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Photo-induced dynamics in heterocyclic aromatic molecules probed by femtosecond XUV transient absorption spectroscopy FLO-RIAN LACKNER, ADAM S. CHATTERLEY, CHAITANYA D. PEMMARAJU, Lawrence Berkeley National Laboratory, DANIEL M. NEUMARK, STEPHEN R. LEONE, UC Berkeley, OLIVER GESSNER, Lawrence Berkeley National Laboratory — We report on the ring-opening and dissociation dynamics of strong-field ionized selenophene (C_4H_4Se), studied by transient XUV absorption spectroscopy at the Se 3d edge. The table-top experiments are facilitated by high-order harmonic generation coupled with a gas phase transient XUV absorption setup that is optimized for the study of organic compounds. Employing element-specific coreto-valence transitions, the ultrafast molecular dynamics are monitored from the perspective of the well-localized Se atoms. Spectral features are assigned based on first principles TDDFT calculations for a large manifold of electronic states. We observe signatures of rapidly (35 fs) decaying highly excited molecular cations, the formation of ring-opened products on a 100 fs time scale and, most notably, the elimination of bare Se⁺ ions in a very rapid multi-step process. A delayed onset of the Se⁺ ions provides direct evidence that both selenium-carbon bonds are broken within only ~130 fs and that a sequential mechanism, presumably an initial ring-opening followed by a subsequent breaking of the second bond, is required to eliminate the atomic fragments.

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