

ULTRAFAST COULOMB EXPLOSION OF FORMIC ACID CLUSTERS AND PRODUCTION OF TRIPLY CHARGED CARBON MONOXIDE

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Multiply charged diatomic molecules are exotic gas-phase species and require high amounts of energy to be produced. Fundamental questions regarding the structures, stabilities, and bonding schemes of small multiply charged ions tests our concepts of bonding. Although uncommon in most chemical settings, the conditions found within the Earth's ionosphere enable such species to be constantly produced, albeit for short periods of time, through the interaction between small atmospheric molecules and cosmic radiation in the extreme ultraviolet regime. We have performed laboratory experiments using intense laser pulses to investigate the stability and production of multiply charged ions from small atmospherically relevant molecules. I will present our recent work where femtosecond laser pulses are utilized to drive multiple ionization in molecular gas-phase formic acid dimers and studied using time-of-flight mass spectrometry. The interaction of formic acid dimer with 200 fs linearly polarized laser pulses of 400 nm with intensities up to 3.7×10^{15} W/cm² produces a carbon monoxide dication and trication. An enhanced ionization is observed in CO ions when the source analyte was switched from the molecular beam to formic acid clusters. Measurements of the kinetic energy release resulting from the Coulomb explosion of clusters are in excellent agreement with our simulations performed over the clusters observed in the mass spectra and suggest that almost no movement occurs during the ionization mechanism. Lastly, potential energy curves for COⁿ⁺, for $n < 4$, have been calculated using high level theory, confirming the existence of a metastable state with a large potential barrier with respect to dissociation of several eV.