$_4$ at the Cl 2p-edge

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Theoretical and Experimental Search for Evidence of Core Hole Localization in X-ray Photoionization of CCl[1] C. S. TREVISAN, California State University Maritime Academy, Vallejo, CA, T. N. RESCIGNO, Lawrence Berkeley National Laboratory, Berkeley, CA, C. W. MCCURDY, University of California, Davis, CA and Lawrence Berkeley National Laboratory, Berkeley, CA, B. GAIRE, Lawrence Berkeley National Laboratory, Berkeley, CA, I. BEN-ITZHAK, Kansas State University, Manhattan, KS, R. DOERNER, Goethe-Universitaet, Frankfurt am Main, Germany, TH. WEBER, Lawrence Berkeley National Laboratory, Berkeley, CA — Recently, unambiguous evidence of core hole localization in X-ray photoionization of CF_4 at the F K-edge was found in the combination of theoretical and experimental determinations of the recoil frame photoelectron angular distributions (RFPADs). In that case, detection of the $CF_3^+ + F^+$ fragments following Auger decay in coincidence with the photoelectron verified that the observed RFPAD arose from ionization of the fluorine atom that was ultimately detected as F^+ [Phys. Rev. A 95, 011401(R) (2017)]. Similar theoretical calculations of RFPADs for ionization of CCl_4 at the Cl 2p L-edge using the Complex Kohn variational method are compared here with COLTRIMS measurements of RFPADs for this case. The localization effect that is evidently related to the strong electronegativity of the F atom was predicted to occur in the case of chlorine which is slightly less electronegative. We explore the comparison of calculated RFPADs from close-coupling calculations for various polarization directions with observations in the $CCl_3^+ + Cl^+$ decay channel to search for evidence of the same effect in this system.

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