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# Attosecond Core-level Photoemission Delays of Organic Molecules

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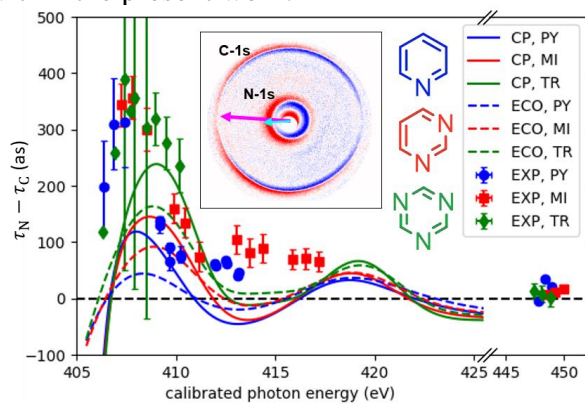
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**Synopsis** We performed angular streaking of the core-shell ionization using the attosecond XLEAP mode of LCLS, determining the relative delays between N-1s and C-1s photoionization for pyridine, pyrimidine, and 1,3,5-triazine on a dense energy grid.

We conducted attosecond angular streaking on the K-shell photoionization of a series of azabenzene (pyridine, pyrimidine, and 1,3,5-triazine) to study the inner-shell electron dynamics of the typical building blocks of biochemical molecules and drugs. The core electrons are ionized by the attosecond soft-X-ray pulses from the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory [1], and the photoelectron momentum is modulated by a co-propagating femtosecond IR dressing field (1300 nm) which encodes the ionization time to the angular distribution into the velocity-map-imaging (VMI) detector perpendicular to the light-propagation direction [2]. The relative photoionization delays between N-1s and C-1s have been measured at photon energies ranging from 400-450 eV. In this energy range, the C-1s delays are negligibly small because of the high kinetic energy of the electrons. The dependence of measured time delays on the molecular structure is interpreted by comparison with our theoretical calculations.

Figure 1 compares the retrieved experimental time delays between N1s and C1s shells (EXP, the error bars correspond to 95% confidence interval) with the computed N1s photoionization time delays (with the Coulomb-laser coupling time delay added). The calculations used the equivalent-core (ECO) method with the optional addition of a correlation potential (CP). Results were obtained for pyridine (PY), pyrimidine (MI), and 1,3,5-triazine (TR), whose chemical structures are presented in the corresponding colors in Fig. 1. The inset shows a typical photoelectron difference image from the coaxial-VMI detector, ob-

tained by subtracting the X-ray-only from the X-ray+IR (streaked) image, encoding the relative photoionization delays of N-1s vs. C-1s into an angular offset between the streaking directions (arrows). Comparison to our calculations reveals that the two maxima in the relative delays are associated with shape resonances [3], which become more symmetric in the sequence PY-MI-TR and display photoionization delays that also increase in this sequence. These results suggest that core-level photoionization delays provide insights into the symmetry of shape resonances that go beyond the information contained in cross sections and asymmetry parameters, which were also measured and calculated within the present work.



**Figure 1.** Experimental and computed time delays. Inner panel: differential signal on the detector.

## References

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