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Observation of double-core-hole continua and ionic fragments of formamide upon irradiation by intense X-ray pulses[1] DIMITRIS KOULENTIANOS, GILLES DOUMY, STEPHEN SOUTHWORTH, Argonne Natl Lab — Doubly core-ionized states of molecules, in which two different atoms have an ionized K shell each, are characterized by enhanced chemical shifts compared to their singly core-ionized counterparts. In this way the chemical environment of an atom in a molecule can be probed in detail [Cederbaum *et al.*, J. Chem. Phys. **85**, 6513 (1986)]. The elusive experimental observation of such states became feasible thanks to the development of third generation synchrotron radiation facilities [Eland *et al.*, Phys. Rev. Lett. **105**, 213005 (2010)] and X-ray free electron (XFEL) lasers [Berrah *et al.*, PNAS **108**, 16912 (2011)]. Using the high-flux, high-intensity, femtosecond X-ray pulses of the Linac Coherent Light Source (LCLS) at Stanford, the doubly core-ionized states of formamide (HCONH2) have been recorded and identified, using an experimental setup which consists of five time-of-flight (TOF) electron spectrometers mounted in different orientations with respect to the polarization of the incoming light, along with an ion TOF detector. This setup allowed us to observe the photoelectron peaks associated with the formation of double-core-hole states involving all three sites of the molecule (C,N,O), as well as the different ionic fragments.

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