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An unambiguous signature in molecular frame photoelectron angular distributions of core hole localization in fluorine K-edge photoionization of CF_4[1] C. W. MCCURDY, T. N. RESCIGNO, Lawrence Berkeley Natl Lab, C. S. TREVISAN, California State University, Maritime Academy , R. R. LUCCHESE, Texas AM University — Molecular Frame Photoelectron Angular Distributions (MFPADs) are calculated using the Complex Kohn variational method for core-hole ionization of the carbon and fluorines in CF_4 at photoelectron energies below 15 eV. The angular distributions for localized versus delocalized core-hole creation on the four equivalent fluorines are radically different. A strong propensity for the dissociation to take place via the mechanism $h\nu + CF_4 \rightarrow CF_4^+ + e^- \rightarrow CF_3^+ + F(1s^{-1}) \rightarrow CF_3^+ + F^+ + 2e^-$ in which a core excited neutral fluorine atom ionizes during or after dissociation creates the conditions for experimental observation of core hole localization. Comparison with recent unpublished experiments at the Advanced Light Source that measured the Recoil Frame Photoelectron Angular Distributions (averaged over CF_3 rotations around the recoil axis) for fluorine K-edge ionization gives unambiguous evidence that these experiments directly observed the creation of an almost completely localized core hole on the dissociating fluorine atom when the molecule was initially photoionized.

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