



Electron-electron coincidence measurements of solvated molecules with a liquid micro-jet device.

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Synopsis Thanks to a magnetic bottle time-of-flight multi-electron spectrometer, we have filtered out the O 1s Auger spectra of the liquid phase and the gas phase in a liquid micro-jet environment. Interesting results are also shown in the C 1s case for a few benchmark molecules.

X-ray Photoelectron Spectroscopy (XPS) has proven to be a powerful asset for surface studies [1]. It is also emerging as the adequate choice to study biological samples [2], especially with the increasing use of liquid micro-jet on synchrotron beamline. These new set-ups can help us to understand the energy transfer processes between organic molecules and the solvent, just after inner-shell ionization.

In this study, we used a new electron time-of-flight magnetic bottle spectrometer [3] [4]. It is composed of two parts: a permanent magnet (B~0.7T) which is placed just beneath the liquid micro-jet and a 1.2 m long flight tube, with a solenoid wrapped around (B~1mT), with a reduce entrance ($\Phi=5\text{mm}$) to allow differential pumping (the vapor pressure around the liquid jet is in the 10^{-4} hPa range). When the Synchrotron light ionizes the molecules in the liquid jet, the electrons are driven by the magnetic field towards the flight tube and detected at the end by a micro-channelplate detector. Their energies are derived from the electrons' time-of-flight.

We studied a 1 molar sodium benzoate solution on the PLEIADES beamline (SOLEIL, France) in the liquid micro-jet. As a first example, we studied the O 1s photoelectron to probe the liquid-gas interface. We have recorded the coincidences between the O1s photoelectrons, and the subsequent Auger and we plot the corresponding two-dimensional map (fig1).

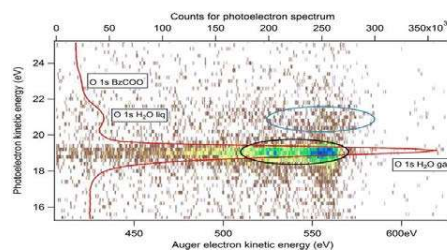


Fig 1: Overlap of two-dimensional electrons coincidence map and XPS spectrum.

Coincidence “islands” allow us to correlate the energies of these two electron types. By projecting the data on the y axis, we obtain the photoelectron spectrum (red curve). In this spectrum we observe three peaks corresponding to contributions from O1s of the gaseous water, the “liquid” water, and the solvated molecule. This first result can be followed by data filtering. In our events, we can separate in the Auger spectra the contribution from gas and liquid phases. We also applied the same coincidence method to other solvated molecules just above the C1s ionization threshold. For a given carbon site, we recorded the corresponding filtered Auger spectra. These spectra are different but, without any strong theoretical support, it is difficult to identify the final states of the solvated dications produced after Auger decay. Such experimental results will provide a severe test for theories.

[1] Siegbahn K 1970, *Phil. Trans. Roy. Soc. Lond. A*, **268**, 33-57

[2] Brown M A *et al* 2013, *Nano. Lett.*, **13**, 5403–5407

[3] Penent F *et al* 2005, *Phys. Rev. Lett.*, **95**, 083002

[4] Pohl M N *et al* 2017, *J. Phys. Chem. B*, **121**, 32, 7709–7714

