

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

On the Aluminum Cluster Superatoms acting as Halogens and Alkaline-earth Metals DENNIS E. BERGERON, PATRICK J. ROACH, A. WELFORD CASTLEMAN, Department of Chemistry and Physics, The Penn State University, College Park PA, 16802, NAICHE O. JONES, J. ULISES REVELES, SHIV KHANNA, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284 — It is shown that a new class of super-polyhalides can be formed by combining the Al_{13} super-halogen with the conventional halogen, I. Experimental reactivity studies demonstrate that the new super-polyhalides, $\text{Al}_{13}\text{I}_x^-$, exhibit pronounced stability for even numbers of I atoms. Theoretical investigations probing the geometry and the electronic structure reveal that the enhanced stability is associated with pairs of I atoms occupying the on-top sites around the Al_{13}^- core. We also demonstrate another series, $\text{Al}_{14}\text{I}_x^-$, that exhibits stability for odd numbers of I atoms. It is shown that this series can be described as consisting of an $\text{Al}_{14}\text{I}_3^-$ core upon which the I atoms occupy on-top locations around the Al atoms. The potential synthetic utility of superatom chemistry built upon these motifs will be addressed.

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Date submitted: 28 Nov 2005

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