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Femtosecond x-ray induced fragmentation of $Ho_3N@C_{80}$

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Synopsis - We report on new data regarding on the photoionization and fragmentation dynamics of gas phase endohedral fullerenes $Ho_3N@C_{80}$ obtained with intense femtosecond X-ray pulses from the Linac Coherent Light Source (LCLS) free electron laser (FEL).

Investigations of ionization and fragmentation dynamics of nano-size fullerenes subjected to ultrashort strong x-ray laser field [1] are very important for understanding the mechanisms of radiation damage and will benefit the development of bio-imaging techniques and radiotherapies. Recently, we reported an investigation on photoionization and fragmentation of C_{60}. Although the dynamics were complicated because of the number of electrons and atoms involved, the experimental results could be well reproduced by molecular dynamics (MD) modeling with electronic structure and nuclear motion taken into account [2]. To understand the dynamics further, we extended our work to endohedral fullerenes, $Ho_3N@C_{80}$.

The experiment was carried out at the AMO hutch at the Linac Coherent Light Source (LCLS) at Stanford. Gas phase $Ho_3N@C_{80}$ molecules were evaporated from a heated oven and interacted with strong x-ray laser pulses. The photon energy of the x-rays was chosen at 1530 eV to optimize the ionization from the Ho atoms, which were encapsulated in C_{80} cages along with a nitrogen atom in the center. The pulse duration of the FEL was set to 80 fs and the pulse energy was nominally 2.2 mJ. The x-rays were focused to a spot approximately 5μm×5μm. A typical mass spectrum is shown in Figure 1. Parent ions up to quintuply charged $Ho_3N@C_{80}^{5+}$ were observed, suggesting a stable structure even with 5 charges on the parent molecule. Atomic Ho^+ ions, originating from the encapsulated Ho_3N molecule, were observed at the highest yield compared to other fragments and parent ions.

In this contribution, we will also present the kinetic energies of fragments and compare them with our prior C_{60} experiment. Furthermore, the correlation between ions will be examined by the covariance mapping technique.

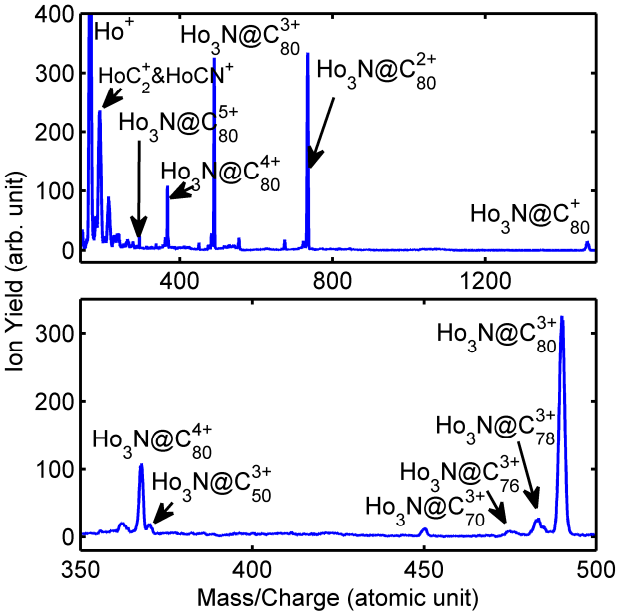

Figure 1. Fragmentation pattern of gas phase $Ho_3N@C_{80}$ exposed to an intense femtosecond X-ray laser beam at 1530eV. The top panel displays the ion fragments from Ho^+ to parent ions while the bottom panel focuses on the triply charged ions.

References

[1] N. Berrah, P.H. Bucksbaum 2014 *Scientific American* **310** 64
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