

# **Ion Mobility Shift of Isotopologues in a High Kinetic Energy Ion Mobility Spectrometer (HiKE-IMS) at Elevated Effective Temperatures**

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Figure S1. Ion mobility spectrum of the reactant ions in nitrogen

Figure S2. HiKE-IMS-MS spectra of the reactant ions in nitrogen

Figure S3. Ion mobility spectra of toluene and toluene- $^{13}\text{C}_7$  in nitrogen

Figure S4. HiKE-IMS-MS spectra of toluene in nitrogen

Figure S5. Ion mobility spectra of benzene and benzene- $^{13}\text{C}_6$  in nitrogen

Figure S6. HiKE-IMS-MS spectra of benzene in nitrogen

Figure S7. Ion mobility spectra of acetone and acetone- $^{13}\text{C}_3$  in nitrogen

Figure S8. HiKE-IMS-MS spectra of acetone in nitrogen

Figure S9. Ion mobility spectra of acetonitrile and acetonitrile- $^{13}\text{C}_2$  in nitrogen

Figure S10. HiKE-IMS-MS spectra of acetonitrile in nitrogen

Figure S11. Reduced ion mobilities for all investigated substances at various reduced drift fields

## SUPPORTING INFORMATION

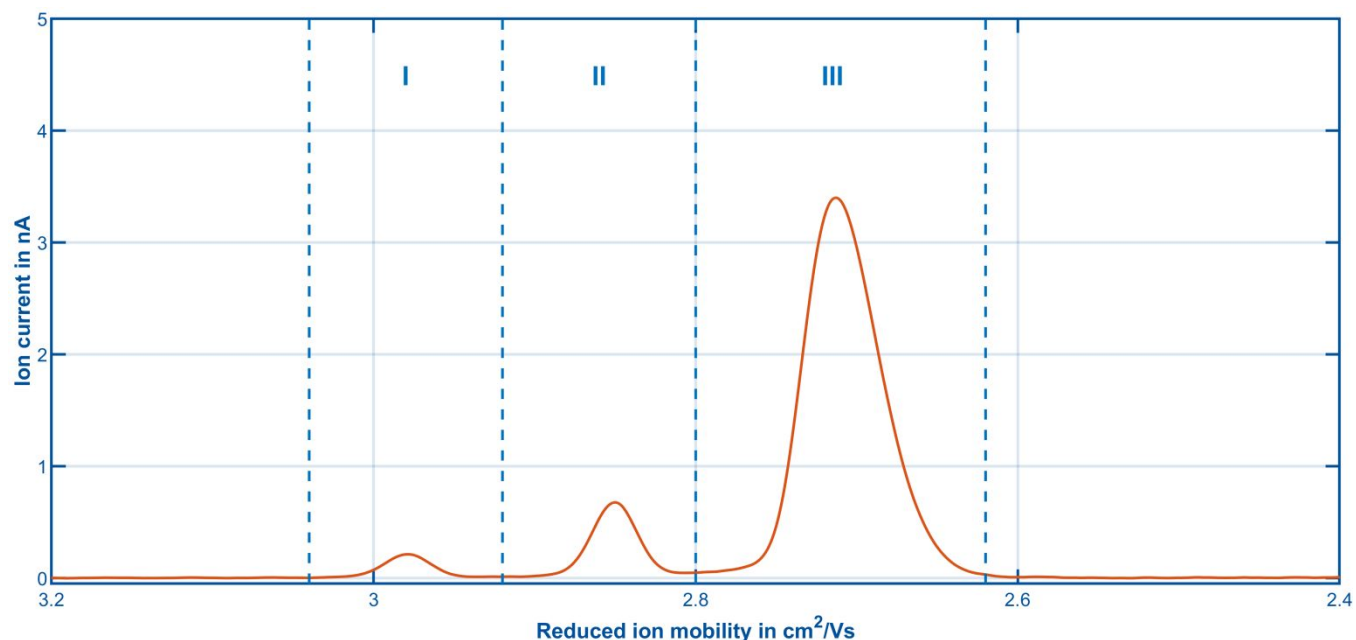


Figure S1. Ion mobility spectrum of the reactant ions in nitrogen at a reduced reaction field of  $E_{\text{RT}}/N = 70$  Td and a reduced drift field of  $E_{\text{DT}}/N = 110$  Td. All other experimental parameters are listed in Table 1 in the article.

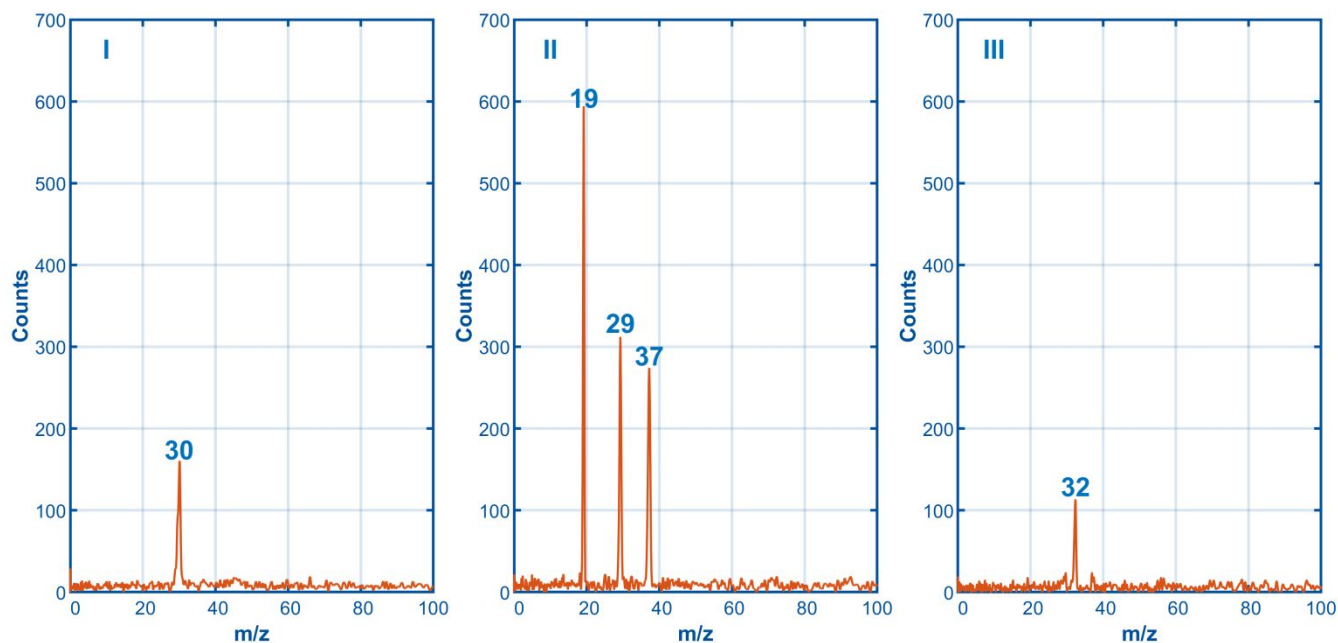


Figure S2. HiKE-IMS-MS spectra of the reactant ions in nitrogen at a reduced reaction field of  $E_{\text{RT}}/N = 70$  Td and a reduced drift field of  $E_{\text{DT}}/N = 110$  Td using the Selected-Mobility Mode. Thus, only the ions from the marked regions in Figure S1 are mass-analyzed. The peak amplitudes in the IMS-MS may differ from those in the IMS in Figure S1 due to different water concentrations in the different devices.

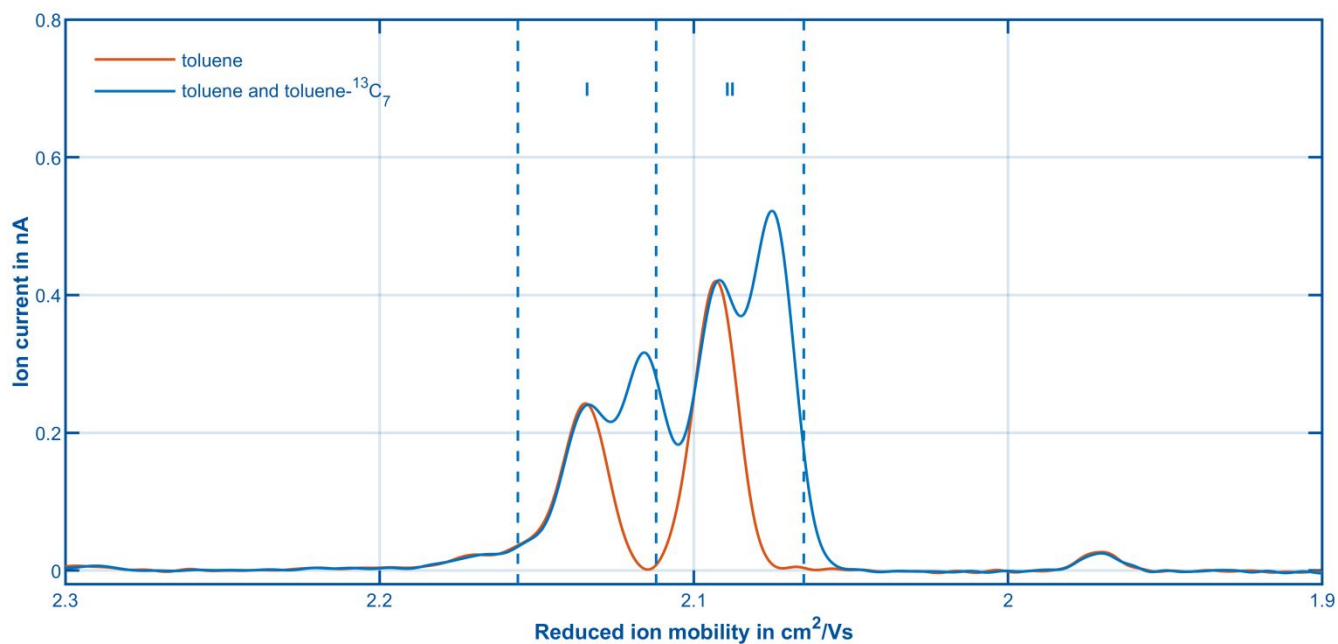


Figure S3. Ion mobility spectra of 900 ppb<sub>v</sub> toluene and 1200 ppb<sub>v</sub> toluene-<sup>13</sup>C<sub>7</sub> in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td. All other experimental parameters are listed in Table 1 **Error! Reference source not found.** in the article.

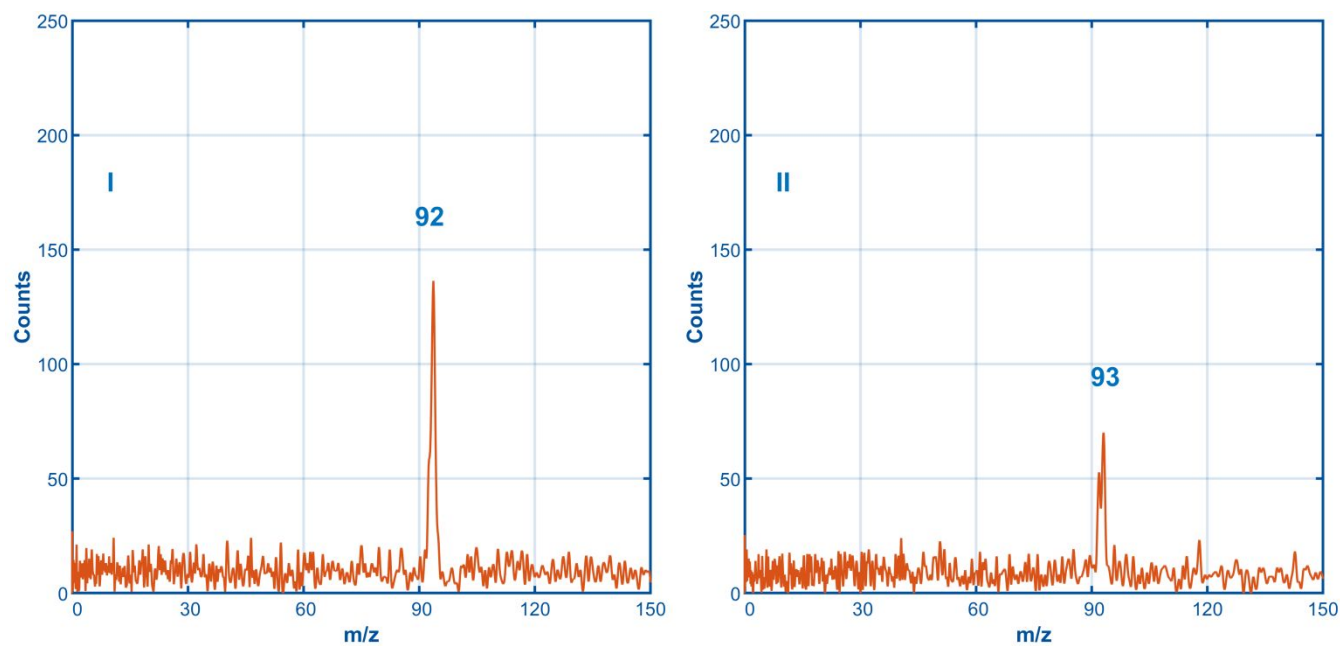


Figure S4. HiKE-IMS-MS spectra of toluene in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td using the Selected-Mobility Mode. Thus, only the ions from the marked regions in Figure S5 are mass-analyzed. Note that only toluene was investigated in the HiKE-IMS-MS.

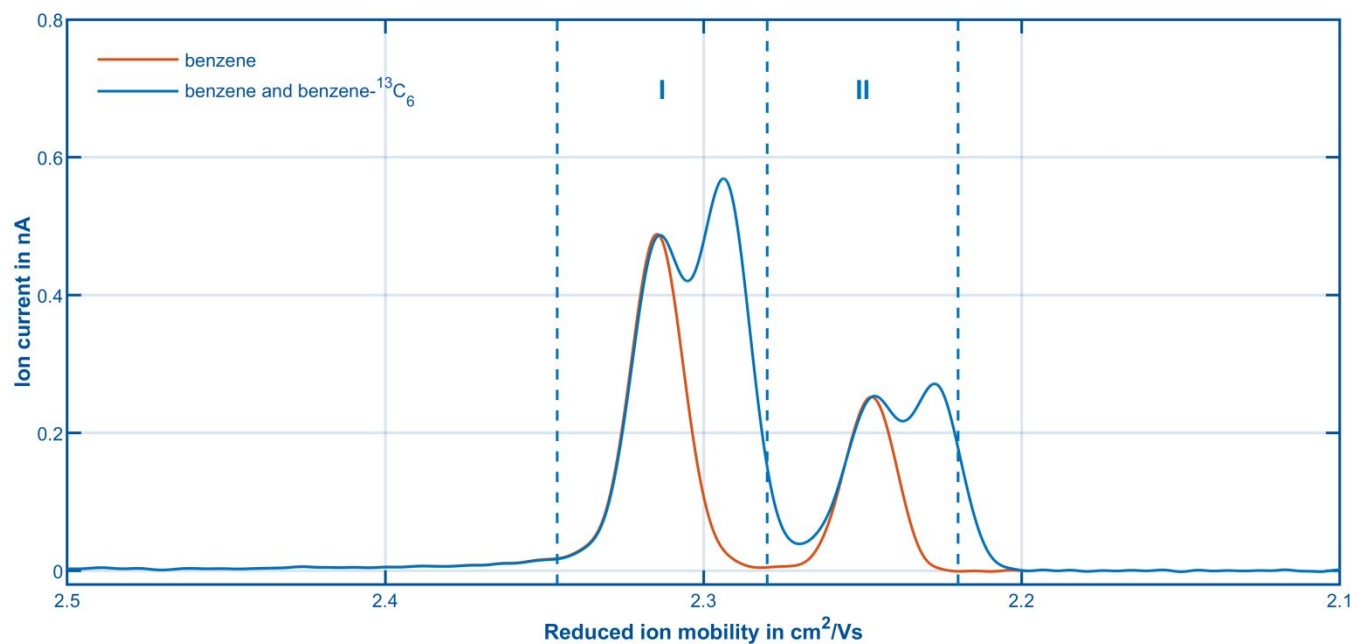


Figure S5. Ion mobility spectra of 950 ppb<sub>v</sub> benzene and 1100 ppb<sub>v</sub> benzene-<sup>13</sup>C<sub>6</sub> in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td. All other experimental parameters are listed in Table 1 in the article.

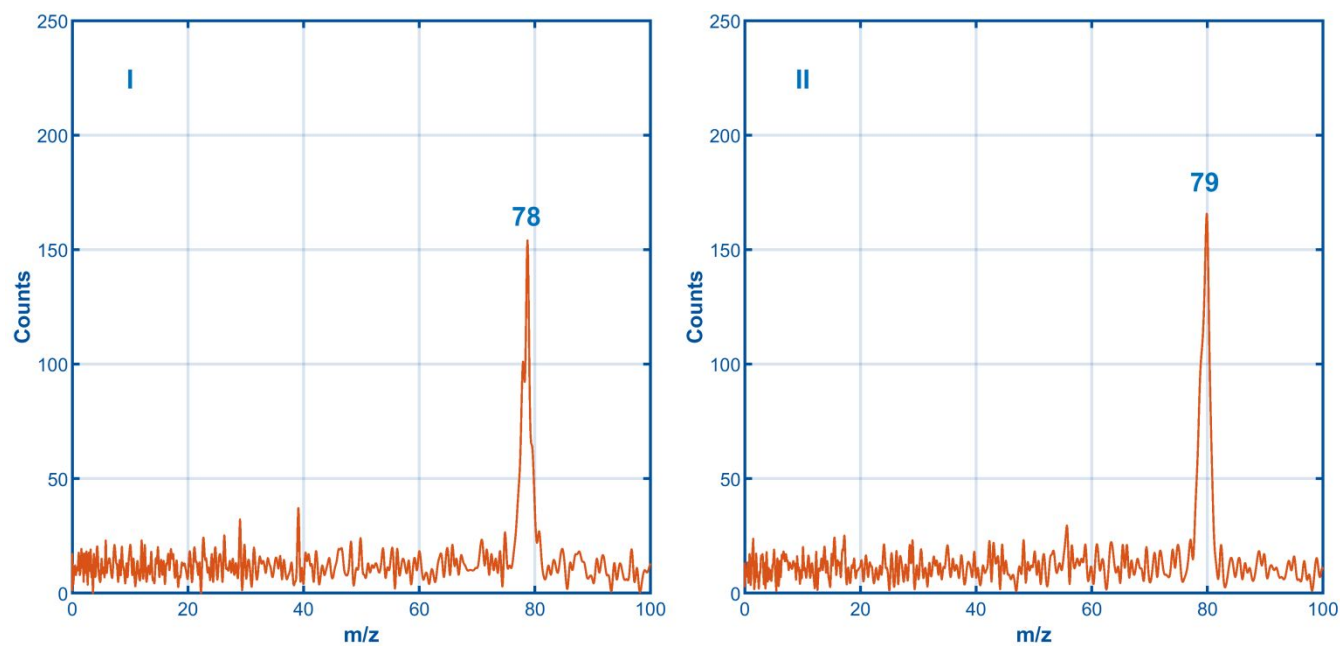


Figure S6. HiKE-IMS-MS spectra of benzene in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td using the Selected-Mobility Mode. Thus, only the ions from the marked regions in Figure S3 are mass-analyzed. Note that only benzene was investigated in the HiKE-IMS-MS.

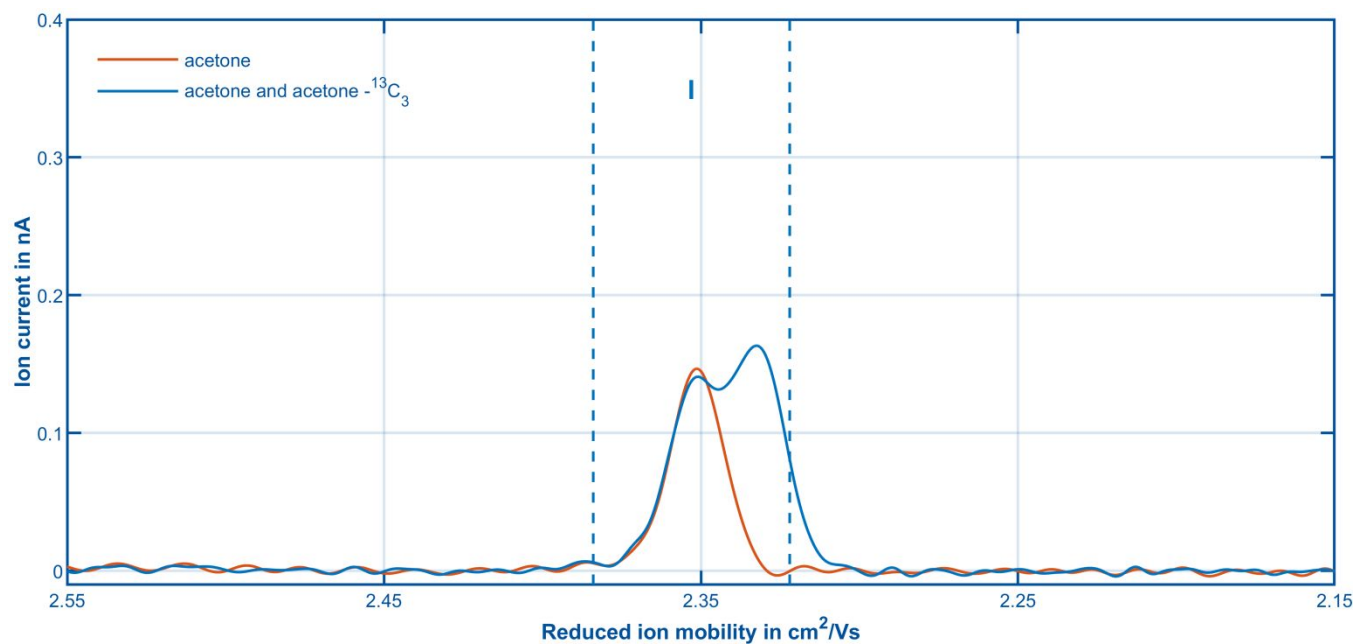


Figure S7. Ion mobility spectra of 150 ppb<sub>v</sub> acetone and 190 ppb<sub>v</sub> acetone-<sup>13</sup>C<sub>3</sub> in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td. All other experimental parameters are listed in Table 1 in the article.

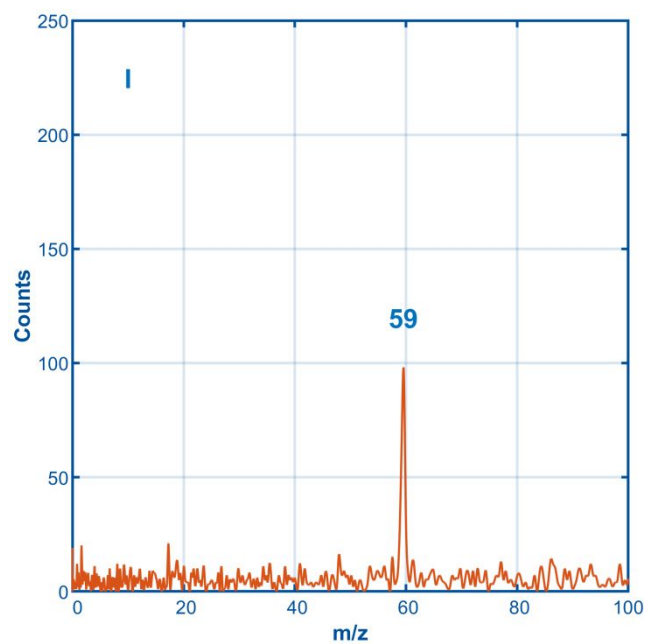


Figure S8. HiKE-IMS-MS spectrum of acetone in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 110$  Td using the Selected-Mobility Mode. Thus, only the ions from the marked regions in Figure S7 are mass-analyzed. Note that only acetone was investigated in the HiKE-IMS-MS.

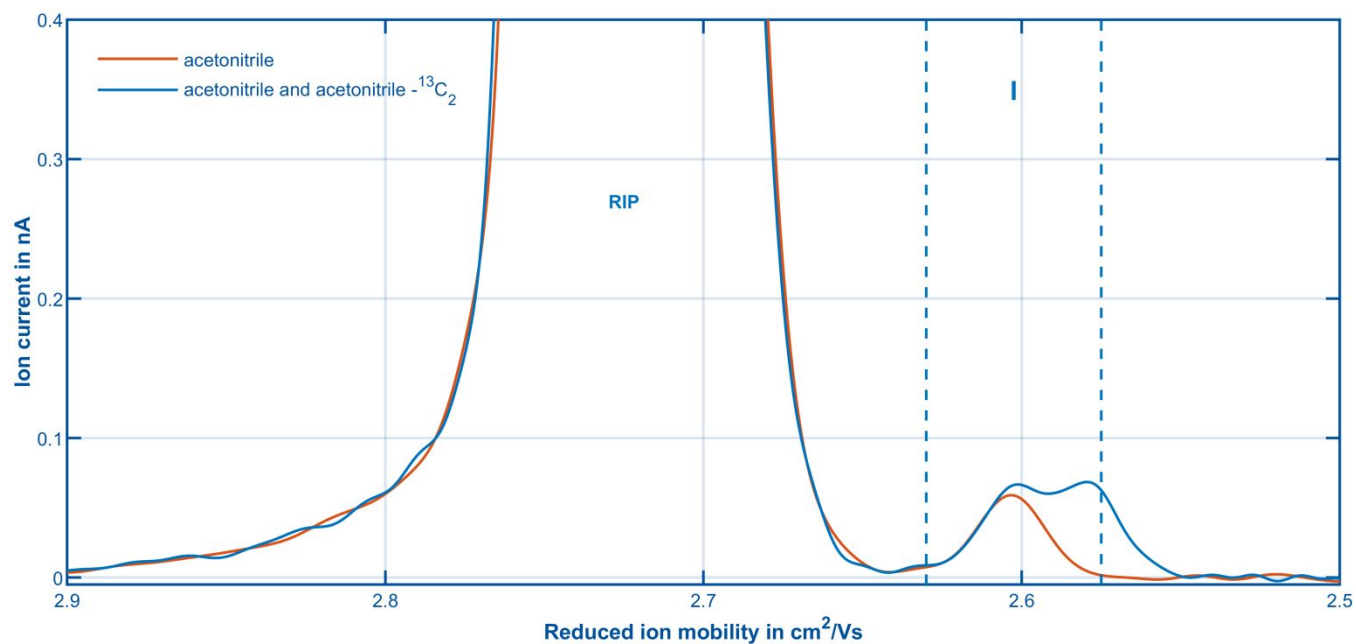


Figure S9. Ion mobility spectra of 130 ppb<sub>v</sub> acetoneitrile and 110 ppb<sub>v</sub> acetoneitrile-<sup>13</sup>C<sub>2</sub> in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 115$  Td. All other experimental parameters are listed in Table 1 in the article.

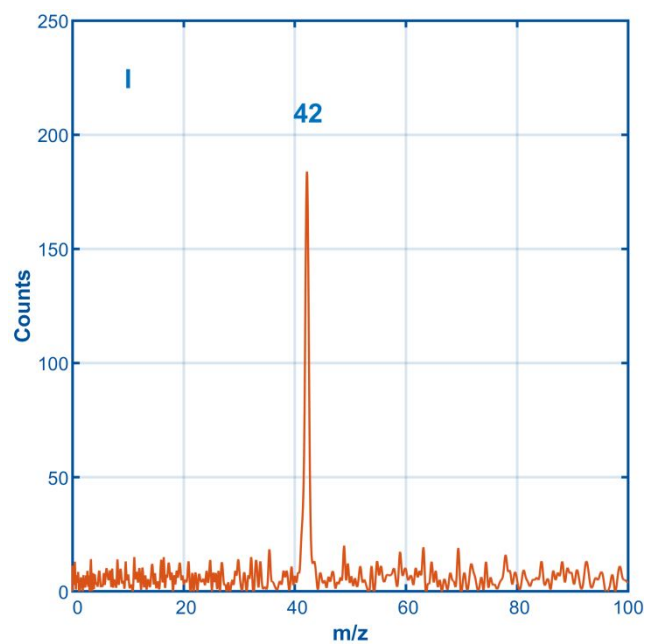


Figure S10. HiKE-IMS-MS spectrum for acetoneitrile in nitrogen at a reduced reaction field of  $E_{RT}/N = 70$  Td and a reduced drift field of  $E_{DT}/N = 115$  Td using the Selected-Mobility Mode. Thus, only the ions from the marked regions in Figure S9 are mass-analyzed. Note that only acetoneitrile was investigated in the HiKE-IMS-MS.

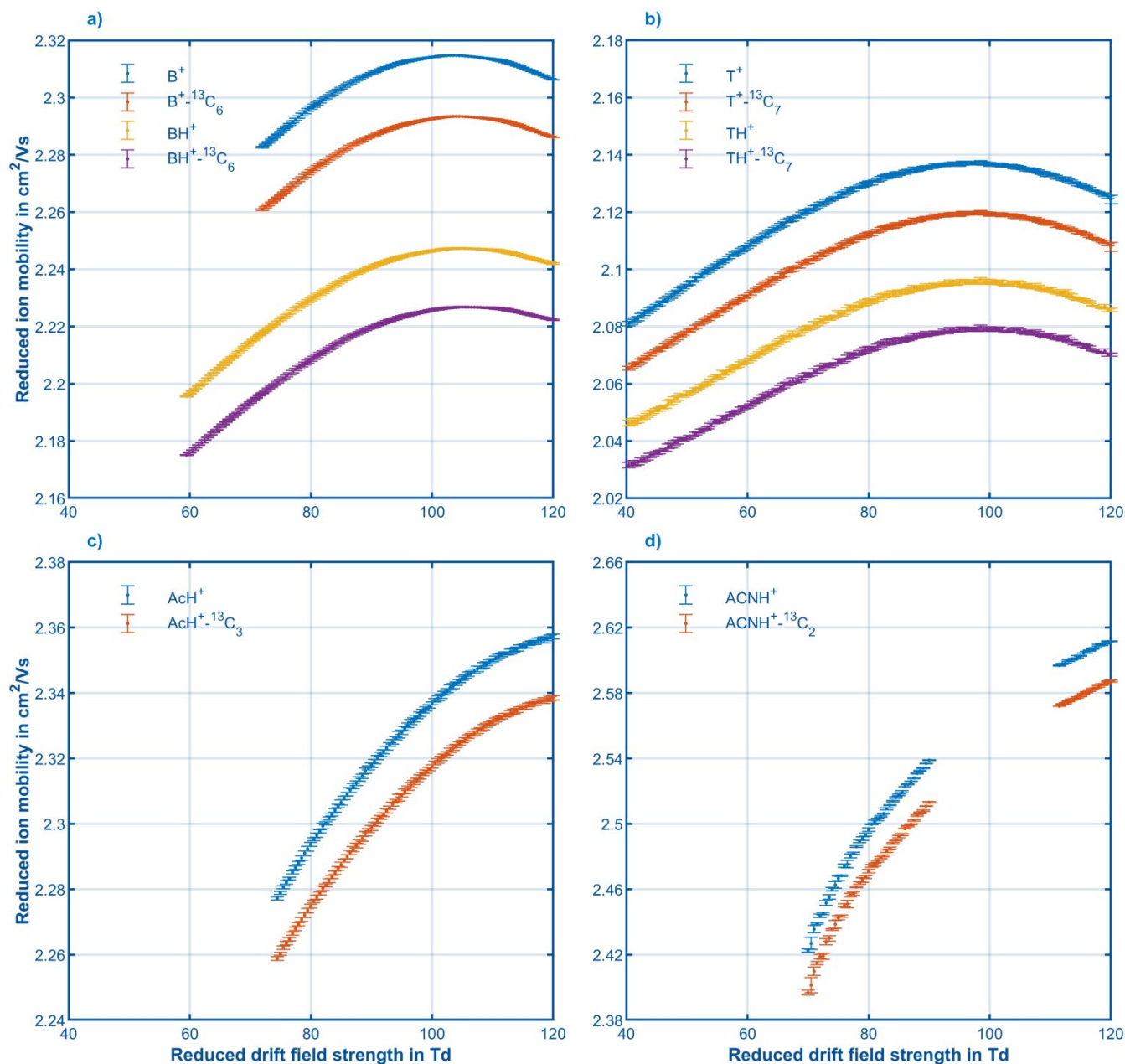


Figure S11. Reduced ion mobility  $K_0$  a) of the directly ionized and protonated monomers of benzene ( $\text{B}^+$  and  $\text{BH}^+$ ) and benzene- $^{13}\text{C}_6$  ( $\text{B}^+ \cdot ^{13}\text{C}_6$  and  $\text{BH}^+ \cdot ^{13}\text{C}_6$ ), b) of the directly ionized and protonated monomers of toluene ( $\text{T}^+$  and  $\text{TH}^+$ ) and toluene- $^{13}\text{C}_7$  ( $\text{T}^+ \cdot ^{13}\text{C}_7$  and  $\text{TH}^+ \cdot ^{13}\text{C}_7$ ), c) of the protonated monomers of acetone ( $\text{AcH}^+$ ) and acetone- $^{13}\text{C}_3$  ( $\text{AcH}^+ \cdot ^{13}\text{C}_3$ ) and d) of the protonated monomers of acetonitrile ( $\text{ACNH}^+$ ) and acetonitrile- $^{13}\text{C}_2$  ( $\text{ACNH}^+ \cdot ^{13}\text{C}_2$ ) at various reduced drift fields in nitrogen at a reduced reaction field of  $E_{\text{RT}}/N = 70$  Td. All other experimental parameters are listed in Table 1 in the article. The reduced ion mobilities were determined by fitting the peaks in the ion mobility spectrum with a gaussian curve. The error bars represent the standard deviation of three individual measurements.