

Thermochemistry and Structural Properties of Extracting Agents for Separations of Lanthanides and Actinides

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The correlation consistent Composite Approach (ccCA) has been a very successful approach for the prediction of thermochemical properties of main group and transition metal species. Recently, we have developed composite strategies for the heavy elements (*f*-ccCA). We apply these strategies, as well as density functional theory to the study of lanthanide- and actinide-containing compounds. Both *f*-ccCA and density functional theory have been utilized to predict thermodynamic properties, and density functionals have been used for structural analysis.