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Diffraction effects in the Recoil-Frame Photoelectron Angular Distributions of Halomethanes

Cédric Bomme^{*1}, Denis Anielski^{*,†}, Evgeny Savelyev^{*}, Rebecca Boll^{*,†}, Benjamin Erk^{*}, Sadia Bari^{*}, Jens Viehhaus^{*}, Mauro Stener[‡], Piero Decleva[‡] and Daniel Rolles^{*,§2}

^{*} Deutsches Elektronen-Synchrotron(DESY), Hamburg, Germany

[†] Max-Planck-Institut f. Kernphysik, Heidelberg, Germany

^{*}European XFEL GmbH, Hamburg, Germany

[‡]Universita' di Trieste, Trieste, Italy

[§]J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, KS, USA

Synopsis We have measured the Recoil Frame - Photoelectron Angular Distributions (RF-PADs) for inner-shell photoionization of CH₃F, CH₃I and CF₃I halomethane molecules for photoelectron energies up to 300 eV detected within a 4 π solid angle in the gas-phase. For high kinetic energies, the RF-PADs are dominated by diffraction effects that encode information on the molecular geometry.

Recoil frame - photoelectron angular distributions supply deep insights into the molecular photoionization process and provide access to an unparalleled level of detailed information such as phases of photoelectron waves [1, 2], localization of core holes [3], and double-slit interference [4, 5]. RF-PADs can also be interpreted in terms of photoelectron diffraction [6, 7] and direct information on the geometric and electronic structure of the molecule can be obtained, e.g., by comparing the measured diffraction patterns and RF-PADs to single and multiple scattering calculations [8, 9, 10, 11, 12].

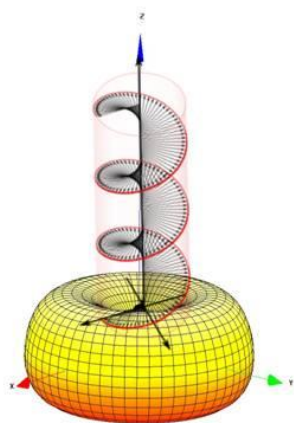


Figure 1: RF-PADs after $F(1s)$ photoionization of CH₃F at 875 eV photon energy, i.e. 180 eV photoelectron energy. Light propagation axis and molecular F-C axis are parallel.

For high kinetic energies of 50 eV and above, the RF-PADs contain diffraction effects that encode information on the molecular geometry in the RF-PADs. In order to illustrate this in more detail, we are comparing our experimental results to single and multiple scattering calculations similar to those used in earlier studies [10, 11, 12] and to DFT calculations [13, 14].

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¹E-mail: cedric.bomme@desy.de

²E-mail: daniel.rolles@desy.de