One-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of crotonaldehyde

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We measured the cationic vibrational spectrum of crotonaldehyde (2-butenal) using one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. The VUV radiation was generated by four-wave difference frequency mixing in Kr gas. From the origin band in the MATI spectrum, the adiabatic ionization energy of crotonaldehyde determined to be 9.7501 ± 0.0005 eV (78642 ± 0.0004 cm^{-1}). This value is in agreement with the previous one. To analyze the cationic vibrational spectrum, we performed the Franck-Condon simulation at M062x/aug-cc-pVDZ level, which revealed to be four stereo isomers of trans-*s-trans*, trans-*s-cis*, cis-*s-trans*, and cis-*s-cis* crotonaldehyde. Most of vibrational peaks observed in the spectrum were assigned to that of trans-*s-trans* crotonaldehyde and the remained peaks were assigned to the vibrational peaks of trans-*s-cis,* cis-*s-trans,* or cis-*s-cis* crotonaldehyde. The adiabatic ionization energies of trans-*s-cis,* cis-*s-trans,* and cis-*s-cis* crotonaldehyde were determined to be 9.7619 ± 0.0005 eV (78737 ± 4 cm^{-1}), 9.7121 ± 0.0005 eV (78335 ± 4 cm^{-1}), and 9.6481 ± 0.0005 eV (77819 ± 4 cm^{-1}), respectively.