

Abstract Submitted  
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**Proton transfer in acetaldehyde and acetaldehyde-water clusters:  
Vacuum ultraviolet photoionization experiment and theoretical calculations** OLEG KOSTKO, TYLER P. TROY, BISWAJIT BANDYOPADHYAY, MUSAHID AHMED, Lawrence Berkeley National Lab — Acetaldehyde, a probable human carcinogen and of environmental importance, upon solvation provides a test bed for understanding proton transfer pathways and catalytic mechanisms. In this study, we report on single photon vacuum ultraviolet photoionization of small acetaldehyde and acetaldehyde-water clusters. Appearance energies of protonated clusters are extracted from the experimental photoionization efficiency curves and compared to electronic structure calculations. The comparison of experimental data to computational results provides mechanistic insight into the fragmentation mechanisms of the observed mass spectra. Using deuterated water for isotopic tagging, we observe that proton transfer is mediated via acetaldehyde and not water in protonated acetaldehyde-water clusters.

Oleg Kostko  
Lawrence Berkeley National Lab

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