

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

On the superhalogen character of Al₁₃ in Al₁₃I⁻ N.O. JONES, T. MORISATO, S.N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, D.E. BERGERON, A.W. CASTLEMAN, Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802 — It is shown that the reaction of aluminum cluster anions with HI in molecular beams leads to the generation of Al_nI_m⁻ clusters. The stability of the clusters, examined by reacting the cluster products with oxygen, led to the observation of a magic cluster corresponding to the composition Al₁₃I⁻. Ab initio calculations indicate that the cluster features a structurally unperturbed Al₁₃⁻ icosahedric core with I occupying an on-top site. An examination of the electronic charge density indicates a region of high charge density on the aluminum vertex opposite from the I atom. As we discuss, this ionically bound magic cluster can be understood by considering that Al₁₃ has an electronic structure reminiscent of a halogen atom. Comparisons to polyhalides are shown to provide a sound explanation for our chemical observations. *Supported by DOE Grant No. DE-FG02-02ER46009

S.N. Khanna
Department of Physics, Virginia Commonwealth University, Richmond, VA 23284

Date submitted: 26 Nov 2004

Electronic form version 1.4