MASS ANALYZED THRESHOLD IONIZATION SPECTROSCOPY OF BENZIMIDAZOLE AND BENZOTRIAZOLE CATIONS

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The vibrationally resolved cation spectra of benzimidazole and benzotriazole have been recorded by using two-color resonant mass-analyzed threshold ionization spectroscopy. The respective adiabatic ionization energies (IEs) are found to be 67552 and 70474 wavenumbers with an uncertainty of about 5 wavenumbers. Comparing these data with that of indole, one finds that the IE of these aza-aromatic bicyclic molecules increases with the number of the N atoms. Most of the active modes of the benzimidazole cation are related to the in-plane ring vibrations. In contrast, the observed spectral bands of the benzotriazole cation correspond to the out-of-plane N2-H and skeleton N1N2N3 bending vibrations. These experimental findings may be attributed to the nature and the N atoms in the five-membered ring.