Abstract Submitted for the GEC07 Meeting of The American Physical Society

Dissociative Electron Attachment to C_2HCl^1 V. NGASSAM, A.E. OREL, Department of Applied Science, University of California Davis — Studies of dissociative electron attachment (DEA) to acetylene have shown a dramatic effect as a function of bending the molecule. We have begun an investigation of such multidimensional effect on mono-chloro substitute of hydrocarbons. This work concentrates on chloroacetylene. We study the system in limited dimensionality (*i.e.* as a diatomic) and then contrast this with multidemension studies. We perform electron scattering calculations using the complex Kohn variational method to determine the resonance parameters of this system. The results show a two low lying resonance state of Σ and Π symmetry. Resonant potential energy surfaces are then constructed as a function of the Cl–C and C–C internuclear distances as well as the Cl–C angle. Stretching the C–H distance does not significantly the position and shape of the resonance states, thus the problem is reduced to 3 active degrees of freedom and the DEA dynamics can be study. The time dependent wave packet method is used to solve the one dimension problem and the Multi-Configuration Time-Dependant Hartree method is used for wavepacket propagation on the computed resonant potential energy surfaces in three-dimension. We discuss the mechanisms leading to dissociation into the product channels and report the computed DEA cross sections.

¹This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Chemical Sciences and the National Science Foundation, PHY-05-55401.

Valery Ngassam Department of Applied Science, University of California Davis

Date submitted: 15 Jun 2007

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