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Conformer-selected photodissociation: Ab Initio Multiple Spawning Dynamics of Excited Propanal Cation HONGLI TAO, Univiersity of Illinois at Urbana-Champaign, TODD MARTINEZ, University of Illinois at Urbana-Champaign — Recent experiments have shown that pure cis and gauche propanal cations can be prepared using REMPI (Resonance Enhanced Multiphoton Ionization Spectroscopy). The H elimination pathway which results when these conformer-selected cations are photoexcited was found to depend on the conformer (cis vs. gauche). This dependence is very surprising since the interconversion barrier of the two conformers is small compared to the excited energy. We use the ab initio multiple spawning (AIMS) method developed in our group to model the conformer-specific photodissociation and to elucidate its origins.

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