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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 Viefhaus[*], Mauro Stener[ʃ], Piero Decleva[ʃ] and Daniel Rolles[*,$2]

[*] Deutsches Electronen-Synchrotron(DESY), Hamburg, Germany

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

[•]European XFEL GmbH, Hamburg, Germany

[ʃ]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 CH_3F, CH_3I and CF_3I halomethane molecules for photoelectron energies up to 300 eV detected within a 4π 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].

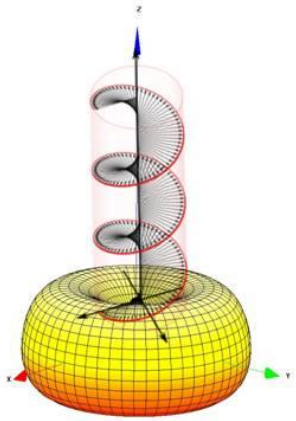

Figure 1: *RF-PADs after F(1s) photoionization of CH_3F at 875eV photon energy, i.e. 180eV photoelectron energy. Light propagation axis and molecular F-C axis are parallel.*

For high kinetic energies of 50eV 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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[1]E-mail: cedric.bomme@desy.de
[2]E-mail: daniel.rolles@desy.de