

## ULTRAFAST COULOMB EXPLOSION AND PROTON TRANSFER DYNAMICS OF FORMIC ACID CLUSTERS

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With increasing concerns over the concentration of carbon dioxide in the atmosphere, new materials are being explored to capture CO<sub>2</sub> for use as a feedstock. The suspected reaction sites of these materials deviates from the bulk phase, such as the quantum confinement of water droplets that happens within pores. The formic acid clusters', (HCOOH)<sub>n</sub>(H<sub>2</sub>O)<sub>m</sub>, minimum energy structures show an evolving cage structure with each additional molecule. The n,m = (5,0) cluster exhibits a much greater stability due to its rigid cage-like structure. This cage structure then encapsulates a water molecule to make an even more stable n,m = (5,1) cluster. The interaction of formic acid clusters with 200 fs linearly polarized laser pulses of 800 and 400 nm with intensities up to 1x10<sup>15</sup> W/cm<sup>2</sup> was studied using time-of-flight mass spectrometry, verifying this trend in stability. An enhanced ionization is observed in clusters, leading to the production of triply charged carbon, oxygen, and CO ions that are not observed when only the formic acid molecule is present. 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. Finally, ultrafast pump-probe spectroscopy was used to investigate how proton transfer dynamics and excited state lifetimes are influenced by the self-solvation of formic acid. These results highlight the role of microsolvation on the excited state dynamics of simple carboxyl groups, specifically formic acid, in producing or capturing carbon dioxide and will help to direct the design of the next generation of carbon capture materials.