CONFORMER SELECTIVE AND VIBRATIONALLY MEDIATED PHOTODISSOCIATION STUDY OF PROPANAL CATION

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We report the conformationally and vibrationally selected imaging study of propanal obtained by resonance-enhanced multiphoton ionization (REMPI). The photoelectron spectra, employing the (2+1) ionization via the (n, 3s) Rydberg transitions in the range from 365 to 371 nm, confirm that there are two stable conformer origins in the lowest ionic state, the cis conformer with a co-planar CCCO geometry and a gauche conformer with a 119 CCCO dihedral angle.
We also study the photodissociation dynamics of propanal cation initially prepared in some certain vibrational modes or conformation. The product kinetic energy distributions for the H elimination channels are bimodal, and the two peaks are readily assigned to propanal cation + H and hydroxyallyl cation + H. The ratio of the fast product with respect to the whole product is varied according to different vibrational mode preparation. However, cis form appears the lowest and gauche form yield the highest ratio. Full 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.