



Glenn T. Seaborg Center Seminar

Structural And Thermodynamic Description of Actinide and Lanthanide Compounds in Solution Site

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Commissariat a l'energie d'atomique, Marcoule

Thursday, September 11, 2008

4:00 - 5:00 pm

Building 70A, Room 3377

The presentation will contain two main parts:

A description of the team LCAM (Laboratoire de Conception des Architectures Moléculaires) in the CEA Marcoule (France). This research group focuses its efforts on the chemistry of f-elements to enhance the knowledge at molecular scale with both a theoretical (quantum chemistry and molecular dynamics) and an experimental approach. A set of equipments linked with glove boxes is available in the laboratory LN1 in the ATALANTE facility to access to fundamental molecular data, to geometric and electronic structures and to the speciation in the chemical systems of interest.

Examples of studies related to actinide separation by liquid-liquid extraction processes. The complexity of biphasic chemical systems makes their description difficult. A prerequisite for the modelling of the thermodynamic properties is the identification of stable species in organic phases. The interactions of metallic ions with chelating systems are at the core of our research, but the influence of the extended surroundings can be an important aspect of a successful separation. Besides the speciation, measurements are carried out to obtain the thermodynamic properties related to the complexation and extraction equilibriums.