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# TESTING NEW DEVICE BASED ON ION MOBILITY

DISSERTATION

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## Summary

The topic of this work is the use of differential mobility spectrometry (DMS) for characterization of explosives and narcotics. Studies were performed for eight explosives and twelve narcotics. Narcotics (cocaine, heroin, amphetamine etc.) have high proton affinity. That is the reason why are these compounds mainly detected in positive channel. Most of the explosives (TNT, PETN, RDX etc.) have high electron affinity. Preferable channel for detection explosives is negative mode. Presented results of analysis have been evaluated by use of special software which communicates with DMS in real time. This tool was developed for visualization, identification and comparison of measured data. Each target molecule appears at a specific compensation voltage under a fixed value of separation voltage which enables differentiation of measured compounds. Calculation of specific alpha coefficients ($\alpha_2$ and $\alpha_4$) to obtain alpha shapes was performed. DMS has proved to be a useful analytical technique for rapid characterization and detection of narcotics and explosives.

## Keywords

Explosives, narcotics, differential mobility spectrometry, compensation voltage, alpha coefficients.

# Introduction

Ion mobility spectrometry (IMS) at high electric field is represented by DMS and high-field asymmetric waveform ion mobility spectrometry (FAIMS). DMS/FAIMS sorts ions according to the difference between ion mobility at high and low electric field with the opposite polarity. Electric field is induced by a periodic asymmetric field which is orthogonal to the ion path. Both DMS and FAIMS techniques separate ions by the difference in their mobility dependence on the applied field strenght. This field dependence is characterized by the alpha function which can be used for ion separation and identification [1, 2]. The electric field applied in FAIMS (DMS) follows high and low asymmetric waveform which can be half sinusoidal [3], bisinusoidal (also called two harmonics) [4] or rectangular [5]. According to theoretical study, rectangular waveform would be ideal for analysis [6]. The crucial difference between DMS and FAIMS is the geometry. DMS use planar electrode [7] whereas FAIMS operates with cylindrical (coaxial) electrode [8].

With the increasing security precautions at the airports, concert halls, or sport stadiums, detection of hidden explosives becomes a challenging branch in analytical chemistry. Most of the explosives (TNT, DNT, PETN, RDX etc.) have high electron affinity. Preferable channel for detection explosives is negative mode.

Identification of narcotic is an important role for toxicological laboratories (both clinical and forensic). Narcotics are psychoactive compounds which can be divided into several classes according their chemical structure, mechanism of action and so on. Narcotics which have had little or no history of medical use are called classical drugs. Cocaine, heroin and amphetamines are representatives of this group. Analogues of these compounds and legal highs are nowadays the most investigated compounds in this branch [9]. Derivatives and analogues of phenethylamines and cathinones belong to the main group of abused stimulants. This work also gives special attention to methiopropamine-structural analogue of methamphetamine (thiophene ring replacing benzene ring) which appears as a drug of abuse since 2011. Stimulant effect of methiopropamine is similar to methamphetamine [10]. Ecstasy (MDMA) is a typical representative of phenethylamines frequently named as a classical recreational drug.

Synthetic cannabinoids and cathinones belong to major class of novel drugs. Synthetic cannabinoids are functionally similar to delta-9-tetrahydrocannabinol (Δ9-THC) and mimic the effects of marijuana when smoked. However, structurally, they are different and include several chemicals such as cyclohexylphenols (CP 47,497), classical cannabinoids (HU-210), naphthoylindoles (JWH-018, JWH-073) or benzoylindoles (JWH 250) [11]. JWH-250 is illegally marketed within “herbal blend” for his psychoactive effects greater than those produced by Cannabis [12]. Synthetic cathinones are structurally related to cathinone, a compound that is naturally observed in the Khat plant [13]. Ethylone and mephedrone are representatives of synthetic cathinones. The reasons for increasing interest in range of cathinone derivatives have been attributed to the low cost and stimulant effect similar to amphetamines [14].

Narcotics were usually analyzed by conventional analytical techniques such as gas chromatography coupled with mass spectrometry (GC–MS) which is considered as a ‘‘gold standard’’ for identification of forensic substance. Narcotics were analyzed by GC–MS using headspace solid-phase microextraction [15], liquid–liquid extraction [16], solid-phase extraction [17]. Coupling liquid chromatography with MS (LC–MS) was used for analysis of narcotics in oral fluids [18], human hair [19], meconium [20], or urine [21]. Low fielded ion mobility spectrometry (IMS) was used for the detection of heroin and cocaine [22], ketamine [9], amphetamines, and other illicit drugs [23]. Analysis of narcotics by high fielded IMS were effected in combination with other analytical techniques: LC–DMS–MS [24], DMS–MS [25], or DTIMS–FAIMS–MS [26].

## Theoretical part

With increasing electric field ion mobility coefficient (K) becomes to be dependent on the ratio of electric field to number of density of the gas (E/N):

$$K = K_0 \;\; 1 + \alpha_2 \; \frac{E}{N}^{\,2} + \alpha_4 \; \frac{E}{N}^{\,4} + \cdots \;\; = K_0 \cdot (1 + \alpha) \qquad (1)$$

$K_0$ is ion mobility coefficient at the low field at standard pressure and temperature. $\alpha$ parameter describes the dependence of K on the electric field. $\alpha_2$ and $\alpha_4$ are specific alpha coefficients. The change in mobility of the ion at elevated E/N is described as alpha function:

$$\alpha \; \frac{E}{N} \; = \; \alpha_2 \; \frac{E}{N}^{\,2} + \alpha_4 \; \frac{E}{N}^{\,4} + \cdots \qquad (2)$$

where $\alpha_2$ and $\alpha_4$ are parameters of ion behaviour in high field strength. Based on these parameters ion mobility coefficient at field strength K (E/N) can be calculated, where E is in ($V \cdot cm^{-1}$) and N is a gas number density in ($cm^{-3}$). For convenience, the values of E/N are reported in Townsend (Td). 1 Td is $1 \times 10^{-17}$ $V \cdot cm^2$. Using experimentally obtained values of compensation voltage (CV) and RF electric field (both in Td units), $\alpha_2$ and $\alpha_4$ can be calculated for bissinusoidal waveform as a result of shortened Taylor expansion [2].

$$-\mathrm{CV} = \quad \mathrm{CV}^3 + \frac{5}{6}\mathrm{CV} \cdot \mathrm{RF}^2 + \frac{1}{9}\mathrm{RF}^3 \quad \alpha_2 + (\mathrm{CV}^5 + \frac{25}{9}\mathrm{CV}^3 \cdot \mathrm{RF}^2 + \frac{10}{9}\mathrm{CV}^2\mathrm{RF}^3 + \frac{55}{72}\mathrm{CV} \cdot \mathrm{RF}^4 + \frac{55}{486}\mathrm{RF}^5)\alpha_4 \tag{3}$$

Eq. 3 can be represented by following equation where only two parameters $\alpha_2$ and $\alpha_4$ are unknown:

$$\begin{array}{c} -c_1 = a_1 \cdot \alpha_2 + b_1 \cdot \alpha_4 \\ -c_2 = a_2 \cdot \alpha_2 + b_2 \cdot \alpha_4 \\ \\ \cdots \\ -c_n = a_n \cdot \alpha_2 + b_n \cdot \alpha_4 \end{array} \tag{4}$$

where $a = \quad CV^3 + \frac{5}{6}CV \cdot RF^2 + \frac{1}{9}RF^3 \quad, b = (CV^5 + \frac{25}{9}CV^3 \cdot RF^2 + \frac{10}{9}CV^2RF^3 + \frac{55}{72}CV \cdot RF^4 + \frac{55}{486}RF^5)$, c = CV.

Recalculation of CV [V] or RF [V] to Td units is based on the facts that 1 Td corresponds to 268.68 $\mathrm{V{\cdot}cm^{-1}}$ at 1 atm and 273.15 K. Alpha is not a number like ion mobility but a function. That is why alpha should be regarded over a wide range of electric field [27]. Under the same experimental conditions the same alpha function could be obtained by any DMS instrument. The alpha function is a characteristic ion property similar to *m/z* in mass spectrometry or ion mobility in IMS.

# Experimental

## Chemicals and sampling

2,4,6-trinitrotoluene (TNT), pentaerythritol tetranitrate (PETN), 2,4,6-trinitrophenol (picric acid), 2,4-dinitrotoluene (DNT), erythritol tetranitrate (ETN), hexamethylene triperoxide diamine (HMTD), 2, 4, 6-trinitrophenylmethylnitramine (tetryl), 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) were purchased from Explosia a.s. Pardubice (Pardubice, Czech Republic). 3 µL of each explosive (1000 ng·µL−1 diluted in acetone) were injected via a syringe to vapour phase generator, where evaporation was realized. The vapour phase generator should maintain a constant flow of the substance for periods longer than a period of one scan. Injected amount of the substance is sufficient for more than one scan (even dozens of scans); however the vapour phase generator is not able to directly regulate the flow. This is not an issue of qualitative analysis (identification).

HPLC-grade methanol was purchased from Sigma-Aldrich St. Louis, MO, USA. Samples of amphetamine, methamphetamine, ketamine, heroin, cocaine, JWH 250, ephedrine, pseudoephedrine, mephedrone, MDMA, methiopropamine and ethylone were purchased from Institute of Criminalistics Prague, Czech Republic. 1 μL of each narcotic (1000 ng· μL diluted in methanol) were injected to DMS prototype manufactured by RS Dynamics.

## Instrumentation

Explosives were measured using a prototype of DMS analyzer with $^{63}$Ni as an ionization source. DMS analyzer is not fully stand-alone device, it downloads basic parameters and configuration from PC, while runtime behavior is controlled by embedded single chip microprocessor. It is responsible for proper timing of critical processes during measurement scans, like RF voltage control, compensation voltage control, synchronous A/D conversion, and data averaging followed by sending it to the PC.

Narcotics were measured using DMS prototype RS Dynamics-Dragon with $^{63}$Ni as an ionization source. Bisinusoidal waveform with frequency 1.247 MHz was used in these experiments. During the low-field portion of the waveform, clusters are formed to changing sizes and shapes that depend on the chemistry of a particular structure of ion. Ions are released from the cluster or reducing their cluster number during the second half of the waveform period owing to increasing electric field. Dried air was used for carrying generated ions to a separation region. Gap between electrodes corresponds to 0.06 cm.

*DMS condition for measurements:* RF was applied from 500 to 1500 V. For one of the RF setting, different CV values are gradually applied varying from −40 V to +15 V. With increasing CV generated effective field decreased. Dried air (purified by activated carbon and dewatered by molecular sieve) was used as carrier gas. Flow rate of carrier gas was 50 ml·min$^{-1}$ and temperature was controlled from 80 °C to 100 °C for explosives and from 75 °C to 120°C for narcotics.

# Results

Reactant ion peak (RIP) is formed by interaction of carrier gas (dried air) with high energy electrons from $^{63}Ni$. This process is simultaneous in positive and negative mode at the same time. $H^+(H_2O)n$ and $O_2-(H_2O)n$ are reactant ions in positive and negative polarity with dried air as a carrier gas. Considering proton/electron affinities of analyte (M), the RIP ions transfer their charge to M by collisions. M replaces water molecule(s) to form monomer or dimer ions, respectively [28]. Explosives were measured in negative channel due to their high electron affinities with the exception of HMTD which has lower electron affinity than other measured explosives. Preferable channel for analysis of HMTD is positive mode. Electron affinity plays the major role in ionization of samples in DMS.

Dispersion plots and compensation voltage scans at fixed separation voltage of explosives measured in negative channel are shown in Fig. 1-3. Dispersion plots show ion intensity and compensation voltage at each separation field. Below the dispersion plots are differential mobility spectra showing ion current as a function of CV for RIP and PIP. Differences in intensities of ions at specific CV in Fig. 1-3 for the same concentration of explosive were observed. The signal intensity at specific RF depends on the amount and chemical properties (proton/electron affinity) of analytes [29].

Compensation voltage of PIP at 1060 RF voltage at 80 °C in negative channel are 1.34 V for PETN, −0.13 V for TNT, −1.61 V for DNT, 1.71 V for ETN, 0.97 V for tetryl and 0.23 V for picric acid (Fig. 1-2). PIP of HMTD at RF = 1060 V appears at CV = 0.23 V. PIP of RDX measured at 100°C appears at CV = 1.34 V (at RF = 1060 V) (Fig. 3).

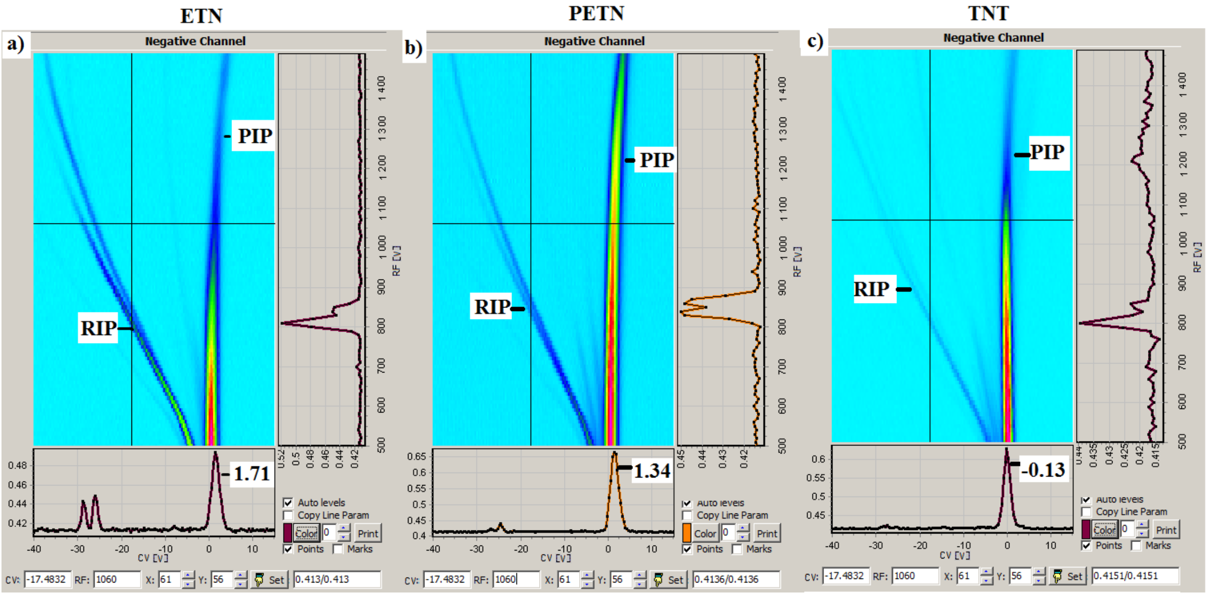


**Fig. 1** DMS fingerprint spectrum (dispersion plot) of ETN (a), PETN (b) and TNT (c) in negative mode at 80 °C. Spectra shown below dispersion plots were isolated at separation voltage of RF = 1060 V

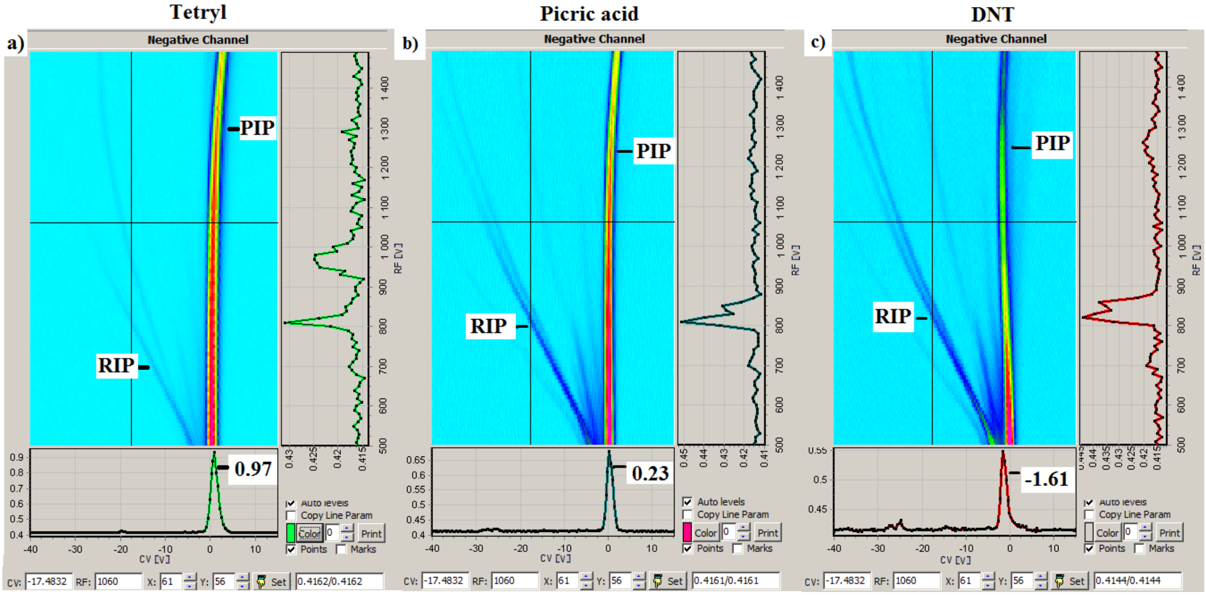
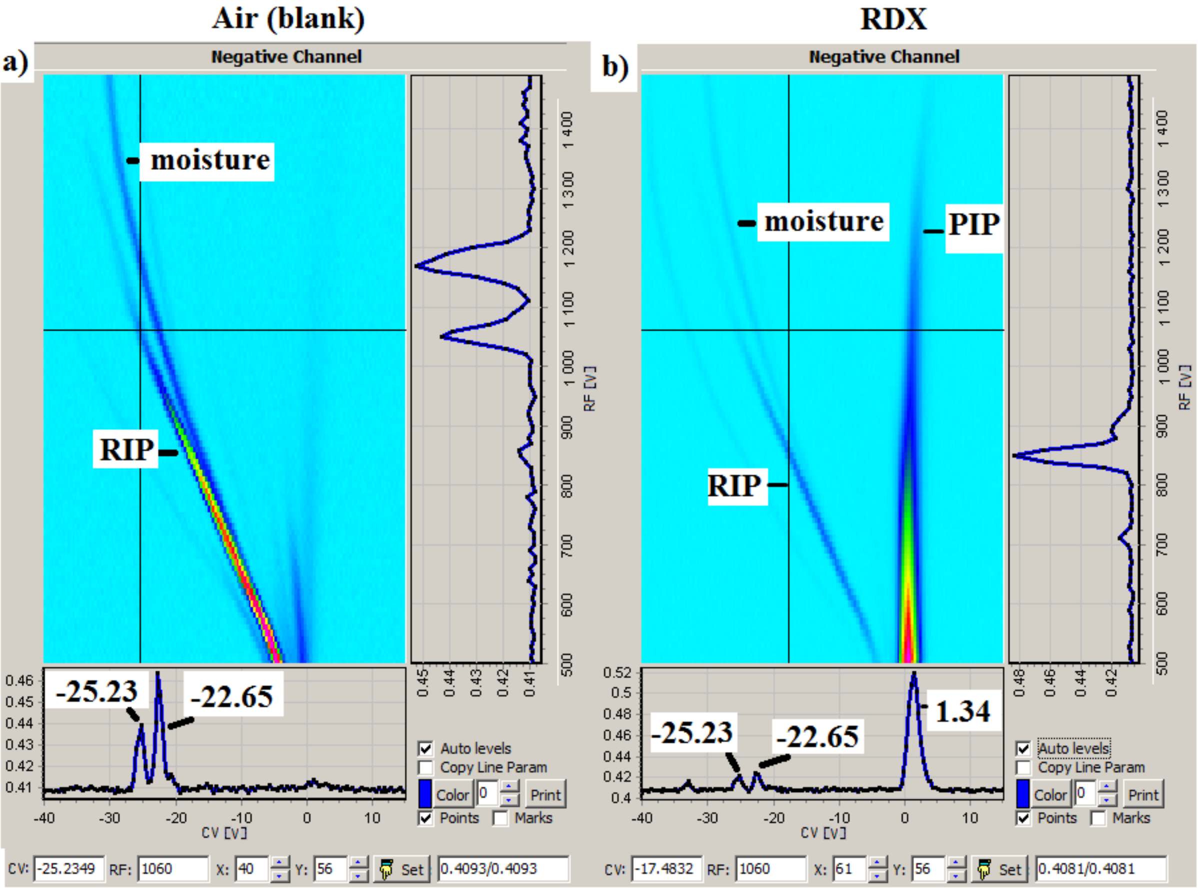


**Fig. 2** DMS fingerprint spectrum (dispersion plot) of Tetryl (a), Picric acid (b) and DNT (c) in negative mode at 80 °C. Spectra shown below dispersion plots were isolated at separation voltage of RF = 1060 V



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CV: -25.2349 RF: 1060 X: 40 Y: 56 Set 0.4093/0.4093

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CV: -17.4832 RF: 1060 X: 61 Y: 56 Set 0.4081/0.4081

**Fig. 3** DMS fingerprint spectrum (dispersion plot) of air (blank) (a) and RDX (b) in negative mode at 100 °C. Spectra shown below dispersion plots were isolated at separation voltage of RF = 1060 V

Nonlinear alpha functions of explosives are summarized in Table 1. Graphical interpretation of alpha shapes of measured explosives for E/N up to 120 Td is portrayed in Fig 4.

**Table 1** The nonlinear alpha functions of explosives

| | |
|---|---|
| **DNT** | $\alpha=3.2138\cdot10^{-6}(E/N)^2-1.7620\cdot10^{-10}(E/N)^4$ |
| **TNT** | $\alpha=2.6164\cdot10^{-6}(E/N)^2-2.8450\cdot10^{-10}(E/N)^4$ |
| **Picric acid** | $\alpha=0.8267\cdot10^{-6}(E/N)^2-1.4897\cdot10^{-10}(E/N)^4$ |
| **Tetryl** | $\alpha=-1.6122\cdot10^{-6}(E/N)^2+0.5013\cdot10^{-10}(E/N)^4$ |
| **PETN** | $\alpha=-1.8191\cdot10^{-6}(E/N)^2+0.1220\cdot10^{-10}(E/N)^4$ |
| **RDX** | $\alpha=-1.4322\cdot10^{-6}(E/N)^2-0.4305\cdot10^{-10}(E/N)^4$ |
| **ETN** | $\alpha=-2.6487\cdot10^{-6}(E/N)^2+0.6459\cdot10^{-10}(E/N)^4$ |
| **HMTD** | $\alpha=1.0525\cdot10^{-6}(E/N)^2-2.1533\cdot10^{-10}(E/N)^4$ |

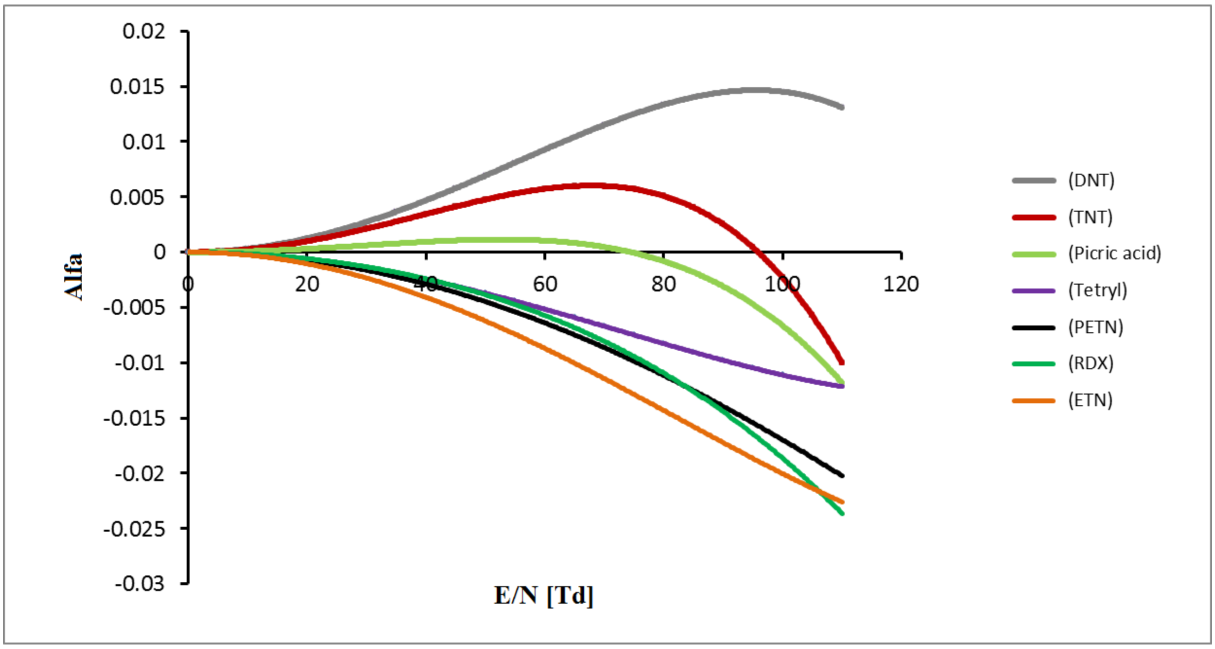

**Fig. 4** Nonlinear function curve of explosives ions in negative channel

Narcotics were measured in positive channel due to their high proton affinities. Values of compensation voltage of product ion peak at RF = 1480 V for cocaine, JWH 250, heroin, ketamine, methamphetamine and amphetamine at 110°C appears at 3.33 V, 3.18 V, 2.43 V, 2.12 V, -0.56 V and -4.9 V, respectively (Fig. 5). Other six narcotics (MPA, pseudoephedrine, mephedrone, MDMA, ephedrine and ethylone) were measured at 90°C. Their characteristic signal of product ion peak at RF = 1480 V appears at -6.28 V, -4.89 V, -4.50 V, -3.85 V, -3.02 V and -1.90 V (Fig. 6).

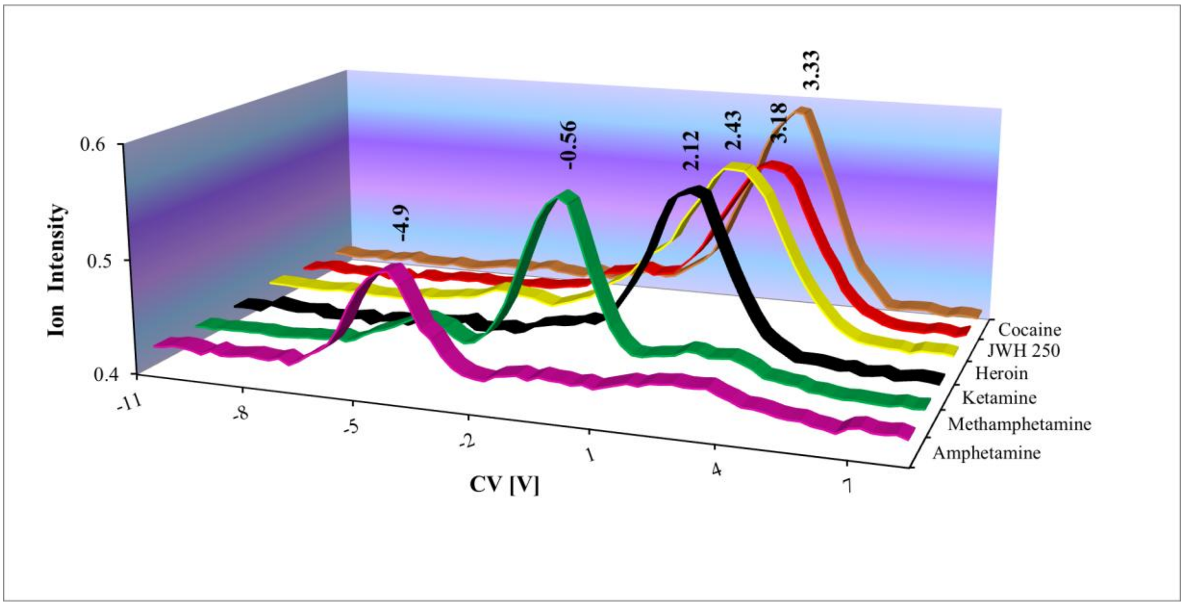

**Figure 5** Differential mobility spectra of narcotics at RF = 1480 measured at 110°C.

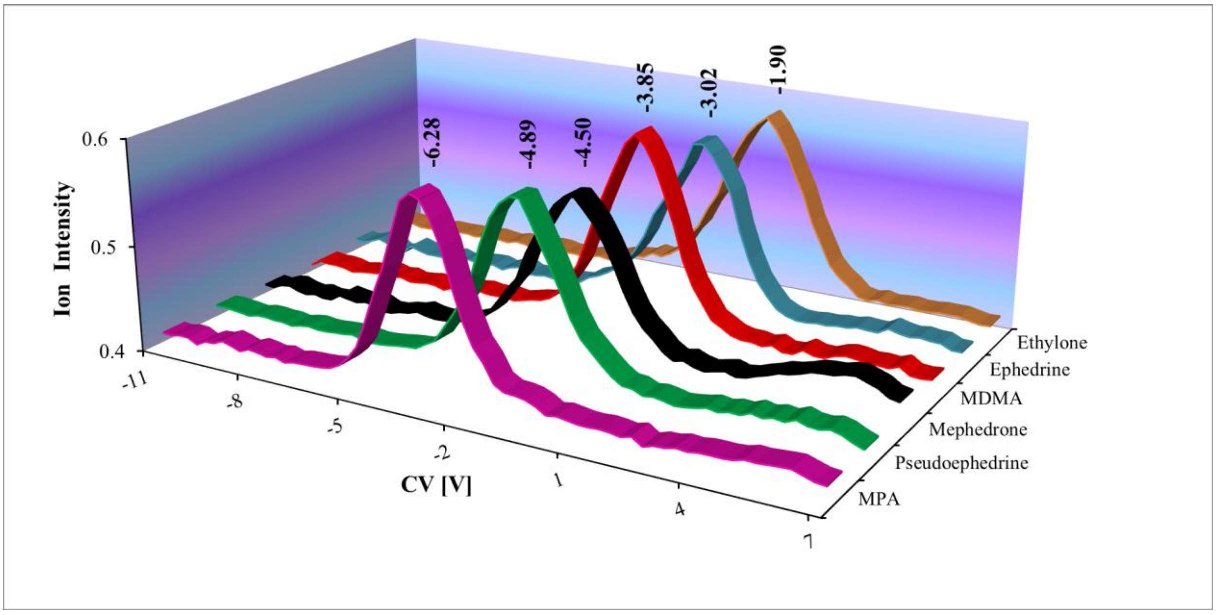

**Figure 6** Differential mobility spectra of narcotics at RF = 1480 measured at 90°C.

Dependence of mobility for measured narcotics ions in electric field at E/N values between 0 and 100 Td were used to graphical differentiation of narcotic (Fig. 7-8).

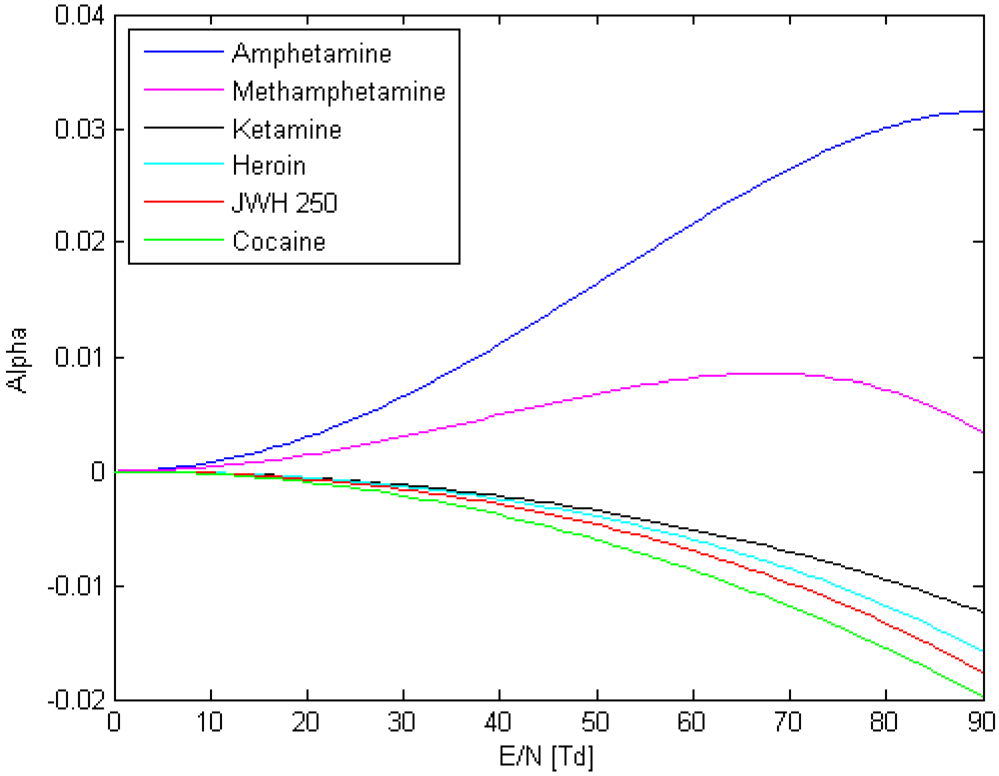

**Figure 7** Nonlinear alpha function curve of narcotics in positive channel measured at 110°C

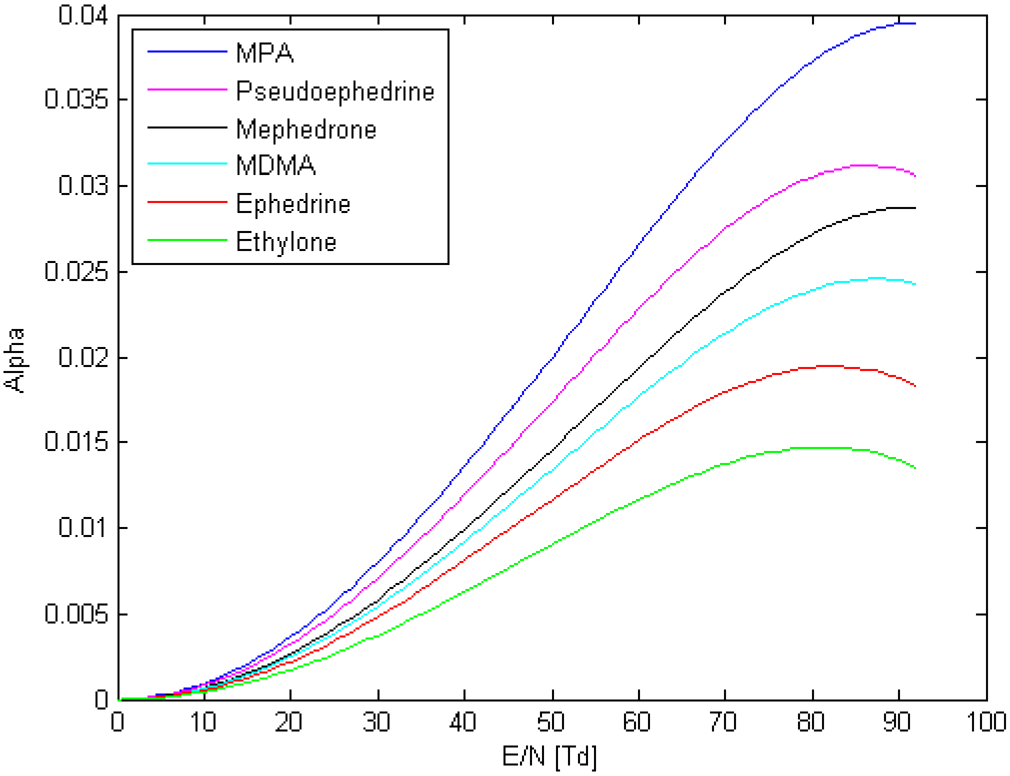

**Figure 8** Nonlinear alpha function curve of narcotics in positive channel measured at 90°C

Summary of nonlinear alpha function for measured narcotics is summarized in Table 2.

**Table 2** Nonlinear alpha functions of measured narcotics

| **Sample** | **Temperature** | **Nonlinear alpha function** |
|---|---|---|
| Cocaine | 110°C | $\alpha = -2.3991 \cdot 10^{-6}\,(E/N)^2 - 0.0503 \cdot 10^{-10}\,(E/N)^4$ |
| JWH 250 | 110°C | $\alpha = -1.7377 \cdot 10^{-6}\,(E/N)^2 - 0.5474 \cdot 10^{-10}\,(E/N)^4$ |
| Heroin | 110°C | $\alpha = -1.4326 \cdot 10^{-6}\,(E/N)^2 - 0.6410 \cdot 10^{-10}\,(E/N)^4$ |
| Ketamine | 110°C | $\alpha = -1.3228 \cdot 10^{-6}\,(E/N)^2 - 0.2539 \cdot 10^{-10}\,(E/N)^4$ |
| Methamphetamine | 110°C | $\alpha = 3.7507 \cdot 10^{-6}\,(E/N)^2 - 4.1207 \cdot 10^{-10}\,(E/N)^4$ |
| Amphetamine | 110°C | $\alpha = 7.7185 \cdot 10^{-6}\,(E/N)^2 - 4.7221 \cdot 10^{-10}\,(E/N)^4$ |
| MPA | 90°C | $\alpha = 9.3895 \cdot 10^{-6}\,(E/N)^2 - 5.5786 \cdot 10^{-10}\,(E/N)^4$ |
| Pseudoephedrine | 90°C | $\alpha = 8.3539 \cdot 10^{-6}\,(E/N)^2 - 5.6011 \cdot 10^{-10}\,(E/N)^4$ |
| Mephedrone | 90°C | $\alpha = 6.8627 \cdot 10^{-6}\,(E/N)^2 - 4.0931 \cdot 10^{-10}\,(E/N)^4$ |
| MDMA | 90°C | $\alpha = 6.4208 \cdot 10^{-6}\,(E/N)^2 - 4.1940 \cdot 10^{-10}\,(E/N)^4$ |
| Ephedrine | 90°C | $\alpha = 5.7183 \cdot 10^{-6}\,(E/N)^2 - 4.2051 \cdot 10^{-10}\,(E/N)^4$ |
| Ethylone | 90°C | $\alpha = 4.4566 \cdot 10^{-6}\,(E/N)^2 - 3.3728 \cdot 10^{-10}\,(E/N)^4$ |

## Conclusions

Characterization of ions from eight explosives using differential mobility spectrometry (DMS) with $^{63}$Ni as an ionization source was performed. Each explosive provides characteristic signal at a specific compensation voltage under a fixed dispersion field. Peaks in DMS spectra for these ions were confined to a range of compensation voltages between −1.61 to +1.71 V at RF = 1060 V. We calculated specific alpha coefficients ($\alpha_2$ and $\alpha_4$) to obtain a nonlinear function of explosives, based on their DMS spectra. Dependence of mobility for measured explosives ions in electric field at E/N values between 0 to 120 Td were used to inspectional graphical differentiation of explosives.

Twelve different narcotics were analyzed by DMS prototype RD Dynamics-Dragon. Each of measured compounds has a characteristic value of compensation voltage at RF = 1480 V. According to peak position and nonlinear alpha curve we are able to detect and differentiate twelve narcotics.

## Acknowledgement

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**Pavlačka M**, Ventura K, Kortánková K, Bláha J, Zástěra M, Mázl R and Bajerová P, Characterization of narcotics using differential mobility spectrometry: Monatsch. Chem. (2017) Received: 3 October 2016/ Accepted: 24 January 2017.

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**Pavlačka M**, Bajerová P and Ventura K, Analysis of gaseous compounds using differential mobility spektrometry and field asymetric waveform ion mobility spektrometry: YISAC 2015: 22 nd Young Investigators Seminar on Analytical Chemistry. Lodž (2015), p. 46, ISBN 978-83-6125-44-8.

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