

Conformer-specific ion spectroscopy of isobutanal

(Kangwon National Univ.) Yu Ran Lee, Hong Lae Kim, and Chan Ho Kwon*

E-mail:chkwon@kangwon.ac.kr

Isobutanal is an aliphatic aldehyde which has been extensively considered as one of important intermediates in isomerization reaction as well as astrochemical relevant models in the interstellar medium. We report conformer-specific ionization dynamics and cationic vibrational spectra of the isobutanal utilizing one-photon mass-analyzed threshold ionization (MATI) spectroscopy using the vacuum ultraviolet (VUV) laser pulse for the first time. The conformational preference of isobutanal in the various supersonic expansion conditions was explored to identify the conformers, from which the intrinsic ionization dynamics were elucidated by directly measuring the VUV-MATI spectrum corresponding to each conformer. The observed conformer-specific vibrational spectra of isobutanal cations could be definitely analyzed through the Franck-Condon simulations at the B3LYP/cc-pVTZ level for isobutanal conformers, trans and gauche. Most of all, we confirm that there exist two stable conformers as gauche and trans in the lowest ionic state as well as the neutral ground state, producing by accurate adiabatic ionization energies of $78,557 \pm 3 \text{ cm}^{-1}$ ($9.7398 \pm 0.0004 \text{ eV}$) and $78,136 \pm 3 \text{ cm}^{-1}$ ($9.6878 \pm 0.0004 \text{ eV}$), respectively. Notably, only gauche conformer undergoes the unique geometrical change upon ionization, resulting in the progression of the CHO torsional mode.