

Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Imaging Molecular Isomerization Using Molecular-Frame Photoelectron Angular Distributions¹ T.N. RESCIGNO, LBNL, A.E. OREL, NICOLAS DOUGUET, UC Davis — Techniques such as X-ray diffraction and ultrafast electron diffraction can potentially be taken to the time domain to image chemical reactions on their natural timescale. Photoelectron diffraction from fixed-in-space molecules, where an electron is launched from an inner shell by photoabsorption, offers a similar promise. We illustrate the idea here with the results of *ab initio* calculations using the complex Kohn variational method of molecular-frame photoelectron angular distributions (MFPADs) on the acetylene monocation (HCCH^+). Photoionization of neutral acetylene, which is linear at equilibrium, in the 20-40 eV range produces ground (X) and excited (A) HCCH^+ in roughly equal amounts. The electronically excited A-state cation can follow a downhill path to a conical intersection with the X-state near a trans-symmetric geometry and from there to a vinylidene (H_2CC) isomeric structure. We will show that the MFPADs produced by C k-shell photoionization of HCCH^+ , while relatively insensitive to the electronic configuration of the valence electrons at a given photoelectron energy, are much more sensitive to nuclear geometry and can therefore be used to track the acetylene to vinylidene isomerization.

¹Work performed under auspices of US DOE by LBNL and supported by OBES Division of Chemical Sciences.

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Date submitted: 24 Jan 2012

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