

Supplementary material

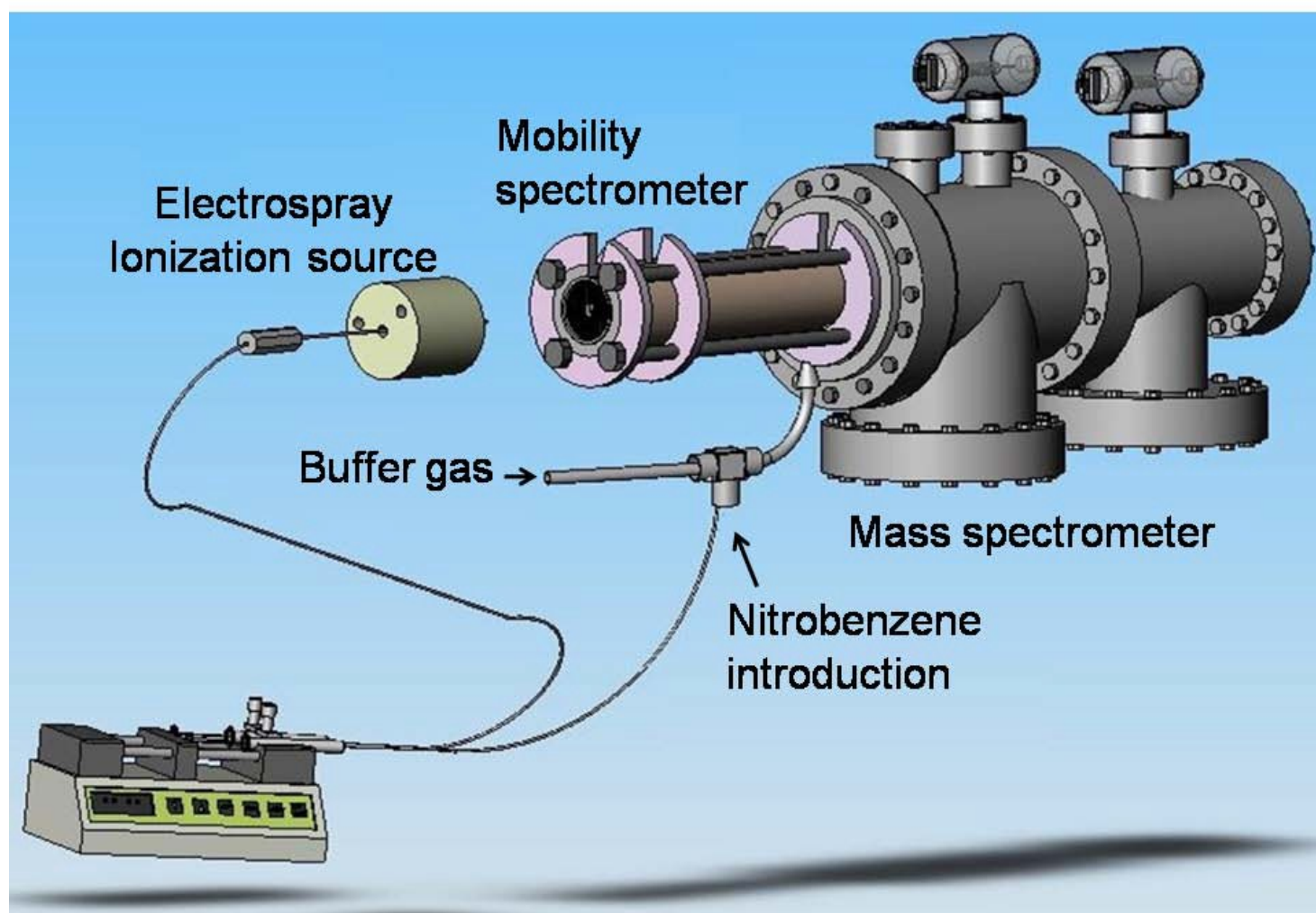


Figure S1 The IMS-MS instrument

A small sample of experiments, in chronological order, that calculated K_0 with respect to the given chemical standard

2,4-lutidine (107 Da)

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Karpas, Z. (1989). Evidence of proton-induced cyclization of α , ω -diamines from ion mobility measurements. *International journal of mass spectrometry and ion processes*, 93(2), 237-242.

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- Rearden P, Harrington PB (2005) Rapid screening of precursor and degradation products of chemical warfare agents in soil by solid-phase microextraction ion mobility spectrometry (SPMEIMS). *Anal Chim Acta* 545(1):13-20
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Karpas, Z., Cohen, G., Atweh, E., Barnard, G., & Golan, M. (2012). Recent applications of ion mobility spectrometry in diagnosis of vaginal infections. *International Journal of Spectroscopy*, 2012.

Karpas, Z., Guamán, A. V., Pardo, A., & Marco, S. (2013). Comparison of the performance of three ion mobility spectrometers for measurement of biogenic amines. *Analytica chimica acta*, 758, 122-129.

Holness, H. K. (2013). The Utilization of Chiral Ion Mobility Spectrometry for the Detection of Enantiomeric Mixtures and Thermally Labile Compounds. PhD dissertation. Florida International University.

Kanu, A. B., & Leal, A. (2016). Identity Efficiency for High-Performance Ambient Pressure Ion Mobility Spectrometry. *Analytical chemistry*, 88(6), 3058-3066.

4-Nitrobenzonitrile (Molecular Weight 148.1)

Fetterolf DD, Clark TD (1993) Detection of trace explosive evidence by ion mobility spectrometry. *J Forensic Sci* 38(1):28–39

Anisole and naphthalene (Molecular Weights 108.1 and 128.2, respectively)

Beitz, T., Laudien, R., Löhmannsröben, H. G., & Kallies, B. (2006). Ion mobility spectrometric investigation of aromatic cations in the gas phase. *The Journal of Physical Chemistry A*, 110(10), 3514-3520

Dipropylene glycol monomethyl ether (DPGME) (Molecular Weight 148.2)

United States Environmental Protection Agency, Office of Research and Development, and N.H.S.R. Centre (2003) Ion mobility spectrometer test/QA plan: verification of portable ion mobility spectrometers for detection of chemicals and chemical agents in buildings.

Hill CA, Thomas CLP (2005) Programmable gate delayed ion mobility spectrometry-mass spectrometry: a study with low concentrations of dipropylene-glycol-monomethyl-ether in air. *Analyst* 130(8):1155–1161.

Diethylphthalate (Molecular Weight 390.6)

Budde KJ, Holzapfel WJ, Beyer MM (1993) Test method for the determination of organic contamination from minienvironments using Ion Mobility Spectrometry (IMS). Semiconductor Equipment and Materials International (SEMI) Documents E46-0301, 2238 & 0307

DTBP (Molecular Weight 191.3)

Viidanoja, J., Sysoev, A., Adamov, A., & Kotiaho, T. (2005). Tetraalkylammonium halides as chemical standards for positive electrospray ionization with ion mobility spectrometry/mass spectrometry. *Rapid communications in mass spectrometry*, 19(21), 3051-3055.

Pedersen CS, Lauritsen FR, Sysoev A, Viitanen AK, Mäkelä JM, Adamov A, Laakia J, Mauriala T, Kotiaho T (2008) Characterization of proton-bound acetate dimers in ion mobility spectrometry. *J Am Soc Mass Spectrom* 19(9):1361

Viitanen AK, Mauriala T, Mattila T, Adamov A, Pedersen CS, Makela JM, Marjamaki M, Sysoev A, Keskinen J, Kotiaho T (2008) Adjusting mobility scales of ion mobility spectrometers using 2, 6-DtBP as a reference compound. *Talanta* 76(5):1218– 1223

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Tadjimukhamedov FA, Stone JA, Papanastasiou D, Rodriguez JE, Mueller W, Sukumar H, Eiceman GA (2008) Liquid chromatography/ electrospray ionization/ion mobility spectrometry of chlorophenols with full flow from large bore LC columns. *Int J Ion Mobil Spectrom* . doi:10.1007/s12127-008-0004-7

Nousiainen, M., Holopainen, S., Puton, J., & Sillanpää, M. (2011). Fast detection of methyl tert-butyl ether from water using solid phase microextraction and ion mobility spectrometry. *Talanta*, 84(3), 738-744.

Crawford, C. L., Graf, S., Gonin, M., Fuhrer, K., Zhang, X., & Hill, H. H. (2011). The novel use of gas chromatography-ion mobility-time of flight mass spectrometry with secondary electrospray ionization for complex mixture analysis. *International Journal for Ion Mobility Spectrometry*, 14(1), 23-30.

Sabo, M., Malásková, M., Harmathová, O., Hradski, J., Masár, M., Radjenovic, B., & Matejčík, S. (2015). Direct Liquid Sampling for Corona Discharge Ion Mobility Spectrometry. *Analytical chemistry*, 87(14), 7389-7394.

All the present author's papers on IMS

Nicotinamide (Molecular Weight 122.1)

Fytche LM, Hupe M, Kovar JB, Pilon P (1992) Ion mobility spectrometry of drugs of abuse in customs scenarios—concentration and temperature study. *J Forensic Sciences* 37(6):1550–1566. Nicotinamide for narcotics

Jackson RA (1998) US Patent 5796099 pressure based calibration correction of an ion mobility spectrometer. Barringer Instruments Ltd, United States

Danylewych-May L, Kuja F (2001) US Patent 6291821—Method of monitoring the status of the gas drying system in an ion mobility spectrometer. Barringer Research Limited

Patchett ML, Minoshima Y, Harrington PB (2002) Detection of gamma-hydroxybutyrate and gamma-butyrolactone by ion mobility spectrometry. *Spectrosc* 17(11):16–24

Bota GM, Harrington PB (2006) Direct detection of trimethylamine in meat food products using ion mobility spectrometry. *Talanta* 68(3):629–635

Wang YS, Nacson S, Pawliszyn J (2007) The coupling of solidphase microextraction/surface enhanced laser desorption/ionization to ion mobility spectrometry for drug analysis. *Anal Chim Acta* 582 (1):50–54

Verkouteren, J. R., & Staymates, J. L. (2011). Reliability of ion mobility spectrometry for qualitative analysis of complex, multicomponent illicit drug samples. *Forensic science international*, 206(1), 190-196.

Demoranville, L. T., Houssiau, L., & Gillen, G. (2013). Behavior and evaluation of tetraalkylammonium bromides as instrument test materials in thermal desorption ion mobility spectrometers. *Analytical chemistry*, 85(5), 2652-2658.

Fullerenes (Molecular Weight 720.6 for fullerene)

Ruotolo BT, Gillig KJ, Stone EG, Russell DH, Fuhrer K, Gonin M, Schultz JA (2002) Analysis of protein mixtures by matrixassisted laser desorption ionization-ion mobility-orthogonal-timeof-flight mass spectrometry. *Int J Mass Spectrom* 219(1):253–267

Woods AS, Koomen JM, Ruotolo BT, Gillig KJ, Russel DH, Fuhrer K, Gonin M, Egan TF, Schultz JA (2002) A study of peptidepeptide interactions using MALDI ion mobility o-TOF and ESI mass spectrometry. *J Am Soc Mass Spectrom* 13(2):166–169

Hexachloroethane (Molecular Weight 236.7)

Patchett ML, Minoshima Y, Harrington PB (2002) Detection of gamma-hydroxybutyrate and gamma-butyrolactone by ion mobility spectrometry. *Spectrosc* 17(11):16–24

Hydrated proton ion (Ion mass 19)

Kebarle, P., Searles, S. K., Zolla, A., Scarborough, J., & Arshadi, M. (1967). The solvation of the hydrogen ion by water molecules in the gas phase. Heats and entropies of solvation of individual reactions: $H^+ (H_2O)_{n-1} + H_2O \rightarrow H^+ (H_2O)_n$. *J Am Chem Soc* 89 (25):6393–6399.

Tabrizchi M (2001) Temperature corrections for ion mobility spectrometry. *Appl Spectrosc* 55(12):1653–1659.

Iodine (Molecular Weight 253.8)

Buryakov IA (2003) Qualitative analysis of trace constituents by ion mobility increment spectrometer. *Talanta* 61(3):369–375

Methylsalicylate (Molecular Weight 152.1)

Buxton TL, Harrington PB (2001) Rapid multivariate curve resolution applied to identification of explosives by ion mobility spectrometry. *Anal Chim Acta* 434(2):269–282

Patchett ML, Minoshima Y, Harrington PB (2002) Detection of gamma-hydroxybutyrate and gamma-butyrolactone by ion mobility spectrometry. *Spectrosc* 17(11):16–24

Verkouteren M, Windsor E, Fletcher R, Maditz R, Smith W, Gillen G (2006) Inkjet metrology and standards for ion mobility spectrometry. *Int J Ion Mobil Spectrom* 9(1):19–23

Miller RA, Nazarov EG, Zapata A, Davis CE, Eiceman GA, Bashall AD (2007) US Patent 7057168 systems for differential ion mobility analysis. S. Corporation, United States

Tetraalkylammonium Ions (Molecular Weight 242.5 for Tetrabutylammonium ions)

Viidanoja J, Sysoev A, Adamov A, Kotiaho T (2005) Tetraalkylammonium halides as chemical standards for positive electrospray ionization with ion mobility spectrometry/mass spectrometry. *Rapid Commun Mass Spectrom* 19(21):3051–5.

Ude S, De la Mora JF (2005) Molecular monodisperse mobility and mass standards from electrosprays of tetra-alkyl ammonium halides. *J Aerosol Sci* 36(10):1224–1237.

Trinitrotoluene (Molecular Weight 227.1)

Buxton TL, Harrington PB (2001) Rapid multivariate curve resolution applied to identification of explosives by ion mobility spectrometry. *Anal Chim Acta* 434(2):269–282

Kanu AB, Hill HH (2007) Identity confirmation of drugs and explosives in ion mobility spectrometry using a secondary drift gas. *Talanta* 73(4):692–699

A small sample of experiments that calculated K_0 from instrumental parameters:

Bush, M. F., Campuzano, I. D., & Robinson, C. V. (2012). Ion mobility mass spectrometry of peptide ions: effects of drift gas and calibration strategies. *Analytical chemistry*, 84(16), 7124-7130.

Kanu, A. B., Kumar, B. S., & Hill, H. H. (2012). Evaluation of micro-versus nano-electrospray ionization for ambient pressure ion mobility spectrometry. *International Journal for Ion Mobility Spectrometry*, 15(1), 9-20.

Hauck, B. C., Siems, W. F., Harden, C. S., McHugh, V. M., & Hill Jr, H. H. (2016). E/N effects on K_0 values revealed by high precision measurements under low field conditions. *Review of Scientific Instruments*, 87(7), 075104.

A small sample of experiments that measured the drift tube temperature, do not mention which temperature (drift gas or drift tube) they measured, do not even mention the temperature of the experiments, or measured the drift gas temperature before entering the drift tube (alphabetical order)

S. H. Kim, K. R. Betty, F. W. Karasek, *Anal. Chem.* 50 (13), 1784-1788 (1978).
<https://doi.org/10.1021/ac50035a018>

Z. Karpas, Z. Berant, O. Shahal, *J. Am. Chem. Soc.* 111 (16), 6015-6018 (1989).
<https://doi.org/10.1021/ja00198a007>

S. J. Valentine, J. G. Anderson, A. D. Ellington, D. E. Clemmer, *J. Phys. Chem. B.* 101 (19), 3891-3900 (1997).
<https://doi.org/10.1021/jp970217o>

D. E. Clemmer, M. F. Jarrold, *J. Mass Spectrom.* 32 (6), 577-592 (1997). [https://doi.org/10.1002/\(SICI\)1096-9888\(199706\)32:6<577::AID-JMS530>3.0.CO;2-4](https://doi.org/10.1002/(SICI)1096-9888(199706)32:6<577::AID-JMS530>3.0.CO;2-4)

A. E. Counterman, S. J. Valentine, C. A. Srebalus, S. C. Henderson, C. S. Hoaglund, D. E. Clemmer, *J. Am. Soc. Mass Spectrom.* 9 (8), 743-759 (1998). [http://dx.doi.org/10.1016/S1044-0305\(98\)00052-X](http://dx.doi.org/10.1016/S1044-0305(98)00052-X)

T. Wyttenbach, J. J. Batka Jr., J. Gidden, M. T. Bowers, *Int. J. Mass Spectrom.* 193 (2), 143-152 (1999).
[http://dx.doi.org/10.1016/S1387-3806\(99\)00113-X](http://dx.doi.org/10.1016/S1387-3806(99)00113-X)

S. C. Henderson, S. J. Valentine, A. E. Counterman, D. E. Clemmer, *Anal. Chem.* 71 (2), 291-301 (1999).
<https://doi.org/10.1021/ac9809175>

G. A. Eiceman, E. G. Nazarov, J. E. Rodriguez, J. A. Stone. Analysis of a drift tube at ambient pressure: Models and precise measurements in ion mobility spectrometry. *Review of Scientific Instruments*, 72(9), 3610-3621 (2001).
<http://dx.doi.org/10.1063/1.1392339>

G. A. Eiceman, E. G. Nazarov, J. A. Stone, *Anal. Chim. Acta.* 493 (2), 185-194 (2003).
[http://dx.doi.org/10.1016/S0003-2670\(03\)00762-1](http://dx.doi.org/10.1016/S0003-2670(03)00762-1)

A. E. Counterman, D. E. Clemmer, *J. Phys. Chem. B.* 108 (15), 4885-4898 (2004).
<https://doi.org/10.1021/jp036454a>

J. Gidden, A. Ferzoco, E. Shammel-Baker, M. T. Bowers. *J. Am. Chem. Soc.* 126 (46), 15132-15140 (2004).
<https://doi.org/10.1021/ja046433+>

A. S. Woods, M. Ugarov, T. Egan, J. Koomen, K. J. Gillig, K. Fuhrer, M. Gonin, J. A. Schultz, *Anal. Chem.* 76 (8), 2187-2195 (2004). <https://doi.org/10.1021/ac035376k>

S. I. Merenbloom, S. L. Koeniger, B. C. Bohrer, S. J. Valentine, D. E. Clemmer, *Anal. Chem.* 80 (6), 1918-1927 (2008). <https://doi.org/10.1021/ac7018602>

R. Fernandez-Maestre, C. S. Harden, R. G. Ewing, C. L. Crawford, H. H. Hill Jr. *Analyst*, 135 (6), 1433-1442 (2010). <https://doi.org/10.1039/B915202D>

R. Fernandez-Maestre, C. Wu, H. H. Hill, *Anal. Meth.* 7, 863-869 (2015). <https://doi.org/10.1039/c4ay01814a>

D. Meza-Morelos, R. Fernandez-Maestre, H. H. Hill, *Int. J. Ion Mobil. Spectrom.* 19 (2), 145-153. (2016).
<https://doi.org/10.1007/s12127-016-0199-y>