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Ultrafast hydrogen migration and induced fragmentation dynamics in propanol[1] RAZIB OBAID, University of Connecticut, JUAN GONZALEZ, Universidad Autnoma de Madrid, DEBADARSHINI MISHRA, University of Connecticut, SERGIO DAZ-TENDERO, Universidad Autnoma de Madrid, NORA KLING, AARON LAFORGE, University of Connecticut, FERNANDO MARTN, Universidad Autnoma de Madrid, NORA BERRAH, University of Connecticut — Carbon backbones play an important role in ultrafast electronic relaxation processes following photoexcitation, particularly in the presence of another functional group such as -OH. We investigated the photoinduced single and double hydrogen migration, leading to formation of H_2O^+ and H_3O^+ respectively, through excitation by intense, ultrashort (˜10 fs), 800 nm laser pulses in two structural isomers of propanol. Our results show changes in the pathways of the time-resolved formation of H_2O^+ and H_3O^+, and the mediated bond dissociation observed at the dicationic states of the two propanol conformers. Using coincidence recoil ion momentum spectroscopy and state-of-the-art molecular dynamics simulations, we show the role of carbon chains in the time-resolved energy redistribution and relaxation mechanisms of photoexcited prototypical hydrocarbons.

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