ESRF	**Experiment title:** Investigating the Compton Effect in Nitrogen in reference to the molecular frame outside the Impulse Approximation	**Experiment number**: CH-5524
Beamline: ID31	**Date of experiment**: from: 13 Aug 2018 to: 28 Aug 2018	**Date of report**: 18/02/2020
Shifts: 18	**Local contact(s)**: Jakub Drnec	*Received at ESRF:*

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Report:

In this beamtime, we measured high-energy photoionization and Compton scattering at N_2 in the gas phase using a portable COLTRIMS Reaction Microscope end-station which we brought from Frankfurt University. This technology allowed us for the first time ever to measure, from each individual ionized molecule, the momenta of the emitted electrons and ions in coincidence at such a high photon energy. The beamtime was highly successful, we succeeded in the detection of a multitude of reactions: First, we observed Compton scattering at the *K*-shell followed by Auger decay and Coulomb explosion of the N_2^{2+} ion. We detected the resulting Auger electron in coincidence with the two ionic N^+ fragments. Second, we observed photoionization of *K*-shell electrons which is also followed by an Auger decay and a Coulomb explosion. We again detected the Auger electron and the ionic fragments. A multitude of interesting phenomena can be extracted from our measured dataset. In particular for photoionization at the present high photon energies, we already published two papers in Physical Review Letters from the data from this one week of beamtime:

Phys. Rev. Lett. **123**, 193001 (2019): *Photon-Momentum-Induced Molecular Dynamics in Photoionization of N_2 at hν=40 keV*

> We investigate K-shell ionization of N_2 at 40 keV photon energy. Using a COLTRIMS reaction microscope, we determine the vector momenta of the photoelectron, the Auger electron and both N^+ fragments. These fully differential data show that the dissociation process of the N_2^{2+} ion is significantly modified not only by the recoil momentum of the photoelectron but also by the photon momentum and the momentum of the emitted Auger electron. We find that the recoil energy introduced by the photon and the photoelectron momentum is partitioned with a ratio of approximately 30:70 between the Auger electron and fragment ion kinetic energies, respectively. We also observe that the photon momentum induces an additional rotation of the molecular ion.

Phys. Rev. Lett. **123**, 243201 (2019): *Recoil-Induced Asymmetry of Nondipole Molecular Frame Photoelectron Angular Distributions in the Hard X-ray Regime*

We investigate angular emission distributions of the 1*s* photoelectrons of N_2 ionized by linearly polarized synchrotron radiation at hν = 40 keV. As expected, nondipole contributions cause a very strong forward-backward asymmetry in the measured emission distributions. In addition, we observe an unexpected asymmetry with respect to the polarization direction, which depends on the direction of the molecular fragmentation. In particular, photoelectrons are predominantly emitted in the direction of the forward nitrogen atom. This observation cannot be explained via asymmetries introduced by the initial bound and final continuum electronic states of the oriented molecule. The present simulations assign this asymmetry to a novel nontrivial effect of the recoil imposed to the nuclei by the fast photoelectrons and high-energy photons, which results in a propensity for the ions to break up along the axis of the recoil momentum. The results are of particular importance for the interpretation of future experiments at x-ray free electron lasers operating in the few tens of keV regime, where such nondipole and recoil effects will be essential.

We got some more yet unpublished preliminary results from the beamtime.

At these high photon energies, the dipole approximation for photonionization does not hold any more. The photon momentum plays a significant role in the processes (as discussed in the two publications above). The photon momentum is imparted onto the sum momentum of the ionic fragments. Interestingly, the mean sum momentum of the ions is backward-directed, i.e. the mean value is in the opposite direction of the photon momentum. Accordingly, the mean value of the photoelectron momentum is forward-shifted along the photon momentum direction. We clearly observe this in Fig. 1.

Status of this result: Paper for submission to PRL in preparation.

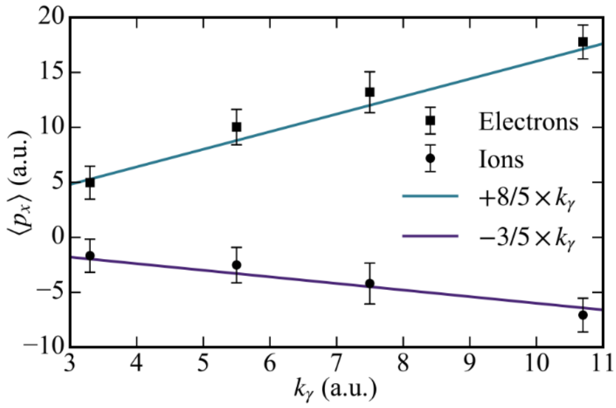

Fig. 1 – Mean electron and ion sum momentum in photon direction. The lines are taken from Chelkowski et al. Phys. Rev. Lett. ***113****, 263005 (2014).*

For Compton scattering we reached a real breakthrough and could measure for the first time Compton scattering from a fixed-in-space molecule (Fig. 2).

We are currently collaborating with the leading theory group in the field, Fernando Martin, Madrid on that topic. More work is needed, in particular we aim for another beamtime after the shutdown to extend this to the H_2 molecule which is currently the only molecule that is theoretically tractable in full detail.

Status of this result: Further beamtime needed after shutdown.

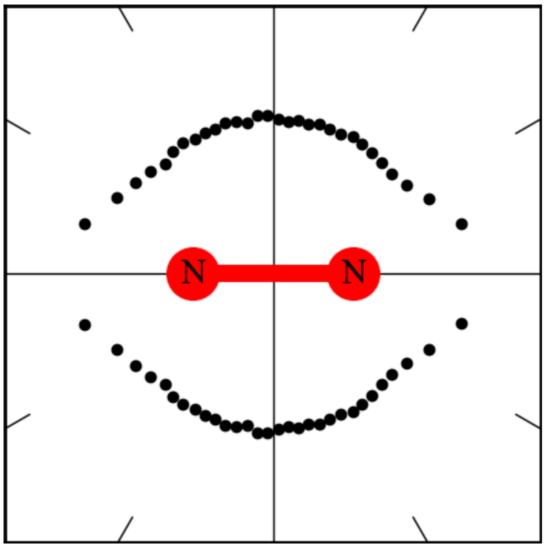

Fig. 2 – Molecular-frame Compton electron angular distributions. The Compton distribution clearly follows the molecular axis.