

# Strong Field Double Ionization of Formaldehyde: Metastable state and dissociative pathways

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Strong field ionization (SFI) has been an integrated part of spectroscopy in order to understand processes involved in excited state dynamics. The Weinacht group used strong field laser pulses to doubly ionize formaldehyde and the momenta {or kinetic energies (KE)} of charged fragments produced from the dication were detected using a velocity map imaging spectrometer. However, experimentally it is very difficult to determine which electronic states contribute to the KE signals of the cations formed. Theory can help address that question as well as better understand the underlying mechanisms and pathways that lead to dissociations. Here, dynamics with trajectory surface hopping (TSH) have been used to study the dynamics on different electronic states of  $\text{CH}_2\text{O}^{2+}$  and capture the kinetic energies of the dissociated cations. Comparisons of the calculated and experimental kinetic energy release data enabled us to determine each state's contribution to the experimental KE signal and consequently determine the states that are populated initially by strong field ionization. One of the most interesting results of this work is that we found that the dication does not dissociate on its first excited state ( $S_1$ ). Experimentally this is confirmed by detection of the parent dication. The ab initio calculations show that the symmetry of the  $S_1$  state ( $A_2$ ) does not allow for non-adiabatic transitions to the ground state thus trapping the population on  $S_1$ . Furthermore, the energy barriers on  $S_1$  limit the dissociation of the dication on that state. Detailed analysis of KE contributions from other electronic states was also performed along the dissociative channels such as ' $\text{H}_2\text{C}^+ + \text{O}^+$ ' and ' $\text{HCO}^+ + \text{H}^+$ '.