THE CHEMICAL PROPERTIES OF EUROPIUM AND AMERICIUM

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To support on-going experimental research directed towards the separation of actinides and lanthanides from nuclear waste, theoretical studies on the molecular chemistry of representative elements from these families have been initiated. Ionization potentials, optical spectra (including $f \rightarrow f$ transitions), and chemical affinities for chloride are compared for isoelectronic cations of Eu and Am. Comparisons are made with experimental data. Multi-configuration SCF and configuration interaction (CI) methods were implemented utilizing ab-initio averaged relativistic effective core potentials (AREPs), spin orbit operators (SOs), and cc-pVDZ Gaussian basis sets to represent valence orbitals. The basis sets were optimized for a balanced representation of the +2 and +3 oxidation states. The importance of utilizing so-called small core AREPs, allowing the outermost occupied s, p and d valence electrons to be included explicitly in the ab-initio calculations, will be discussed. Calculations of each of the above chemical properties will be contrasted at various levels of computational sophistication, in particular, the effects of including SO within the valence electrons as well as the number and type of configurations included in the CI. Because of the size and computational complexities associated with such large-scale ab-initio SOCI calculations on systems with many open shells, parallel processing codes are critical to effective implementation.