

Abstract Submitted
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Understanding the lack of site-specificity in molecular inner-shell photofragmentation¹ LINDA YOUNG, Argonne National Laboratory, LUDGER INHESTER, Center for Free-Electron Laser Science, BART OOST-ENRIJK, Lund University, MINNA PATANEN, ESKO KOKKONEN, University of Oulu, STEPHEN SOUTHWORTH, CHRISTOPH BOSTEDT, Argonne National Laboratory, OKSANA TRAVNIKOVA, TATIANA MARCHENKO, MARC SIMON, Sorbonne Universites, UMPC, ROBIN SANTRA, SANG-KIL SON, Center for Free-Electron Laser Science, STACEY SORENSEN, Lund University — In many cases fragmentation of molecules upon inner-shell ionization loses the specificity associated with the initially localized ionization site. Often this is interpreted in terms of an equilibration of internal energy into vibrational degrees of freedom after Auger decay. Here we investigate the x-ray photofragmentation of ethyl trifluoroacetate, the iconic ESCA molecule, upon core electron ionization at environmentally distinct carbon sites using photoelectron-photoion-photoion coincidence measurements and ab-initio electronic structure calculations. For all the 4 carbon ionization sites, the Auger decay weakens the same bonds and transfers the two charges to opposite ends of the molecule, which leads to a rapid dissociation into 3 fragments followed by further fragmentation steps. The lack of site-specificity is attributed to the character of the dicationic electronic states after Auger decay, instead of a fast equilibration of internal energy.

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