

# Molecular-Frame Photoelectron Angular Distributions of OCS Molecules

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Molecular-frame photoelectron angular distributions (MFPADs) provide deep insights into the molecular photoionization process that give access to an unprecedented level of detailed information such as phases of photoelectron waves [1, 2], localization of core holes [3], and double-slit interference [4, 5]. When interpreting MFPADs in terms of photoelectron diffraction [6, 7], direct information on the geometric and electronic structure of the molecule can be obtained, e.g., by comparing the measured diffraction patterns and MFPADs to multiple scattering calculations [8, 9, 10, 11].

We have determined the MFPADs of sulphur 2p and oxygen 1s photoelectrons from OCS molecules at beamline BW3 at DORIS by means of angle-resolved photoelectron-photoion coincidence spectroscopy. Our measurements extend existing experimental data [10, 11] to higher photoelectron kinetic energies of up to 70 eV in order to allow a more systematic comparison to theory. Fig. 1 shows exemplary experimental results for a relatively low photoelectron kinetic energy in comparison to the results from multiple scattering calculations. The calculations are similar to those used in earlier studies [10, 11] but were extended to include angular averaging effects due to the non-perfect alignment of the molecules.

These experimental and theoretical studies are a part of our effort to perform time-dependent photoelectron diffraction experiments at Free-Electron Lasers.

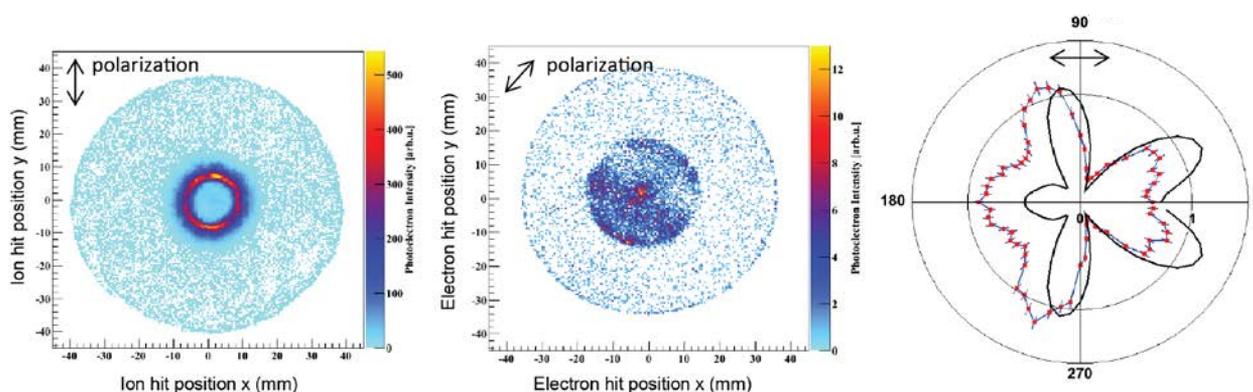


Figure 1: Photoion and photoelectron angular distributions after O(1s) photoionization of OCS molecules at 555 eV photon energy. *Left*: Ion detector image for O<sup>+</sup> fragment ions emitted parallel to the detector plane. *Middle*: Electron detector image of photoelectrons detected in coincidence with O<sup>+</sup> fragment ions emitted along the light polarization direction. *Right*: Polar plot of the experimentally determined molecular-frame photoelectron angular distribution (symbols) of 15 eV photoelectrons compared to the results of a multiple scattering calculation (solid line). Light polarization and molecular axis are along the horizontal axis.

## References

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