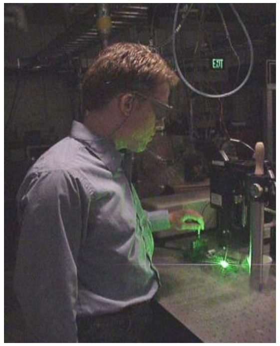

Detection of Trace Explosives by Ion Mobility-Mass Spectrometry

C.L. Beppler, Ph.D.

Explosive Technologies Group

Unclassified-Unlimited Release

Sandia National Laboratories

Explosives Detection

http://www.securityinfowatch.com/root+level/1281760
RKB Database, www.rkb.us

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Ion Mobility Spectrometry

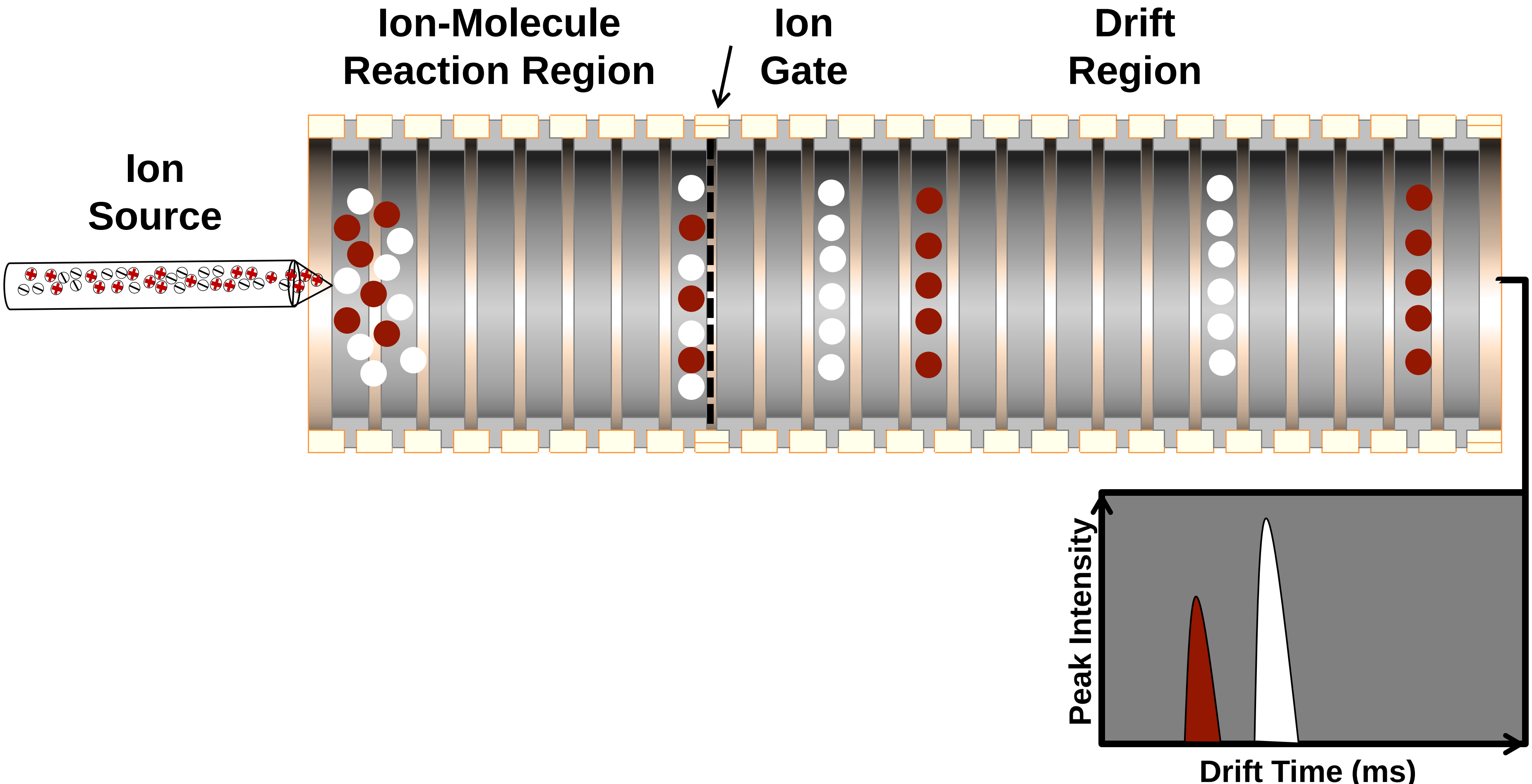
Commercial ^{63}Ni-IMS System

Advantages of IMS

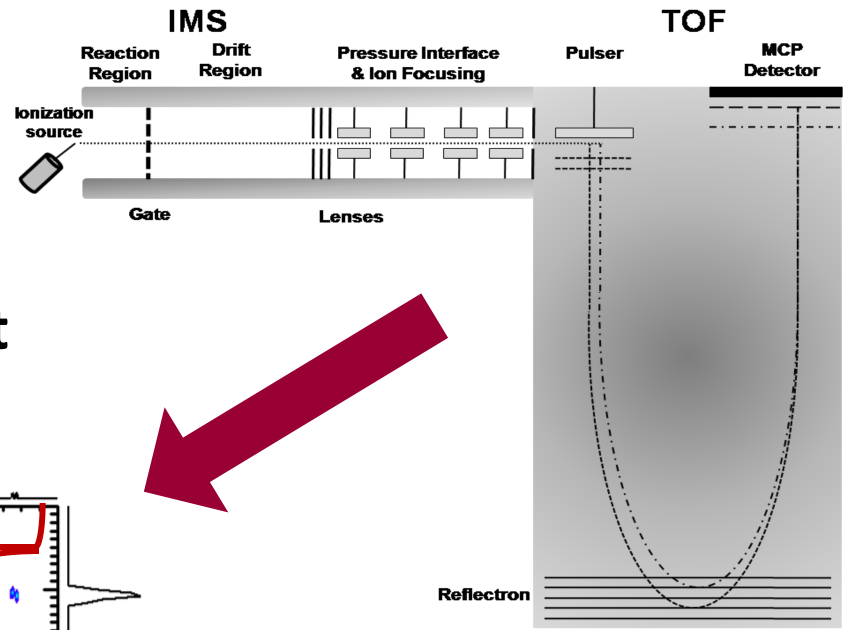
- Gas phase ion separation by size/charge
- Quick analysis cycle (under 6 seconds)
- Commercial systems easy to operate; currently deployed worldwide
- Air is carrier gas
- Good qualitative instrument
- Sub ppb detection limit for many explosives

http://www.smithsdetection.com/IONSCAN_400B.php

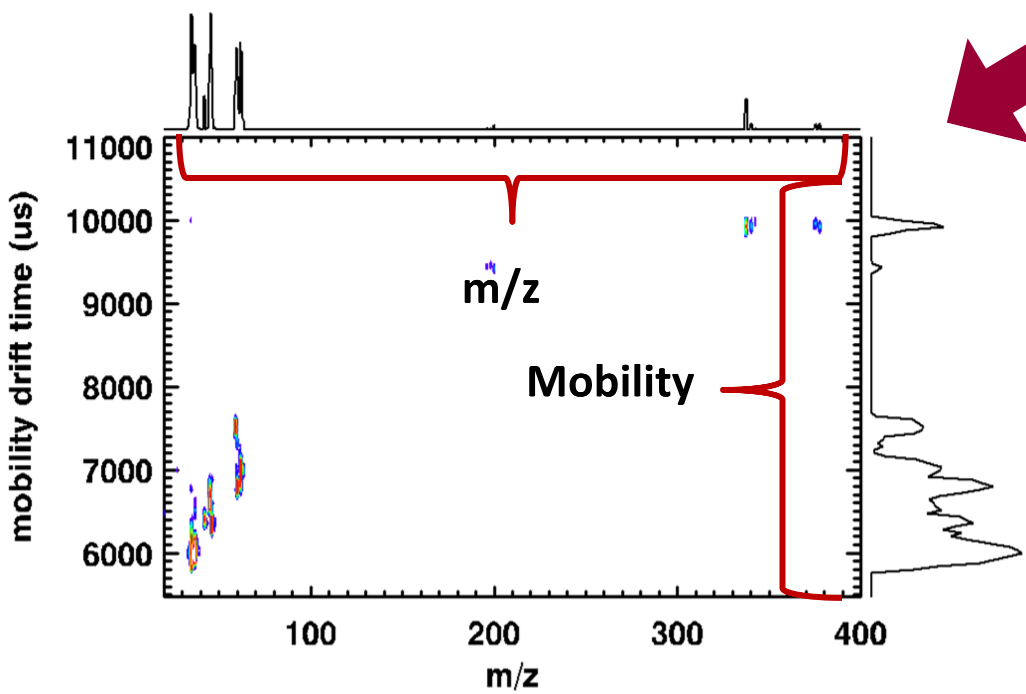
Ion Mobility Spectrometry



Simultaneous Mobility-Mass ID



2D Mobility-Mass Plot



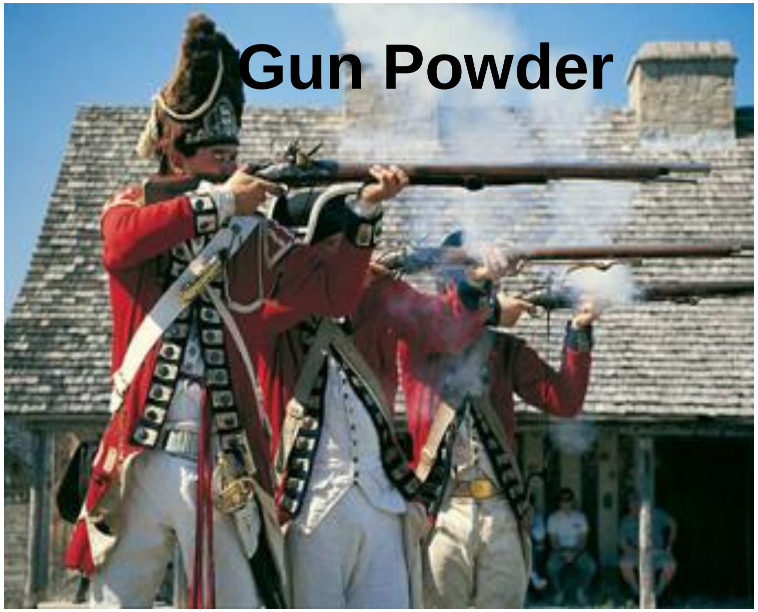
Reduced Mobility values identify analytes in IMS

$$K_0 = \left(\frac{L^2}{Vt_d}\right)\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)$$


Fireworks


Obscurants


Incendiary
Devices


Gun Powder

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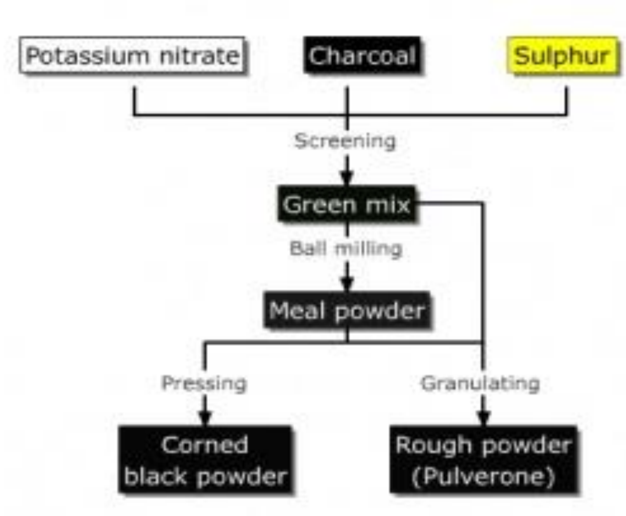
Black Powder by IMMS

- Obtain a K_0 value for black powder
- Mass ID the ion species that make up the mobility peak
- Determine differences in K_0 values for black powders from differing origins
- Published in *Analytical Chemistry*



Anal. Chem. ***2010*, *82*, 387–393**

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Previous Black Powder Detection Methods

Direct Chemical Methods

- Chemical spot testing: using a reagent that confirms presence of potassium nitrate or sulfur

Spectroscopic Methods

- Refractive Index measurements, x-ray powder diffraction, emission spectrography, polarizing microscopy

Chromatographic Methods

- TLC, ion chromatography/conductivity detection

IMS

- Barringer IONSCAN Model 200

MS

- TOF-SIMS & LDI-TOF-MS

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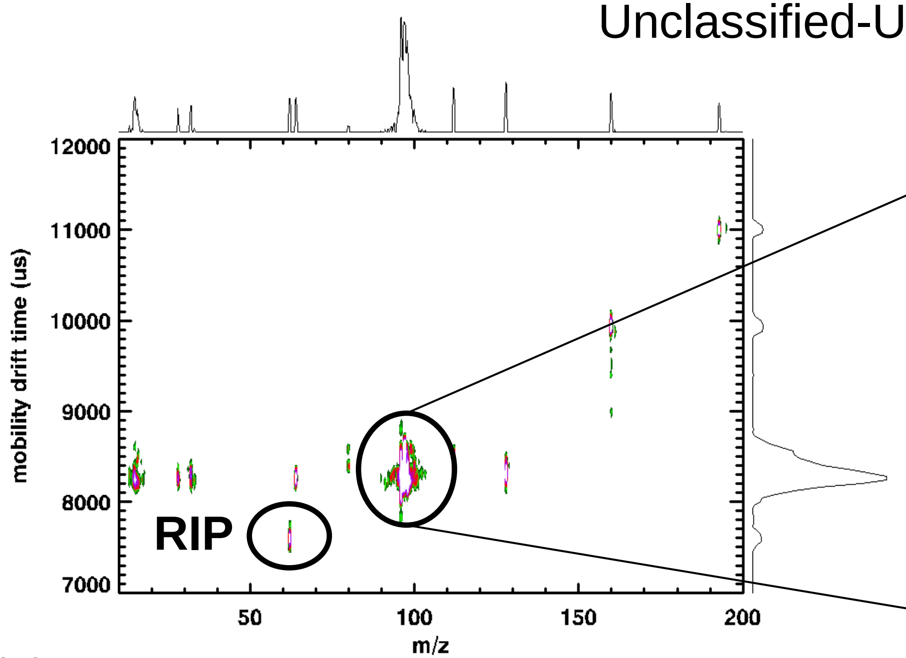
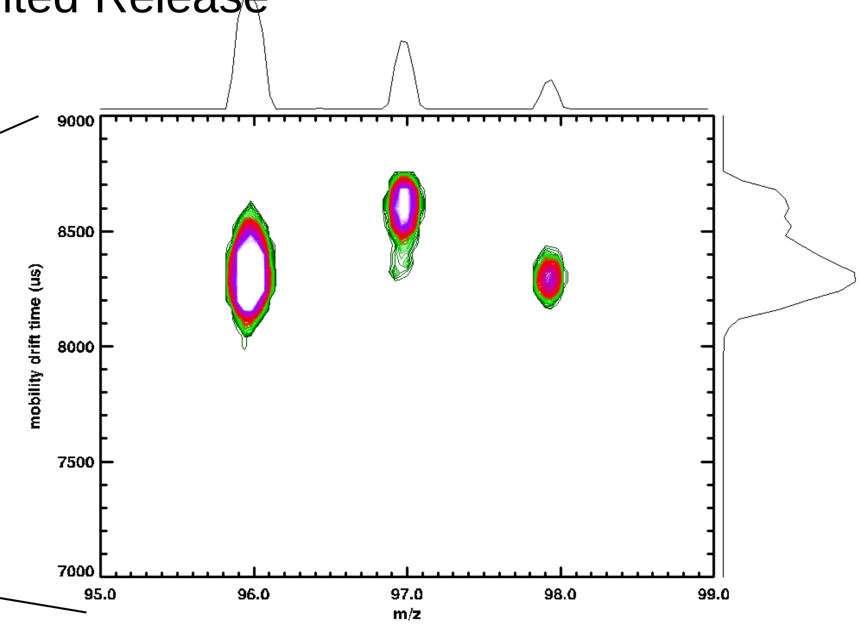
Results & Conclusions

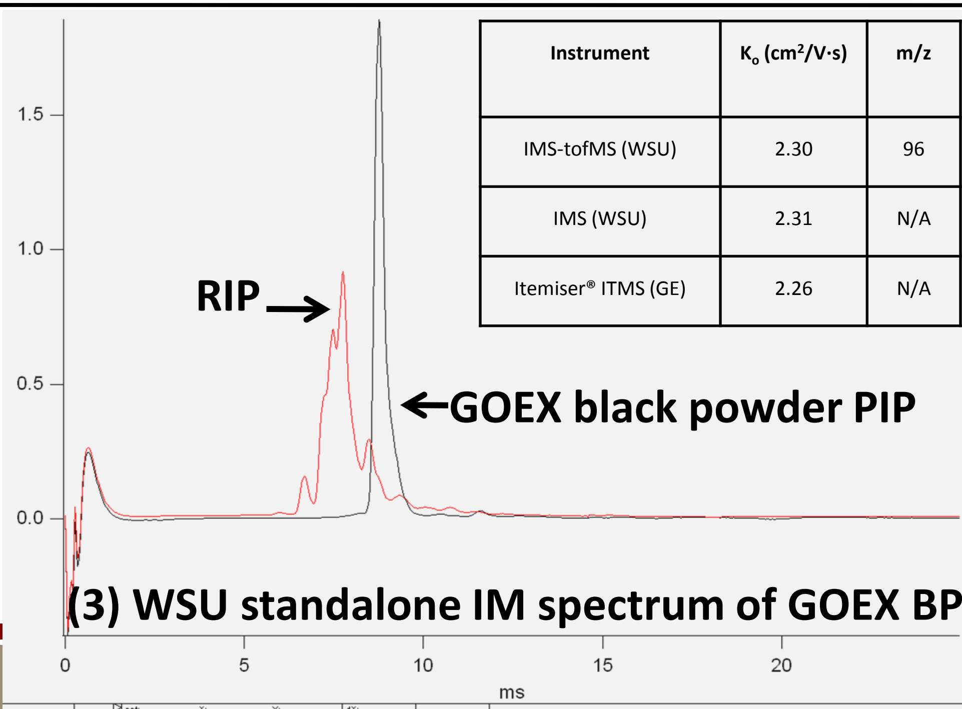
- Black powder successfully detected using ^{63}Ni-IM-TOFMS
- *First reported* K_0 value for the primary black powder mobility peak at 2.28±0.02 $cm^2V^{-1}s^{-1}$
  - S_n^- clusters where n=1-4
- Regardless of origin, each BP sample produced the same product ions
- ^{63}Ni-IM-TOFMS should be used in future black powder analyses



(1) 2D Mobility-Mass plot of GOEX Black Powder

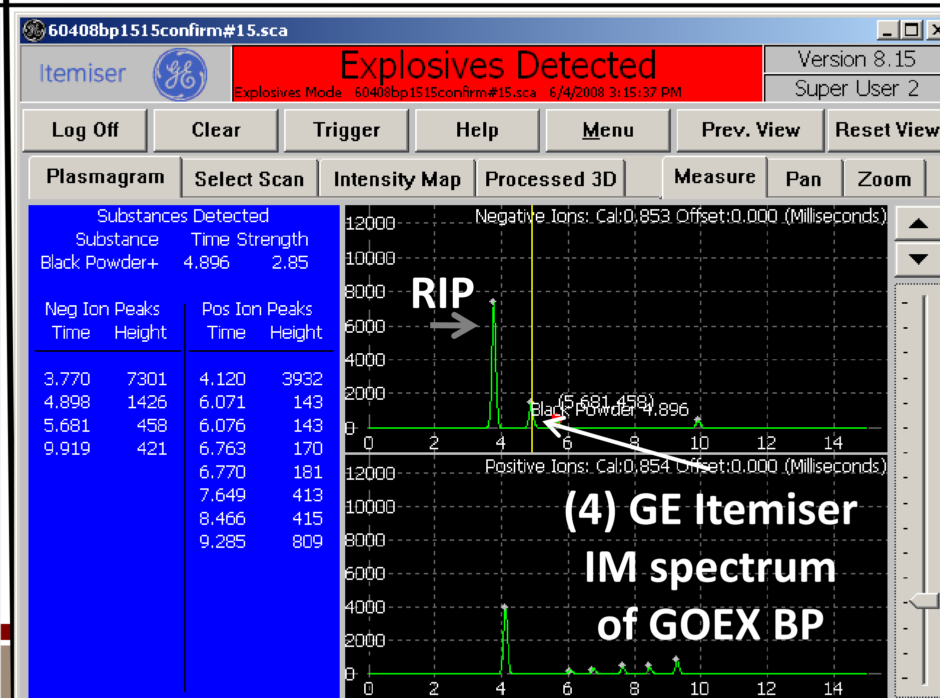


(2) Inset showing most intense peak from plot (1)



Instrument	K_o (cm²/V·s)	m/z
IMS-tofMS (WSU)	2.30	96
IMS (WSU)	2.31	N/A
Itemiser® ITMS (GE)	2.26	N/A

(3) WSU standalone IM spectrum of GOEX BP



(4) GE Itemiser IM spectrum of GOEX BP

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Reproducibility of BP Measured K_0 Values

- GOEX black powder on three IMS systems: IM-TOFMS, standalone IMS and GE Security's ITEMISER IMS
- Intense broad mobility peak sample with a K_0 of *2.29 ± 0.03 cm²V⁻¹s⁻¹*

Instrument	System Type	Drift Time	K_o ($cm^2V^{-1}s^{-1}$)	Nominal m/z value
IM-TOFMS (WSU)	Hybrid	8.331±0.025	2.30	128
IMS (WSU)	Standalone	8.750±0.000	2.31	Not applicable
Itemiser® ITMS (GE)	Standalone	4.176±0.022	2.26	Not applicable

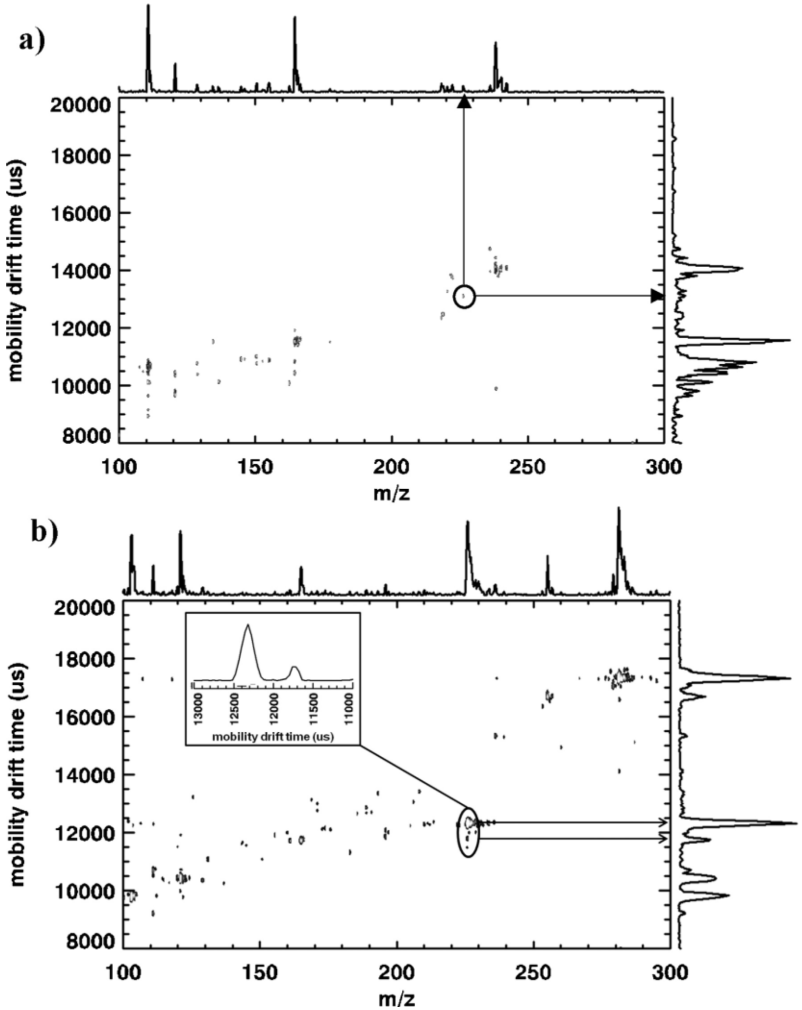
Evaluation of Interferences with Explosives by IMMS

- Evaluate ingredients in common household products for mass and mobility interferences with explosives
- Demonstrate a need for simultaneous mobility-mass measurements for accurate threat detection in complex mixture analysis
- Published in Analytica Chimica Acta

Analytica Chimica Acta, 2013. 795: p. 36-43.

Results & Conclusions

- Two common household ingredients influenced IMMS response for TNT and RDX
  - Enhanced and suppressed IMMS response
- Ions from the ingredients shared a similar m/z and drift time range for the common explosives
- The mobility separation often produced several K_0 values for each m/z identified ion species
- The samples were rich in isomeric species
  - The mobility separation found several more examples of isobaric species for the identified ions
- Reported new K_0 values for PCP ingredients



Summary & Overall Conclusions

- Ion Mobility Spectrometry (IMS) is a proven trace explosives detection technology
- Mass spectrometry coupled to IMS enhances both the IMS and MS data output
- The future of IMS and IMMS
  - Complex mixture characterization
  - Detection of trace, non-explosive threat compounds
  - Further hybridization with separation techniques (GC,LC, CE, etc.) and mass spectrometers (TOFs, etc.)

Acknowledgements

Sandia National Laboratories

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Institutional Support

- Washington State University (Pullman, WA)
- Dr. Herbert H. Hill, Jr. Research Group (Chemistry Dept.)

Funding Support

- National Science Foundation
- SAIC
- Savannah River National Laboratory
- Safran Morpho (formerly GE Security)

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Morpho
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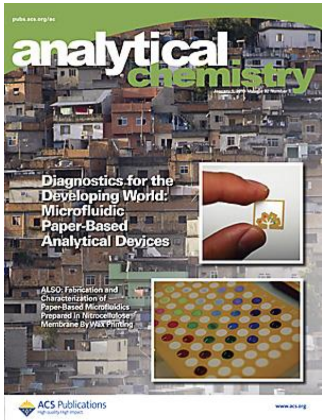
Relevant References



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