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Dynamics of Molecular Fragmentation Mediated by Charge-Transfer States ROBERT LEVIS(1,*), DMITRI ROMANOV(2,*), ALEXEI MARKEVITCH(1,*), (1) Department of Chemistry, (2) Department of Physics, (*) Center for Advanced Photonic Research, Temple University, STANLEY SMITH, Department of Chemistry, Wayne State University, DUSAN LORENCZ, DUSAN VELIC, Comenius University, Bratislava, Slovakia — Dissociative ionization of large organic molecules caused by ultrashort strong-field laser pulses is largely predetermined by nonadiabatic electron dynamics during the pulse. The key element of the nonadiabatic process is the bottleneck transition from the systems ground state to the charge-transfer doorway state of the excited-state manifold. The induced charge transfer across large distances in polyatomic molecules and ions evolves into a complicated dynamics that can include prolong charge localization and sequential ionization. This electron-charge dynamics affects essentially the ensuing nuclear motion and thus determines the fragmentation pattern and charge distribution among the fragments. We observed manifestations of nonadiabatic electron-nuclear dynamics mediated by charge-transfer states in a series of experiments on related polyaromatic molecules, including study of the fragmentation threshold as a function of the laser intensity, the proton kinetic energy distributions, and the relative yield of ionized fragments as a function of the carrier wavelength. In all these cases our model calculations agree quantitatively with the experimental data.

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