Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Energetic Lanthanide Complexes: Coordination Chemistry and Explosives Applications VIRGINIA MANNER, BEAU BARKER, ERIC SANDERS, KENNETH LAINTZ, BRIAN SCOTT, DANIEL PRESTON, MARY SANDSTROM, BETTINA REARDON, Los Alamos National Laboratory — Metals are generally added to organic molecular explosives in a heterogeneous composite to improve overall heat and energy release. In order to avoid creating a mixture that can vary in homogeneity, energetic organic molecules can be directly bonded to high molecular weight metals, forming a single metal complex with Angstrom-scale separation between the metal and the explosive. To probe the relationship between the structural properties of metal complexes and explosive performance, a new series of energetic lanthanide complexes has been prepared using energetic ligands such as NTO (5-nitro-2,4-dihydro-1,2,4-triazole-3-one). These are the first examples of lanthanide NTO complexes where no water is coordinated to the metal, demonstrating novel control of the coordination environment. The complexes have been characterized by X-ray crystallography, NMR and IR spectroscopies, photoluminescence, and sensitivity testing. The structural and energetic properties are discussed in the context of enhanced blast effects and detection. Cheetah calculations have been performed to fine-tune physical properties, creating a systematic method for producing explosives with "tailor made" characteristics. These new complexes will be benchmarks for further study in the field of metalized high explosives.

Virginia Manner
Los Alamos National Laboratory

Date submitted: 20 Dec 2012 Electronic form version 1.4