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Photodissociation of Acetylacetone: Photoionization and Threshold Photoelectron Spectroscopy Reveal Much More Than OH Radicals

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The absorption of light by an organic molecule, and the subsequent pathways for energy transformation and release, are fundamental processes governing life on earth. Two of the most important electronic chromophores in organic systems are C=O bonds (carbonyl molecules) and C=C bonds (alkenes and polyenes). Carbonyl molecules, such as acetaldehyde (CH_3CHO) also have enol tautomers ($\text{H}_2\text{C}=\text{CHOH}$, vinyl alcohol). This tautomerization converts the weakly absorbing C=O chromophore to a strongly absorbing C=C chromophore. We have studied the photodissociation of acetylacetone (AcAc), which exists at 300 K in the gas phase mostly as the enolone tautomer, rather than the diketo tautomer. The enolone tautomer is stabilized by both π -conjugation and an internal hydrogen bond. Previous studies have concluded that OH loss is the dominant (or only) channel when AcAc is excited in the ultraviolet at 266 or 248 nm. However, truly universal detection techniques have not been used in these studies. By combining multiplexed photoionization mass spectrometry (MPIMS), threshold photoelectron photoion coincidence spectroscopy (TPEPICO), and time-resolved infrared absorption spectroscopy of OH radicals, we have discovered that photodissociation of AcAc is much richer than previously presumed, and that OH production is not even energetically allowed following one-photon 266 or 248 nm excitation. This work demonstrates the power of multiplexed, universal detection of charged particles in photodissociation studies, and lifts the veil on the photodissociation of a molecule that is both an enol and a ketone.

Summary

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