Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Long-distance proton transfer induced by a single ammonia molecule: ion mobility mass spectrometry of protonated benzocaine reacted with NH_3

Keijiro Ohshimo, Shun Miyazaki, Keigo Hattori, Fuminori Misaizu*

Department of Chemistry, Graduate School of Science, Tohoku University, 6–3 Aoba, Aramaki, Aoba-ku, Sendai 980–8578, Japan

*Corresponding author: misaizu@tohoku.ac.jp (F. Misaizu)

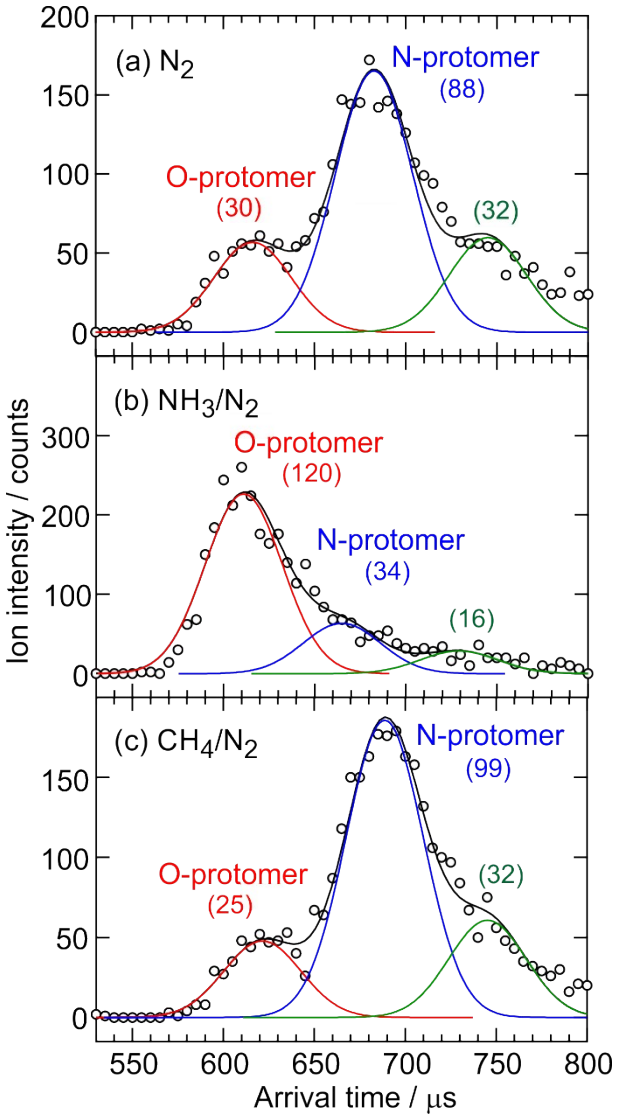

Fig. S1 Arrival time distributions of $BC{\cdot}H^+$. (a) N_2 buffer gas in the ion drift tube (Pressure in the drift tube P_{DT} = 0.11 Torr), (b) 0.5% NH_3/N_2 buffer gas (P_{DT} = 0.10 Torr), (c) 1% CH_4/N_2 buffer gas (P_{DT} = 0.11 Torr). Red, blue and green curves are Gaussian functions for fitting the experimental plots (black circles). Red, blue and green curves represent the O-protomer, N-protomer, and $BC{\cdot}H^+$ fragments caused by the dissociation of acetonitrile-solvated N-protomers. Each area of bands with red, blue and green curves is shown in parenthesis.

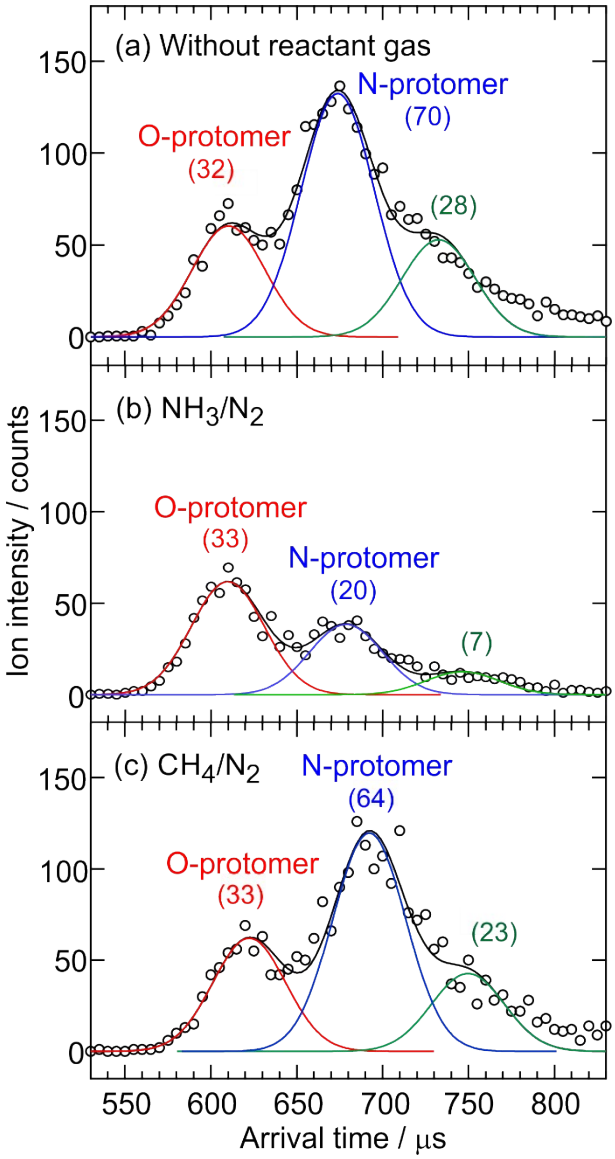

Fig. S2 Arrival time distributions of BC·H$^+$. (a) Without reactant gas in the ion guide, (b) 20% NH_3/N_2 gas in the ion guide (ΔP = 3.1×10^{-3} Pa), (c) 20% CH_4/N_2 gas in the ion guide (ΔP = 3.0×10^{-3} Pa). The pressure of N_2 buffer gas in the ion drift tube was P_{DT} = 0.11 Torr. Red, blue and green curves are Gaussian functions for fitting the experimental plots (black circles). Red, blue and green curves represent the O-protomer, N-protomer, and BC·H$^+$ fragments caused by the dissociation of acetonitrile-solvated N-protomers. Each area of bands with red, blue and green curves is shown in parenthesis.

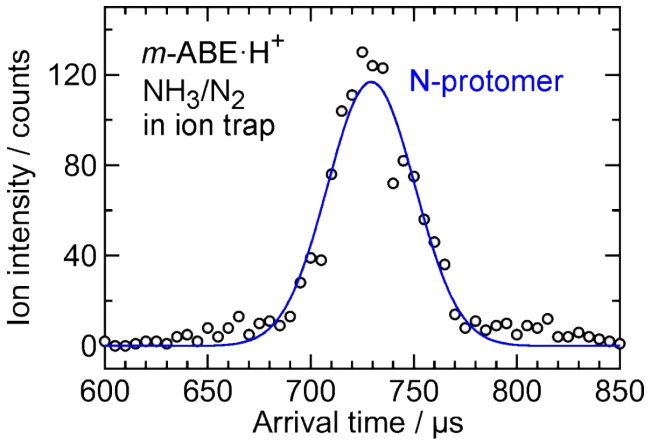

Fig. S3 Arrival time distributions of *m*-ABE·H$^+$ with 1% NH_3/N_2 gas in the ion trap. The partial pressure of NH_3/N_2 gas (ΔP = 2.7×10^{-3} Pa) was monitored by the vacuum gauge of the chamber. The pressure of N_2 buffer gas in the ion drift tube was P_{DT} = 0.20 Torr. The blue curve is Gaussian functions for fitting the experimental plots (black circles).