Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of hydrazoic acid (HN₃)

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We obtained the vibrational spectrum of hydrazoic acid (HN₃) cation in the electronic ground state by utilizing the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy for the first time. For the one-photon ionization of hydrazoic acid, the tunable and coherent vacuum ultraviolet (VUV) radiation in the 86200-88100 cm⁻¹ (10.687-10.923 eV) range was generated by non-resonant four-wave sum frequency mixing ($\omega_{\text{VUV}} = 2\omega_{\text{UV}} + \omega_{\text{Vis}}$) in Xe and Ar mixture. The accurate ionization energy of HN₃ was determined to be 86,591 \pm 5 cm⁻¹ from the 0-0 band position in the MATI spectrum. To assign the peaks observed in the MATI spectrum, we carried out the Franck-Condon simulations employing various methods and levels, from which the precise structure of HN₃ could be determined. It revealed that the observed spectrum displayed mainly totally symmetric vibrational modes of A' for the linear HN₃.