Molecules Illuminated from Within: Photoelectron diffraction from light molecules fixed in space

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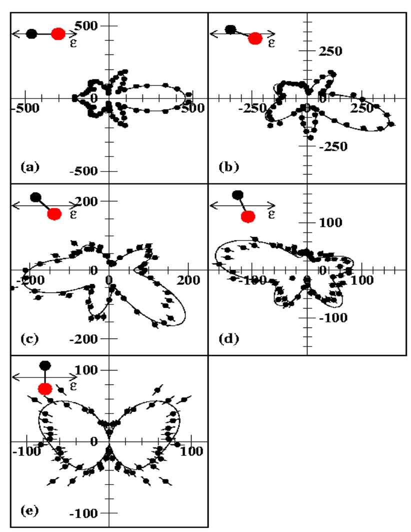
The goals of this aspect of the JRM program are to explore the dynamics of photoelectron emission from and the instantaneous structure of small molecules. We measure the diffraction patterns of photoelectrons issuing from core photoionization of fixed-in-space light molecules. The electron emanates from a known site within the molecule and "illuminates" the structure from within. The diffraction patterns are shaped by the interaction of the electron with the instantaneous potential presented by the remaining nuclei and electrons of the molecule. The data provide an extremely comprehensive picture of the diffraction patterns, which in turn probe the overall charge density distribution within the molecule at the time of photoelectron emission. The experiments also provide information on the subsequent modes of breakup of the doubly-charged molecule. The experiments are carried out at the Advanced Light Source (ALS) on beamlines 4.0 and 9.3.2. The K shells of the target molecules (CO, N_2, C_2H_n) are photoionized slightly above threshold. The molecule subsequently undergoes Auger decay, and the doubly charged molecule dissociates. COLTRIMS techniques are used to measure the coincident photoelectron and two charged molecular fragments. The charged products are projected by an electric field onto the surfaces of time- and position-sensitive multichannelplate detectors, and their full coincident momentum vectors are reconstructed on an event-by-event basis. The molecule is "fixed in space" on an *a posteriori* basis, assuming a radial two-body dissociation. Further information on this project is provided in the research summaries.

A representative result for CO is shown in the figure to the right, where angular distributions of photoelectrons are plotted in the laboratory-fixed coordinate system with the linear polarization of the light parallel to the x-axis, and for various orientations of the molecule with respect to the polarization vector. The photon energy is 10.2 eV above the C-K edge, near the maximum of the well-known f-wave sigma shape resonance for this molecule. The f-wave character of the distribution is evident in the upper left-hand figure. The resonance is clearly weaker for the lowest figure (molecule perpendicular to polarization).



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