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Ultrafast Dynamics of Single and Double Hydrogen Migration in Ethanol

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Hydrogen plays an important role in the chemistry of hydrocarbons, proteins and peptides, as well as most biomolecules. Intramolecular reactions where a hydrogen migrates from one bonding site to another has considerable impact on the chemical behavior of the molecule. Similarly, in molecules containing more than one hydrogen, multiple hydrogen migrations can occur, further altering the molecule's functionality or original identity. Using a pair of ultrashort (9 fs), intense ($I \sim 10^{14}$ W/cm²) laser pulses in a pump-probe scheme, combined with 3D coincidence ion imaging (COLTRIMS), we explore the rich dynamics of the single and the double hydrogen migration reactions taking place in ethanol, CH₃CH₂OH. Four reaction channels are studied for this purpose, including three double coincidence channels: C₂H₅⁺ + OH⁺, C₂H₄⁺ + H₂O⁺, C₂H₃⁺ + H₃O⁺, and one triple coincidence channel: H⁺ + H₂O⁺ + C₂H₃⁺. The double coincidence channels are attributed to dynamics occurring in the ethanol cation. Simultaneously tracking the ion yields as a function of time between the pump and probe pulses for the three channels, we investigate the chemical kinetics for 'no', single, and double hydrogen migration reactions. Furthermore, we investigate correlations between the different channels. The triple coincidence channel is attributed to dynamics occurring in the ethanol dication. Three precursor channels are identified through monitoring the kinetic energy release and momenta of the involved fragments. Newton and Dalitz plots help to decipher the relevant molecular motions at different pump-probe delays. Compared to some of the processes leading to single hydrogen migration, the probability of observing double hydrogen migration in the experiment is quite significant, suggesting that double hydrogen migration might play a more important role in the chemistry of charged organic compounds than generally assumed. The conclusions are supported by state-of-the-art molecular dynamics calculations. This work is funded by the NSF under grant No. 1700551.