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Vibrationally resolved B 1s photoionization cross section of BF₃

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Synopsis We present a study of the vibrationally resolved B 1s photoionization cross section of the BF₃ molecule. A combination of high-resolution photoelectron spectroscopy measurements and of state-of-the-art calculations shows the evolution of the photon energy dependence of the cross section from a complete trapping of the photoelectron wave (low energies) to oscillations due to intramolecular scattering [1, 2]. These diffraction patterns allow to access structural information of both the neutral molecule and the core-hole species generated upon photoabsorption [3].

The advent of third-generation synchrotron radiation facilities, in combination with high energy-resolution detection techniques, has opened the way for the investigation of vibrationally-resolved inner-shell photoionization in small molecules, where an electron is emitted from a 1s orbital of a first-row atom. We present a study on B 1s photoionization of BF₃, comparing experimental results with full first-principle calculations and showing that the most relevant features can be understood by means of simple models.

In order to calculate vibrationally-resolved cross sections, we have evaluated (bound and continuum) electronic wave functions using the static-exchange and the time-dependent DFT methods [4], developed by Decleva and collaborators, for different molecular geometries along the totally symmetric stretching mode. This mode is the most affected by the structural rearrangement accompanying core ionization [1, 2]. Our theoretical results are in good agreement with experimental measurements from SOLEIL synchrotron and, at high energies, qualitatively agree with a first-Born approximation model.

We have found that the relative cross sections show clear oscillations in the high-energy region as a function of photoelectron momentum which are due to an intramolecular scattering mechanism: in its way out of the molecule, the photoelectron is diffracted by the surrounding atomic centers, encoding the geometry of the molecule [1, 2, 3]. Very close to the photoionization threshold a complete trapping of the photoelectron is observed, manifesting itself

as an emission angle dependent shape resonance feature [1, 2].

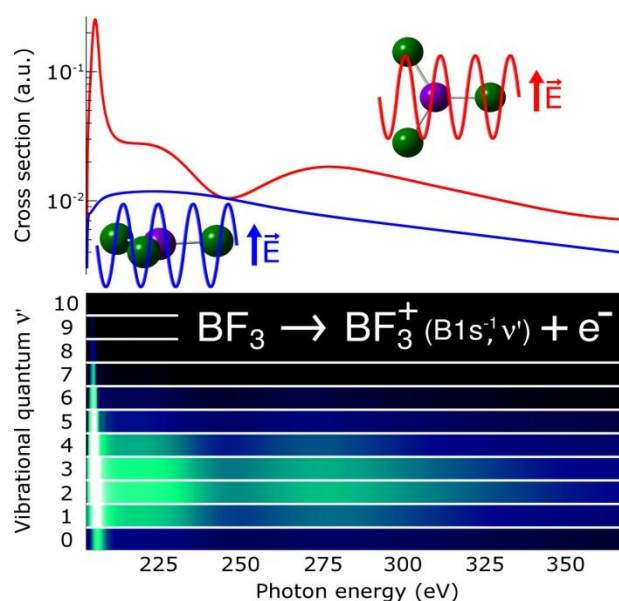


Figure 1. Calculated cross section (upper panel) for different molecular orientations and vibrationally resolved cross section in the totally symmetric stretching mode (lower panel) for the case of randomly oriented molecules.

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