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Gas-Phase Ion-Neutral Reactions of Cerium Cluster Ions with Deuterium.[1] MANUEL MANARD, Special Technologies Laboratory, PAUL KEMPER, University of California, Santa Barbara, RUSTY TRAINHAM, Special Technologies Laboratory, PETER ARMENTROUT, University of Utah, Salt Lake City, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — The gas-phase interactions of cerium cluster cations and deuterium neutrals have been investigated using a temperature-dependent reaction cell embedded between two quadrupole mass analyzers. Ce_m^+ (m = 1 – 20) have been generated with our instrumentation and evidence for reaction of these clusters with D_2 to form cerium-deuterium adducts has been obtained. No evidence for fragmentation of cerium clusters via reaction with D_2 was found. Accordingly, rate constants for the reaction of Ce_m^+ with D_2 to form $Ce_mD_{2m}^+$ (m = 1 – 3) products have been acquired as a function of temperatures ranging from approximately 235 – 515 K. Arrhenius analysis of the data indicate activation energy barriers exists along the potential energy surfaces (PESs) for the reaction of Ce_2^+ and Ce_3^+ with D_2, while a negative temperature dependence is observed for the rate constants of the Ce^+/D_2 reaction. Electronic structure calculations were performed using density functional theory (DFT) to characterize all reactant and product species. This combination of experimental and theoretical results suggest the cerium cluster ions dissociate the deuterium sigma bond to form Ce^+-D bonds in an overall exothermic process. Preliminary data for extending these methods to larger cerium clusters is also presented.

[1]Site-Directed Research and Development (SDRD), Mission Support Test

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