

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

On the Reactivity of $\text{Al}_{13}\text{I}_n^-$ and $\text{Al}_{14}\text{I}_n^-$ Clusters with Methanol¹ M.B. ABREU, A.C. REBER, S.N. KHANNA, Department of Physics, Virginia Commonwealth University — Al_{13} and Al_{14} cluster anions act as halogen or alkaline earth superatoms respectively when bound by I atoms. $\text{Al}_{13}\text{I}_2^-$ and $\text{Al}_{14}\text{I}_3^-$ have enhanced resistance to oxidation by oxygen because of the clusters' closed electronic shells, however the reactivity of aluminum clusters with methanol depends on the presence of complementary active sites. We have examined the reactivity of $\text{Al}_{13}\text{I}_n^-$ and $\text{Al}_{14}\text{I}_m^-$ with methanol to identify if the presence of electronegative Iodine may induce active sites on the cluster. The presence of a single Iodine atom on Al_{13}^- is insufficient to activate the cluster, however two adjacent ligands induce an active site and makes the cluster highly reactive. The $\text{Al}_{14}\text{I}_m^-$ clusters are found to be reactive with methanol highlighting the importance of geometric shell closures in ligand protected clusters.

¹We gratefully acknowledge financial support from Air Force Office of Scientific Research (AFOSR) through grant #FA9550-09-1-0371.

M.B. Abreu
Department of Physics, Virginia Commonwealth University

Date submitted: 13 Nov 2011

Electronic form version 1.4