trivalent f-Block Metal Complexes with Weakly-Binding Metalloligands

Jamin L. Krinsky
Molecular Graphics and Computation Facility, University of California, Berkeley

Complexes of heavy, open-shell ions displaying weak metal-ligand bonding interactions still present a formidable challenge to current computational methods. This part of the seminar will focus on the use of density functional theory in the modeling of trivalent f-block species, specifically in the context of their bonding interactions with the monovalent group 13 dative metalloligands CpE (Cp = cyclopentadienyl, E = Al, Ga). Electronic contributions to Ln-E and An-E bonding will be explored, as well as the feasibility of using simplified model systems to predict the binding strengths observed experimentally and those for which no experimental data are available. Topics to be covered include the selection of appropriate computational methods, differences in the behavior of Ln vs. An centers toward dative coordination of CpE, and trends in Ln-E interaction strengths.

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