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Fragmentation of Small Molecules by Photo-Double Ionization[1]

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Molecular structure, formation, breakup pathways and recombination formed the subject of many theoretical and experimental studies. Among molecular species like H_2, CO, N_2, O_2 recently great attention has been paid to the dynamics of the fragmentations and rearrangements of C_2H_2 molecule. Nature's smallest stable hydrocarbon, the symmetric linear acetylene molecule, C_2H_2, is an important polyatomic system for the study of photo initiated processes. Important features of the intramolecular dynamics in neutral acetylene have been revealed over many years through numerous spectroscopic studies. More recently, the availability of synchrotron radiation and intense laser sources has lead to intriguing studies of the ionization, isomerization and breakup dynamics of acetylene ions. Of particular interest are the yields into the symmetric (CH^+/CH^+), deprotonation (HCC^+/H^+) and quasi-symmetric (HHC^+/C^+) channels, the latter involving isomerization from the neutral acetylene structure into the vinylidene configuration prior to breakup. One expects that the products of dissociation, their kinetic energy releases (KER) and the isomerization times will depend on the particular initial electronic states of the dication involved, but such detailed information has heretofore not been available. We will present the results of the experiment where the dication of acetylene is prepared by Auger decay following core-level X-ray photoionization. Cold Target Recoil Ion Momentum Spectroscopy technique was used to measure the corresponding 3d momentum vectors of Auger electrons and recoil ions in coincidence. We will show that this experimental approach, in combination with *ab initio* quantum mechanical calculations, can yield a comprehensive map of the two-body dissociation pathways including transition through different electronic energy surfaces, barriers to direct dissociation and the associated rearrangement channels. Work done in collaboration with T. Rescigno, T. Weber, S. Miyabe, M. Hertlein, B. Feinberg, M. Prior, and A. Belkacem, Lawrence Berkeley National Laboratory; T. Jahnke, O. Jagutzki, L. Schmidt, M. Schöffler, L. Foucar, S. Schössler, T. Havermeier, S. Voss, and R. Dörner, Institut fur Kernphysik, J. W. Goethe-Universitat Frankfurt am Main; A. Landers, Auburn University, Alabama; A. Alnaser, Kansas State University; and L. Cocke, Kansas State University.

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