RESEARCH ARTICLE

Ion Mobility Spectrometry - High Resolution LTQ-Orbitrap Mass Spectrometry for Analysis of Homemade Explosives

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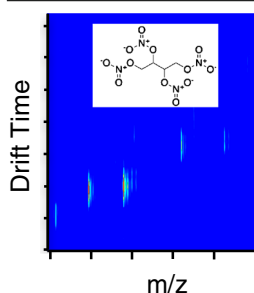
Abstract. The detailed chemical characterization of homemade explosives (HMEs) and other chemicals that can mimic or mask the presence of explosives is important for understanding and improving the performance of commercial instrumentation used for explosive detection. To that end, an atmospheric-pressure drift tube ion mobility spectrometry (IMS) instrument has been successfully coupled to a commercial tandem mass spectrometry (MS) system. The tandem MS system is comprised of a linear ion trap and a high resolution Orbitrap analyzer. This IMS-MS combination allows extensive characterization of threat chemical compounds, including HMEs, and complex real-world background chemicals that can interfere with detection. Here, the composition of ion species originating from a specific HME, erythritol tetranitrate, has been elucidated using accurate mass measurements, isotopic ratios, and tandem MS. Gated IMS-MS and high-resolution MS have been used to identify minor impurities that can be indicative of the HME source and/or synthesis route. Comparison between data obtained on the IMS/MS system and on commercial stand-alone IMS instruments used as explosive trace detectors (ETDs) has also been performed. Such analysis allows better signature assignments of threat compounds, modified detection algorithms, and improved overall ETD performance.

Keywords: Homemade explosive, ETN, Ion mobility, Mass spectrometry, ETD

Introduction

Ion mobility spectrometry (IMS) is one of the most widely used screening tools to identify potentially hazardous materials, such as drugs, chemical weapons, or explosives [1–4]. More than 30,000 stand-alone IMS systems have been deployed worldwide in military and homeland protection applications. However, these deployed IMS instruments typically have lower resolving power than laboratory IMS instruments, resulting in potential for false positive or false negative detections, particularly when the threat is present in a complex mixture [5]. Additionally, newly emerging threats may be misidentified or completely missed. These include a variety of HMEs, which can be synthesized from or contain commonly available ingredients (including peroxides, sugars, ammonium nitrate, etc.). Owing to the relative ease and low cost for its large-scale synthesis, erythritol tetranitrate (ETN, 1,3,4-trinitrooxybutan-2-yl nitrate, Scheme 1) has become a popular HME [6]. ETN is the nitrate ester of erythritol and is structurally analogous to the more well-known explosive pentaerythritol tetranitrate (PETN, Scheme 1). Instructions for ETN synthesis are easily accessible on the internet. The availability of the main starting material (erythritol, a main ingredient in some commercial "alternative" sweeteners) and ETN's chemical and physical properties (e.g., relatively low melting point) make it a desirable component in melt cast mixtures with other high explosives [7] such as PETN and 1,3,5-trinitro-1,3,5-triazinane (RDX).

On-line coupling between IMS and MS instruments has proven to be a powerful analytical platform with a multitude of successful applications from physics to biology [4, 8–10]. These include characterization of complex mixtures in

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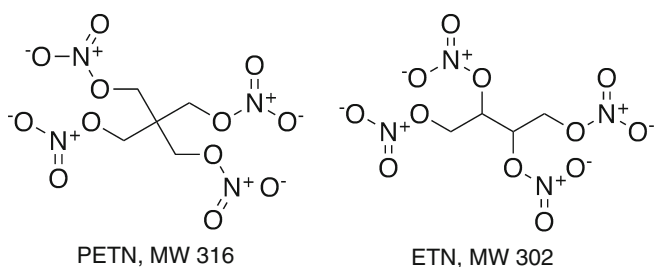
Scheme 1. PETN (pentaerythritol tetranitrate) and ETN (erythritol tetranitrate) structures

proteomics and metabolomics, as well as 3-D structural elucidation of large biomolecules and their complexes [11–20]. A number of IMS-MS studies aimed at elucidating various aspects regarding traditional IMS analysis of explosives and other threat compounds have also been reported [21–26]. IMS can provide chemical separation based upon differences in the size, shape, and charge of analyte ions, and their effective interactions with drift gas molecules. In addition to IMS-derived information, MS can provide unequivocal identification of chemical species using high mass accuracy in combination with tandem MS. Drift-tube ion mobility (DTIMS) as well as differential ion mobility (DIMS) instruments have been interfaced with different types of mass analyzers (including time-of-flight, magnetic sector, and ion trap) resulting in powerful multidimensional analytical combinations [27]. Here we utilize a DTIMS instrument coupled to a tandem high-resolution/accurate mass (HRAM) MS instrument for characterization of threat materials. We illustrate the advantages of this system for characterization of gas-phase ion chemistry processes occurring during IMS analysis of explosives using ETN, synthesized from different starting materials and by different routes. In parallel, data have been acquired with a commercial stand-alone DTIMS-based explosives trace detection (ETD) system. The flexible atmospheric pressure IMS-MS interface readily allows for "gold standard" comparison with and characterization of current generation DTIMS-based ETD instruments, as well as future IMS threat detection systems that are in development. The IMS-MS instrument presented here is equipped with three different ionization sources – electrospray ionization (ESI), corona discharge (CD), as well as ^{63}Ni. In addition, the IMS interface allows for modification of reagent/drift gases and the introduction of dopant materials, which can be used to alter the ionization chemistry or ion transport processes. Currently deployed ETD systems utilize ^{63}Ni for ionization, whereas newer models rely on CD and other non-radioactive methods. Replacing ion sources in commercial ETDs may require alterations to the detection bands or algorithms used by these instruments. Therefore, a combined IMS-MS approach is also valuable to study the effects of alternate ionization sources on threat material identification. Although IMS combined with low resolution MS and MS/MS analyzers have been previously used to probe the gas phase ion chemistry of explosives [2, 21–24, 28, 29], this is to our knowledge the first such study of explosives using a higher resolution DTIMS coupled to a high resolution MS/MS instrument.

Experimental

Sample Preparation

Certified reference standard samples of explosives (PETN, ETN, TNT, RDX) were purchased from Accustandard (New Haven, CT, USA) as 1 mg/mL stock solutions in acetonitrile or methanol and were diluted as needed. In an effort to approximate clandestine preparation of explosives, small quantities of ETN were also synthesized in-house. Either food grade (Truvia brand sweetener, purchased from a local food store) or analytical grade erythritol were nitrated by reaction with acetyl nitrate or with mixed sulfuric and nitric acids, according to procedures detailed in Oxley et al. [30]. All required chemicals and solvents, including erythritol, acetyl nitrate, ammonium nitrate, sulfuric acid, isopropanol, and acetone, were purchased from Sigma Aldrich (St. Louis, MO, USA).

IMS, IMS-MS, and MS Analyses

IMS-MS analyses were performed using an Excellims (Acton, MA, USA) MA3100 HPIMS coupled to a Thermo Fisher (San Jose, CA, USA) LTQ-Orbitrap Velos mass spectrometer. The IMS instrument (Figure 1) can be readily installed in place of the standard IonMax ESI ion source provided with the MS instrument, requiring no additional hardware changes or modifications, and is controlled using a simple graphical user interface. Multiple sample introduction and ionization methods can be utilized, including direct infusion ESI and thermal desorption with subsequent CD or ^{63}Ni ionization. Changing ionization modes requires only a few minutes to exchange the ion source chamber (Figure 1). IMS resolving power in excess of 100 has been reported for this instrument [31].
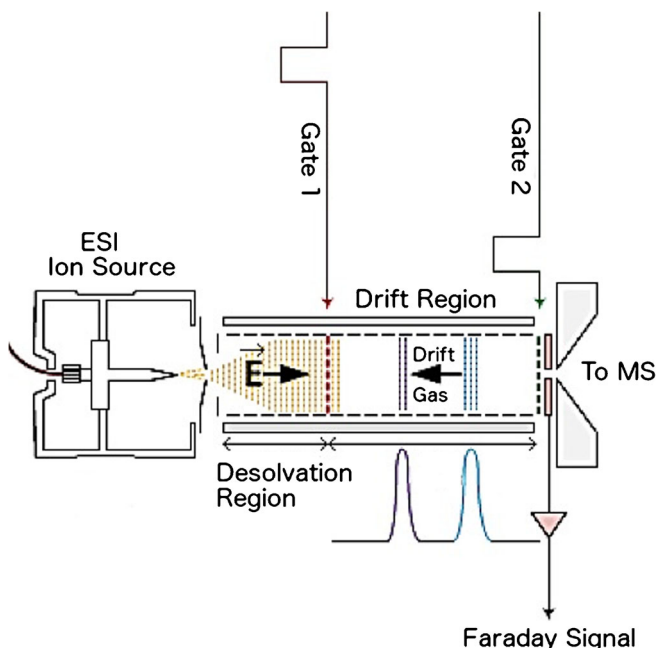

Figure 1. Schematic of the DTIMS portion of the instrument (ESI source configuration shown)

For most experiments, explosive samples were ionized directly from solution by ESI operated at ~2.5 kV relative to the entrance of the IMS desolvation region. In some cases (specifically noted in the text), samples were first deposited on swabs (DSA Detection, North Andover, MA, USA) and then thermally desorbed at 180°C. Desorbed sample molecules (including products of thermal degradation) were ionized either by CD (operated at 1.8 kV in negative ion mode and 2.2 kV in positive ion mode; voltages relative to IMS desolvation region) or ^{63}Ni. For all ionization sources, ions were sampled through an aperture into an intermediate desolvation/reaction region before injection through the entrance gate into the drift region (Figure 1). A cylinder of compressed, dry air (Ultra zero-grade; Airgas, Dallas, TX, USA) was used as an IMS drift gas, which was set to a flow rate of 2.5 L/min. (It is estimated that approximately 1.5 L/min of this gas flow is directly drawn into the mass spectrometer inlet, resulting in an effective drift gas flow of approximately 1 L/min.) In several experiments, approximately 1 ppm$_v$ dichloromethane was added directly to the drift gas using a temperature-controlled permeation tube heater (Excellims) to explore the effects of drift gas modifiers (dopants) on ion formation and ion transport processes. The temperatures of the ionization region, drift gas, and IMS housing were all adjusted to 150°C, which was found to be important for observation of stable chloride ion adducts with explosive standards such as PETN and RDX. Two Bradbury-Nielsen gates – entrance (BNG1, operated at 45 V relative to the drift tube) and exit (BNG2, operated at 150 V relative to the drift tube) – were used to inject ion packages into the 10.56 cm drift region and control the exit of separated ions, respectively. The gates were opened and closed by applying voltage across the wire electrodes with a typical gate pulse width of 70 μs. The drift tube was operated at 10 kV potential. BNG1 was at 62.94% and BNG2 at 7.67% of the total operating potential, resulting in 5.53 kV drop between the two gates (typical field strength of 525 V/cm). While these conditions were optimized for sensitivity and to achieve comparable results to the stand-alone ETD rather than high resolution, a resolving power of greater than 50 was readily achieved. Both positive and negative ion mode spectra were acquired, utilizing multiple detection modes for acquisition of IMS-MS data (see Discussion below). Measured drift times for unknown species were calibrated against well-characterized chemical standards (TNT and 2,6-di-tert-butylpyridine for negative and positive modes, respectively) in order to determine the respective reduced mobilities (K_0) [32]. High-resolution MS-only data were also collected on the Orbitrap at better than 60,000 resolving power, allowing typical mass accuracy better than 3 ppm, following the manufacturer's standard external calibration procedure. Elemental composition assignments from the accurate mass data were determined using the calculators built into the Xcalibur software (Thermo Fisher Scientific). Two-dimensional (2-D) IMS-MS data analysis and plotting was performed using the Excellims developed software, VisIon Trap.

Stand-alone IMS data were collected using a Smiths Detection ETD (Ionscan 500DT; London, UK). This ETD instrument thermally desorbs samples from swabs for ionization in a ^{63}Ni source and detects both positive and negative ions. All instrument parameters were under the control of the manufacturer software and could not be adjusted [33]. Instead, parameters for the hybrid IMS-MS system (e.g., desorber and drift tube temperatures) were adjusted as described above to allow observation of similar ion species in both systems for explosive standards such as RDX and PETN. A resolving power of ~40 has been reported for this standalone IMS instrument [29, 34]. Drift gas was supplied from room air that had been passed through a drying column to eliminate significant humidity effects. In some experiments, the manufacturer-supplied drift gas dopant cartridge that enhances explosive detection through formation of chloride adducts was removed to allow for direct comparison with the IMS-MS instrument. K_0 values included in the manufacturer-supplied software package were cross-calibrated against published K_0 values for well-characterized explosive standards.

Safety Precautions

Small-scale syntheses of energetic materials should only be conducted by appropriately trained personnel following all necessary safety protocols. Althugh solutions containing trace quantities of explosives are safe for manipulation and analysis outside of a fume hood, all such samples should be handled with caution. The radioactive ^{63}Ni ionization source should be used only by appropriately trained personnel.

Results and Discussion

IMS-MS Coupling

We have utilized DTIMS-MS in parallel with traditional stand-alone ETD systems for characterization of threat materials. Typical drift times for a DTIMS are on the order of 10 ms. However, in order for a combined IMS-MS system to provide sufficiently resolved IMS data upon reconstruction, a mass spectrum must be acquired on the order of 10 to 100 μs. Such time scale "nesting" requirements typically restrict the type of mass analyzers that can be directly interfaced with DTIMS to time-of-flight (TOF) mass spectrometers. When IMS is combined with mass analyzers acquiring spectra on the order of hundreds of milliseconds, such as linear quadrupoles and ion traps, the combined system is generally operated in a low duty-cycle "scanning mode" (see below) in order to

accommodate the disparate time scales. Several atmospheric pressure DTIMS combinations with ion trap mass analyzers, including an FTICR spectrometer, have been previously reported [10, 35–38]. Recently, linear frequency chirping of the IMS beam and subsequent Fourier transform decoding of the MS signal has resulted in an increased overall duty cycle of the DTIMS-ion trap system [31]. This approach utilizes multiplexing schemes for ion beam modulation in the IMS including Fourier [39] and Hadamard [40] transforms, also utilized in hybrid DTIMS-TOF instruments [41–43].

The dual gate DTIMS-MS combination [35, 44] used here can operate in four distinct modes. In "open mode," ions drift continuously and unrestricted through both ion gates allowing conventional mass spectral data acquisition. Since ion signal is necessarily reduced in other IMS modes due to reduced duty cycle, high-resolution mass spectra on the Orbitrap are typically collected in "open mode." In addition, this mode facilitates adjustment and optimization of source operating parameters without removing the IMS. In "scan mode," the selected ion mobility range can be scanned by sequentially stepping the delay between the opening of the entrance and exits gates across the chosen range of drift times. This allows the generation of a comprehensive 2-D IMS-MS plot, which is of particular importance for the correlation of specific ion drift times with their corresponding mass spectra and for the multidimensional separation of components of complex mixtures. In "gated mode," mass spectra can be collected at individually specified ion mobilities by applying a predetermined delay between the opening of the entrance and exit gates respectively. This mode uniquely allows for the removal of contaminants and also targeted accumulation of ions in the trap for improved sensitivity and enhanced MS^n fragmentation. Finally, the addition of a Faraday plate detector behind the IMS exit allows the DTIMS to function in "Faraday mode" as an independent, stand-alone instrument. This mode was used for comparison to the ETD system and for concurrent collection of full-scan IMS and MS data. Although the system is capable of operating in an "FT mode" [31], this mode was not utilized for these studies.

ETN Analysis by IMS-MS

The IMS-MS system can interrogate liquid phase samples directly and with minimal sample preparation. Solutions containing ETN have been analyzed directly by ESI, or by CD and ^{63}Ni ionization, after deposition on a swab, drying, and thermal desorption. The ETN samples produce similar anionic species in all three types of ion sources (Figure 2). Elemental composition assignments were confirmed to be $C_4H_7N_4O_{13}$ and $C_4H_6N_5O_{15}$ using accurate mass measurements on the Orbitrap (m/z at 319.0029 and 363.9857, respectively).

The species at m/z 364 is identified as $[ETN + NO_3]^-$, which is consistent with previous studies of ETN and PETN [30]. Formation of the ETN–nitrate anion complex at m/z 364 is more pronounced under CD ionization conditions compared with ESI and ^{63}Ni, perhaps due to a higher concentration of nitrate anions generated by CD under ambient conditions. Although nominally denoted as $[ETN + OH]^-$ in some studies [45], the elemental composition of the anion observed at m/z 319 is also consistent with the in vacuo loss of NO_2 from an ETN anion adduct with HNO_3, analogous to ions observed during IMS-MS studies of PETN [23]. Furthermore, the m/z 319 species may reflect the presence in solution of erythritol trinitrate (ETriN), forming the $[ETriN + NO_3]^-$ anion. ETriN (containing only three NO_3 groups) can be a by-product of incomplete ETN synthesis as well as an ETN degradation product [30, 46]. While it is hypothesized that this ion is at least partially due to the presence of ETriN in solution (see below), it is likely a combination of multiple species and will be referred to by the empirically determined elemental formula. Upon addition of a Cl-atom containing dopant with the ^{63}Ni source, the respective $[ETN + Cl]^-$ and $[ETN + 2Cl]^-$ anion adducts can be readily identified based on characteristic Cl isotopic distribution patterns as well as accurate mass measurements (Table 1).

Evidence for the possible presence of ETriN in solution is further provided by the observation of additional ion species during the IMS-MS analysis of ETN by CD or ^{63}Ni ionization (Table 1). Analogous to m/z 319 species, the Cl adduct ion at m/z 292 can be a mixture of two ions having the same elemental composition, ETriN and a gas-phase ETN fragment, resulting from the loss of NO_2 (as denoted in Table 1). While nominally the anion at m/z 303 is denoted as $[ETN + H]^-$, ion formation by hydride addition to ETN seems much less likely compared with the formation of the $[ETriN + NO_2]^-$ anion adduct with the same elemental composition. Moreover, based on accurate mass measurements, a species at m/z 370 can be interpreted only as an anion adduct of ETriN with trifluoroacetic acid (TFA), plausibly present as a trace impurity either during synthesis or analysis. Indeed, tandem MS data confirmed this assignment, where the sole strong fragment ion was found to have an elemental composition ($C_2F_3O_2$) corresponding to $[TFA – H]^-$ (Table 1). No $[ETN + TFA – H]^-$ adduct was observed. Presumably TFA ion pairing occurs only with ETriN that contains a free hydroxyl group. The ETriN adduct species was observed to be present only in ETN samples synthesized in-house as well as in commercially produced ETN stored for an extended period of time past the stated expiration date, suggesting that the ETriN ions originate predominantly from ETN sample impurities.

ESI IMS-MS spectra obtained for PETN and ETN in "scan mode" are shown in Figure 3. Using TNT as a standard, K_0 values
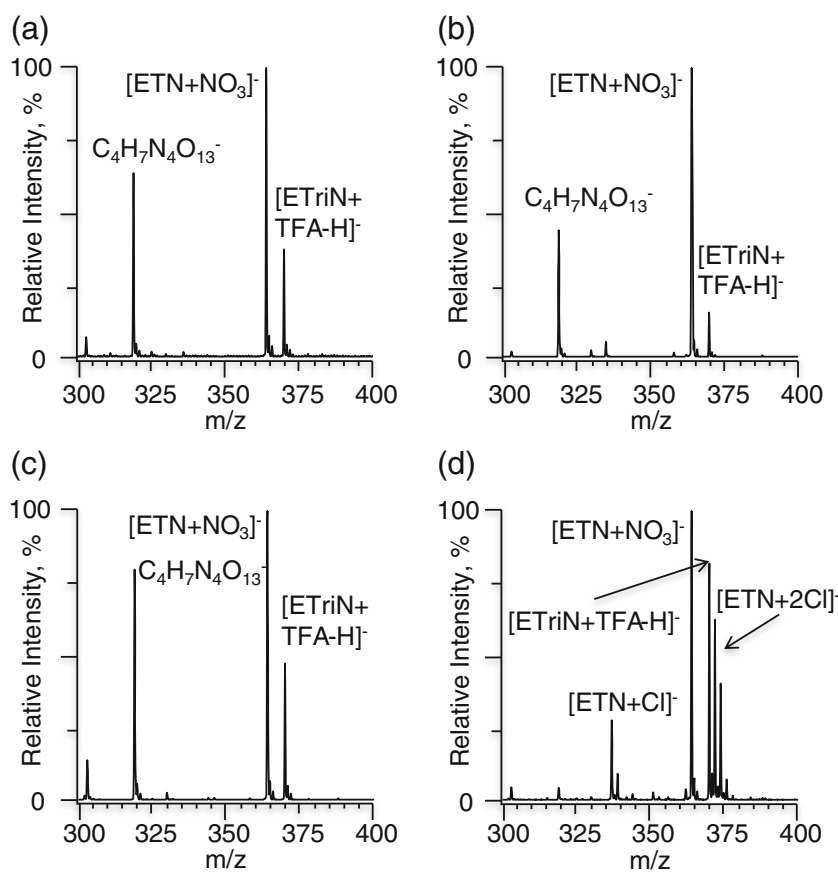
Figure 2. Negative ion mass spectra for purchased ETN obtained in three different ionization modes: ESI (**a**), CD (**b**), and ^{63}Ni – without (**c**) or with Cl-containing dopant (**d**)

for the major ion species observed for PETN ([PETN-NO$_2$ + H + NO$_3$]$^-$, [PETN + NO$_3$]$^-$), and ETN (C$_4$H$_7$N$_4$O$_{13}$$^-$ and [ETN + NO$_3$]$^-$) were determined to be 1.22, 1.16, 1.27, and 1.20, respectively, using the measured drift times and $K_{0,TNT}$ = 1.54. Additional K_0 values for all ion species identified from ETN analyses are given in Table 1. The K_0 values for PETN are in good agreement with previous studies [23], whereas those for ETN have not been previously determined. Although some ETN species may be sufficiently resolved by IMS alone, confident

determination of the identities of each of the species is only possible using the combination of IMS with high resolution MS.

Ion mobility spectra obtained for purchased ETN on the IMS-MS system after desorption from a swab are similar to those collected on a standalone IMS-based ETD system, based on the major peaks observed (Figure 4). K_0 values for each of the three major peaks in the mobility spectrum (indicated as A, B, and C in the figure) were compared with K_0 values determined from the hybrid IMS-MS system (Table 1). Peak A, with

Table 1. Summary of Ion Species Observed in IMS-MS Analysis of ETN Using Different Ionization Modes. Chemical Formulas for Each Species were Confirmed Using Accurate Mass Measurements and Isotopic Distribution Patterns. MS/MS Fragments for ESI-Generated Species are Shown

Anion species	Elemental composition	Experimental accurate mass (Δ from calculated)	K_0	Ionization mode	MS/MS fragments (ESI only)
[ETN–NO$_2$ + H + Cl]$^-$ [ETriN + Cl]$^-$	C$_4$H$_7$N$_3$O$_{10}$^{35}Cl	291.9818 (3 ppm)	1.35	^{63}Ni (with dopant)	
[ETN + H]$^-$ [ETriN + NO$_2$]$^-$	C$_4$H$_7$N$_4$O$_{12}$	303.0058 (3 ppm)	1.31	ESI, CD, ^{63}Ni	241, 261, 259, 271, 285
[ETN + OH]$^-$ [ETN–NO$_2$ + H + NO$_3$]$^-$ [ETriN + NO$_3$]$^-$	C$_4$H$_7$N$_4$O$_{13}$	319.0029 (4 ppm)	1.27	ESI, CD, ^{63}Ni	125, 229, 255, 275, 301, 303
[ETriN + SO$_3$-H]$^-$	C$_4$H$_6$N$_3$O$_{13}$S	335.9635 (2 ppm)	1.27	ESI	139, 151, 164, 179, 227
[ETN + Cl]$^-$	C$_4$H$_6$N$_4$O$_{12}$^{35}Cl	336.9660 (5 ppm)	1.25	^{63}Ni (with dopant)	
[ETN + NO$_3$]$^-$	C$_4$H$_6$N$_5$O$_{15}$	363.9857 (2 ppm)	1.20	ESI, CD, ^{63}Ni	142, 255, 347
[ETriN + TFA-H]$^-$	C$_6$H$_7$N$_3$O$_{12}$F$_3$	369.9994 (2 ppm)	1.15	ESI, CD, ^{63}Ni	113 (112.9854)
[ETN + 2Cl]$^-$	C$_4$H$_6$N$_4$O$_{12}$^{35}Cl$_2$	371.9346 (5 ppm)	1.20	^{63}Ni (with dopant)	

ETriN erythritol trinitrate (a synthetic impurity and potential degradation product), *TFA* trifluoroacetic acid
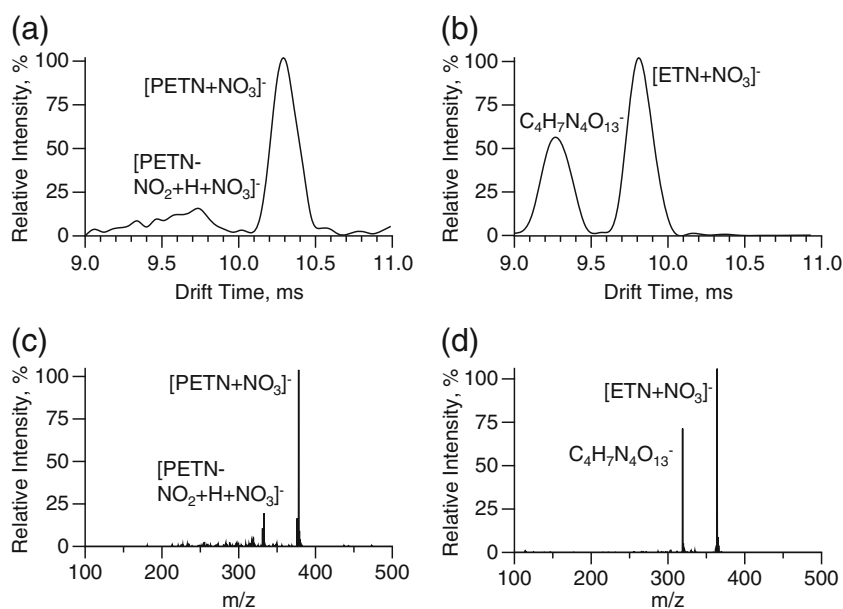
Figure 3. Negative ion ESI ion mobility (**a**), (**b**) and mass spectra (**c**), (**d**) obtained for purchased PETN (**a**), (**c**) and ETN (**b**), (**d**)

a K_0 of 1.36, is consistent with an assignment of $[ETN - NO_2 + H + Cl]^-$. Peak B likely represents $[ETN + Cl]^-$ with a K_0 of 1.29. Peak C (K_0 = 1.22) may be a combination of two overlapping species: $[ETN + NO_3]^-$ with some contribution from $[ETN + 2Cl]^-$. Further support for these assignments was obtained from experiments in which the Cl-containing dopant tube was removed, resulting in an increased relative signal for the nitrate-adducted species (not shown). This qualitative similarity between the stand-alone IMS and IMS-MS results demonstrates that IMS-MS can be a valuable tool for characterization of the ion chemistry occurring in standalone benchtop IMS systems.

Differentiation of Homemade ETN by IMS-MS

ETN that was synthesized in-house from Truvia or erythritol yields similar ^{63}Ni and CD ionization IMS-MS signatures to the purchased ETN standard (Figure 5).
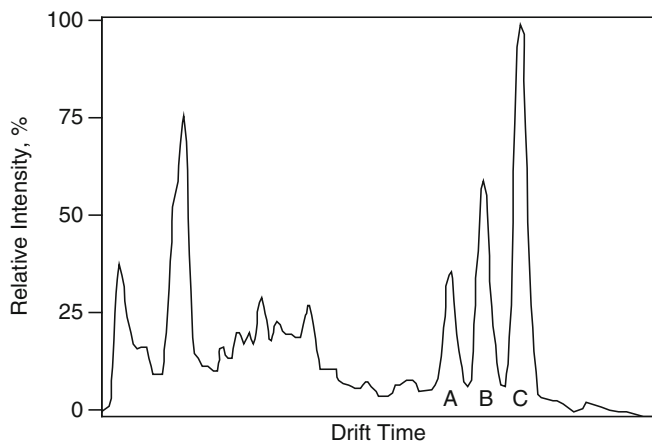

Figure 4. Ion mobility spectrum of purchased ETN acquired on a Smiths Detection 500DT ETD with ^{63}Ni source in negative ion mode; peaks labeled A, B, C are discussed in the text

However, a strong peak at *m/z* 336 is observed with ESI at relatively low source voltages (<2.5 kV) from the in-house synthesized ETN. The elemental composition of this species has been confirmed by accurate mass and isotope distribution measurements as containing one S atom (Supplementary Data, Figure S1). The ion at *m/z* 335.9635 corresponds to an anion with composition ($C_4H_6N_3O_{13}S$), which is quite similar to ETN ($C_4H_6N_4O_{12}$). We interpret it as the sulfate adduct of ETriN. The elemental composition similarity of *m/z* 336 to ETN suggests a structure similar to ETN (Scheme 1) in which one nitrate group is removed. Since *m/z* 336 is only observed with the in-house synthesized ETN samples, a sulfate adduct may be generated during ESI due to the presence of trace amounts of H_2SO_4, which was utilized in the relatively crude ETN synthesis. ESI spectra of ETN synthesized using a route not involving H_2SO_4 did not contain the *m/z* 336 species. The species at *m/z* 336 is relatively unstable compared with either $C_4H_7N_4O_{13}$ or $[ETN + NO_3]^-$ since it is not observed upon desorption and subsequent ionization by either CD, ^{63}Ni, or ESI at higher source voltages. A 2-D plot (Figure 6) of ESI IMS-MS data from in-house synthesized ETN shows that the $C_4H_7N_4O_{13}$ and the *m/z* 336 species have similar drift times (i.e., cross-sections), while the $[ETN + NO_3]^-$ anion is bulkier. If an ETN sample were analyzed by IMS alone, the *m/z* 336 species (i.e., the ETriN impurity) would not be resolved. The presence and identity of this component can be characterized only by IMS-MS analysis, and may provide information on the sample origin and method of synthesis that have important forensic implications. Based on these initial findings, additional studies are currently being conducted in which the synthetic methods and reagents are systematically varied.
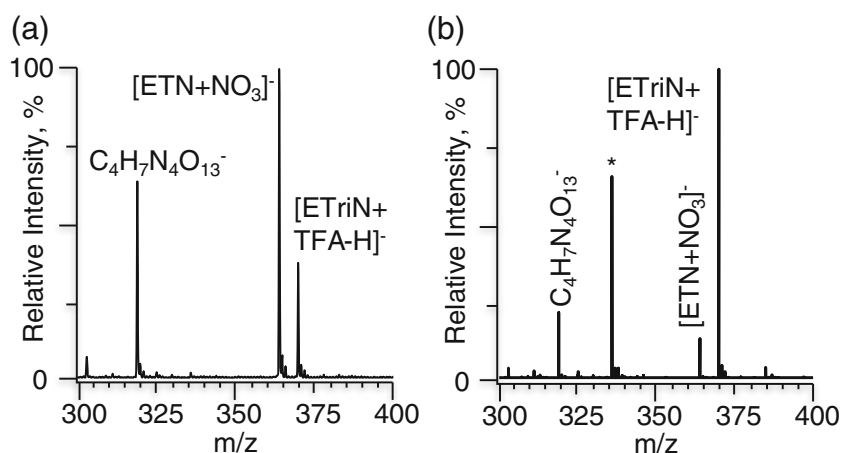
Figure 5. ESI MS comparison of purchased ETN (**a**) versus ETN synthesized from Truvia (**b**); the impurity at *m/z* 336 observed in only the in-house synthesized preparation is denoted by an asterisk

An ESI-MS spectrum of the in-house synthesized ETN, obtained by applying an appropriate IMS gating scheme to remove major ETN peaks ($C_4H_7N_4O_13^-$ and $[ETN + NO_3]^-$), is shown in Supplementary Data, Figure S2. In this mode, only minor anionic species, originating most probably from sample impurities, are detected. These impurities include the previously putatively identified sulfate adduct of ETriN at *m/z* 336, as well as other unidentified species. These impurities can act as fingerprint signatures, and potentially be used to readily differentiate between various samples. Elemental composition could likewise be determined using accurate mass measurements and tandem MS. Specialized threat compound databases from such data could complement other forensically relevant information that is available.

Conclusions

High resolution/accurate mass MS combined with IMS is a valuable tool for analysis of HMEs. IMS-MS allows identification of the ion species generated during sample introduction that may be otherwise impossible if limited to IMS alone. We have found that IMS-MS spectra are similar to those collected on a stand-alone ETD system for characterization of HME samples. ETN ionized by ESI, CD, and ^{63}Ni forms similar anionic species, analogous to PETN ions documented in the literature. Although ETN synthesized by relatively crude methods yields very similar IMS-MS signatures to purchased ETN standards, gated IMS and high-resolution MS have been used to identify minor ETN impurities that may be
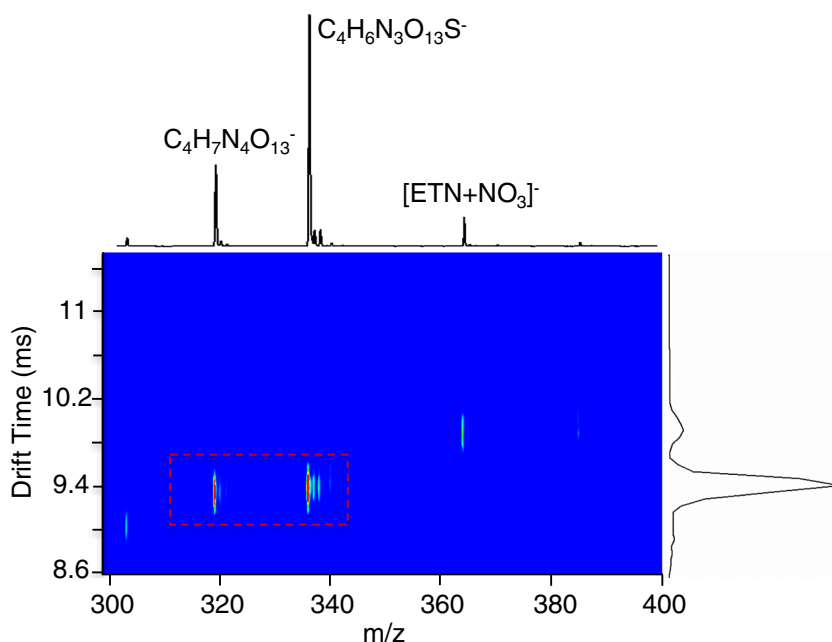

Figure 6. 2-D ion mobility-mass spectrum of synthesized ETN, obtained in negative ion ESI with the IMS operated in "scan mode"

indicative of the chemical source and the synthetic methods used to manufacture the threat. This information allows successful differentiation between, e.g., commercial explosives from homemade formulations, which is of great utility for forensic and attribution purposes. We envision that comprehensive IMS-MS analysis of both threats and common background chemicals could also be used to improve threat identification and reduce false positive results that are often encountered in stand-alone IMS ETD systems.

Acknowledgements

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