Abstract Submitted
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Conformationally controlled chemistry: Excited state dynamics dictate ground state dissociation ARTHUR SUITS, Wayne State Univ, MYUNG-HWA KIM, UC Santa Barbara, LEI SHEN, BAILIN ZHANG, Wayne State Univ, HONGLI TAO, TODD MARTINEZ, UIUC — Ion imaging results show distinct photodissociation dynamics for propanal cations initially prepared in either the *cis-* or *gauche-* conformation, even though these differ only slightly in energy and there is a small barrier between them. The product kinetic energy distributions for the H elimination channels are bimodal, and the two peaks are readily assigned to propanoyl cation + H and hydroxyallyl cation + H. Ab initio multiple spawning dynamical calculations show that distinct ultrafast dynamics in the excited state leads to internal conversion to the ground state in isolated regions of the potential surface for the two conformers, and from these distinct regions, conformer interconversion does not effectively compete with dissociation.

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