Abstract Submitted for the MAR12 Meeting of The American Physical Society

Breaking Carbonyl Bonds in Formaldehyde via Complementary Active Sites¹ SHIV N. KHANNA, ARTHUR C. RE-BER, Department of Physics, Virginia Commonwealth University, W. HUNTER WOODWARD, JORDAN C. SMITH, A. WELFORD CASTLEMAN JR., Departments of Chemistry and Physics, Pennsylvania State University — We had recently shown that the complementary active sites in homonuclear clusters may stimulate the breaking of polar bonds enabling an atomic level control of reactivity. However, such bond cleavage has only been observed in hydroxyl bonds. In this work, we present experimental and theoretical evidence that demonstrates that the stronger C=O carbonyl bond of formaldehyde is split by complementary active sites on size selective aluminum cluster anions. The resonance structure in which the carbonyl is reduced to a single bond is stabilized by the paired active sites establishing the potential use of these geometrically driven centers in devising precursors for synthesizing chemicals or radicals that might find use in production of fine chemicals.

¹We gratefully acknowledge financial support from Air Force Office of Scientific Research through grants #FA9550-10-1-0071 and FA9550-09-1-0371.

Arthur Reber VCU

Date submitted: 16 Nov 2011 Electronic form version 1.4