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Probing Delayed C–I Bond Fission in the UV Photochemistry of 2-iodothiophene with Core-to-Valence Transient Absorption Spectroscopy[1] B.W. TOULSON, M. BORGWARDT, Lawrence Berkeley National Laboratory, D. FACCIALA, CRN-IFR, D.M. NEUMARK, S.R. LEONE, UC Berkeley and Lawrence Berkeley National Laboratory, O. GESSNER, Lawrence Berkeley National Laboratory — UV pump – XUV probe femtosecond transient absorption spectroscopy is used to study the dynamics of 2-iodothiophene (C_4H_3IS). Iodine N-edge core-to-valence transitions probe changes in valence electronic structure from the perspective of the iodine atom, with ultrafast time resolution. A key question we wish to address is, to what extent ring-opening occurs prior to C-I bond fission. In 2-iodothiophene, the initial $\pi\pi^*$ electronic excitation is localized on the thiophene ring, rather than the halogen atom, resulting in singly occupied molecular orbitals (SOMO) that are "dark" to our probe. Significant electronic and nuclear rearrangement (and perhaps ring-opening) must occur before the localized I(4d) core-to-valence transitions are observed. While 2-photon ionization of 2-iodothiophene leads to the prompt appearance of I^+ ions, within the instrument response function, the onset of neutral atomic I fragments is delayed by over 100 fs relative to the I^+ and parent bleach signals. A global fit approach is used to separate the spectral contributions of each fragmentation channel. The observation of delayed absorption features is similar to that reported in iodobenzene, where the parent depletion occurs 50 fs prior to the emergence of atomic iodine [L. Drescher et al., J. Chem. Phys. 145, 011101 (2016)].

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