Univerzita Komenského v Bratislave

Fakulta matematiky, fyziky a informatiky

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Autoreferát dizertačnej práce

Detection of Trace Amounts of Substances using Ion Mobility Spectrometry Mass Spectrometry (IMS-MS) Technique

na získanie akademického titulu philosophiae doctor

v odbore doktorandského štúdia:
4.1.6. Fyzika plazmy

Bratislava 2019

Dizertačná práca bola vypracovaná v externej forme doktorandského štúdia

na Katedre experimentálnej fyziky, Fakulte matematiky, fyziky a informatiky v Bratislave

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1. *Introduction*

In these days physicists and chemists have an opportunity to take the advantage of various analytical techniques[1, 2, 3]. Different methods allow to investigate almost full range of chemical compounds. These methods can be applied in medicine, pharmacy, environmental protection, food industry, homeland security etc [3, 4, 5]. Detecting chemicals like explosives, drugs, pollutants nowadays is not an issue[6, 7, 8]. Nevertheless, there is no an ideal analytical method and for each method several disadvantages can be listed.

In our research ion mobility spectrometry (IMS) [9] coupled with orthogonal acceleration time of flight mass spectrometry (oaTOF-MS)[10] have been applied to study not only volatile organic compounds (VOC's) [11, 12] but also chemicals with high boiling points and low vapour pressures [8, 13]. This tandem arrangement allows to use profits from both techniques and eliminate deficiencies. The ion mobility spectrometry is known as a high sensitivity technique with fast time of analysis (milliseconds) and is inexpensive. Simplicity and speed of TOF measurements completes whole setup and provide one of the most valuable analytical technique. The addition of mass information to mobility information opens new horizons for both ion mobility spectrometry and mass spectrometry (MS) [9]. The combination of mass and mobility provides information on ion structure that is not possible with IMS or MS alone. By adding IMS information to mass information, the structure of an ion as well as its mass may be measured. Usually, mass spectrometry is blind to low levels of ions in complex mixtures because of the chemical noise of the matrix and to isomeric components of the mixture. Thus, the addition of size information to mass information can be used for ion detection. Of course, the primary advantage of coupling IMS with MS is that ion mobility provides a rapid pre-separation step prior to MS.

In this work several chemical compounds have been investigated using the IMS-oaTOF apparatus in several research projects. Detection of whisky lactone by IMS and identification of generated ions by TOF-MS has been done. Furthermore, studies of organic solvents (acetone, methanol, ethanol, propan-2-ol, diethyl amine, ethyl acetate) by IMS-TOFMS to determine generated ions in APCI source (corona discharge) have been conducted. Another project has dealt with detection and distinction of isomers and conformers of dimethyl phthalate. Another study has dealt with protonation, hydration, and cluster formation of ammonia, formaldehyde, formic acid, acetone, butanone, 2-ocatanone, 2-nonanone, acetophenone, ethanol, pyridine, and its derivatives and finally, study of Atmospheric Pressure Chemical Ionization Mechanism in Corona Discharge Ion Source with and without NH_3 dopant by Ion Mobility Spectrometry combined with Mass Spectrometry for 2-nonanone, cyclopentanone, acetophenone, pyridine, and di-tert-butyl pyridine has been done.

2. *Objectives*

The main aim of this dissertation thesis was to detect different chemical compounds by means of ion mobility spectrometry and mass spectrometry and to study processes between ions and neutral molecules in Corona Discharge at atmospheric pressure. The research part can be divided into few subsections:

I. Fast Quantification of Whisky Lactone in Oak Wood by Ion Mobility Spectrometer.

In this part application of IMS to determine the concentration of β-methyl-γ-octolacton alsko known as Whisky Lactone in oak wood samples has been demonstrated. This work shows that IMS has the potential to be applied in the industry.

II. Investigation of selected volatile organic compounds (VOCs) solvents by Atmospheric Chemical Ionization Ion Mobility Spectrometry coupled with orthogonal accelerated Time of Flight Mass spectrometry

This topic deals with several volatile organic compounds (VOCs) i.e. methanol, ethanol, propan-2-ol, acetone, diethylamine and ethyl acetate. These chemicals are used as solvents for example in the Thin Layer Chromatography (TLC) technique. Using IMS and IMS-oaTOF-MS has been carried out a study focused on the identification of the VOCs present in the TLC analysed samples and also to understand the processes of the formation of the VOC’s originating ions in IMS as they may interact with the analytes.

III. Phthalates

This project raises the subject of phthalates which are a group of chemicals widely used mainly as a plasticizers. Importance of this study relates to phthalates' potential risk to human health due to their presence in soil and water or in indoor environment.

IV. Study of Atmospheric Pressure Chemical Ionization Mechanism in Corona Discharge Ion Source with and without NH3 Dopant by Ion Mobility Spectrometry combined with Mass Spectrometry: A Theoretical and Experimental Study

In this part, an ionization of 2-nonanne, cyclopentanone, acetophenone, pyridine and di-tert-butylpyridine in Corona Discharge (CD) - an atmospheric pressure chemical ionization (APCI) source was studied in the presence and the absence of ammonia dopant.

V. Effect of Basicity and Structure on the Hydration of Protonated Molecules, Proton-Bound Dimer and Cluster Formation: An ion Mobility- Time of Flight Mass Spectrometry and Theoretical Study

Finally, in this part, protonation, hydration and cluster formation of ammonia, formaldehyde, formic acid, acetone, butanone, 2-octanone, 2-nonanone, acetophenone, ethanol, pyridine were investigated.

3. *Experimental equipment*

4. *Ion Mobility Spectrometer used at Department of Experimental Physics – Comenius University*

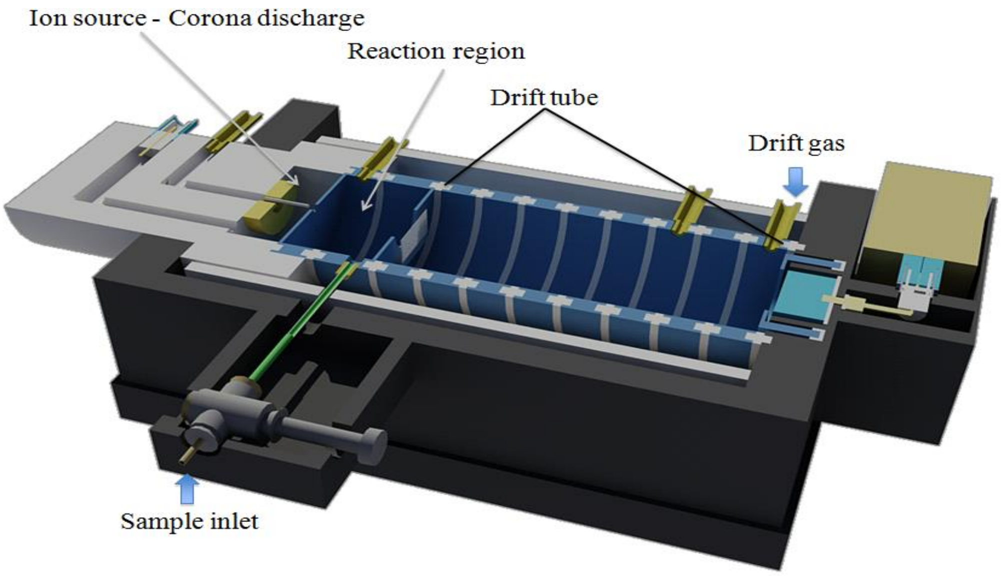

Figure 1. A 3D scheme of ion mobility spectrometer

Figure 1 shows a scheme of the ion mobility spectrometer used in our laboratory [14]. This is an example of standard IMS with linear electric field. The drift tube is constructed of a series of stainless-steel ring electrodes insulated by Teflon rings to ensure tightness. Every stainless-steel ring is connected with next one by resistors (5 MΩ or higher). The high voltage is applied to the first ring which is at the same time an electrode of corona discharge. High voltage is set at the level to achieve magnitude of electric field in the order of hundreds of V/cm. In our case corona discharge (CD) was used as an ionization source however many other sources are being used and electrospray (ESI), photoionization and isotope ^{63}Ni are only examples of sources which can be used in IMS. Each of ionization source produce reactive particles which react with analyte inside reaction region sometimes called reaction chamber and ionize investigated molecules. During the absence of the sample only reactant ions (RI) are detected. Subsequently, within the drift tube ionized molecules are drifting directed by electric field in a counter-stream of a grift gas and reach the detector.

Before ions from reaction region reach drift tube they have to pass through the shutter grid (SG). It is a Bradbury-Nielsen type shutter which allows to dose ions inside drift tube. When shutter have the same potential as drift tube it is mean that ions can enter the drift tube but when voltage is applied on SG ions are stopped. Shutter grid is usually open for 30-110 μs or so. After crossing SG ions are separated in drift tube depending on their mobilities and before they reach the detector (Faraday plate) they must go through the last obstacle- an aperture grid which is made of Ni mesh.

Ion mobility (K) can be related to the structure of molecule and according to the Chapman-Enskog theory, can be described by the Mason-Champ equation:

$$K = \frac{3e(2\pi)^{1/2}(1+\alpha)}{16N\left(\mu k T_{eff}\right)^{1/2}\Omega_D\left(T_{eff}\right)} \qquad (51)$$

where e is the charge of the electron, α is a correction factor; N - number density of neutral gas molecules; μ is the reduced mass of the pair of diffusing ions and carrier gas molecule; T_{eff} - effective temperature of the ion determined by thermal energy and the energy acquired in the electric field; $\Omega_D(T_{eff})$ - effective collision cross section of the ion at the temperature of the supporting atmosphere.

5. *Ion Mobility Spectrometry - Orthogonal Acceleration Time of Flight Mass Spectrometry*

In our laboratory ion mobility spectrometer is coupled with time of flight mass spectrometry (TOF-MS) resulting in Corona Discharge Ion Mobility Spectrometry Orthogonal Acceleration Time of Flight Mass Spectrometry (CD IMS-oaTOF). Ion Mobility Spectrometer was fully described in previous chapter, this part is dedicated to the Orthogonal Acceleration Time of Flight Mass Spectrometry (oaTOF-MS).

Ions after traveling whole drift tube hit detector but some of them can pass the 100 μm pinhole in the centre of the detector and enter first vacuum chamber where ion optic guide them to the orthogonal acceleration chamber of linear time of flight mass spectrometer located in the second vacuum chamber. The mentioned ion optic consists of five electrodes and the skimmer. While applied voltage on skimmer was 1,8 V the other electrodes were on potential in range 3,5-8,0 V. The orthogonal acceleration chamber is made of two parallel electrodes with 5 mm gap between them. Front electrode is partially shielded by stainless steel mesh with 60% of transmittance and rear electrode acts as push electrode. From the orthogonal acceleration region ions are pushing and uniformly accelerating to the drift region (tube) of the spectrometer. Acceleration region of TOF consists of seven electrodes with 7 mm separation between, electrodes are connected with high precision vacuum resistors. The drift tube is made of perforated stainless steel with length of 547 mm and during measurements was on the potential of – 3,53 kV. As a detector microchannel plate (MCP) was used (frontal electrode with applied voltage of – 3.61 kV and back electrode + 1.01 kV for positive ions detection). Signal registered on detector was subsequently processed by preamplifier (Surface Concept GmbH) and collected by a multiscalar PCI card (FASTComTec GmbH, model P – 7888). Software provided with the PCI card (FASTComTec) was used for TOF calibration.

The push out electrode was pulsed with 1 μs pulse width and 32,5 μs period and was controlled by high voltage transistor switch (Behlke GmbH) (voltage in range from + 120 V to +160 V was applied during the pulse). HV switch was managed by pulse generator (HAMEG HM8035). This same pulse generator was also used for the triggering of a FASTComTec PCI card. The multiscalar PCI card was able to generate a synchronic TTL signal additionally modified by a delay gate generator (TENELEC, TC410A) to manage the high voltage switch (Behlke GmbH) of IMS. The IMS was synchronically operated with the TOF spectrometer. The scheme of IMS-MS setup is shown in Figure 3 [9].

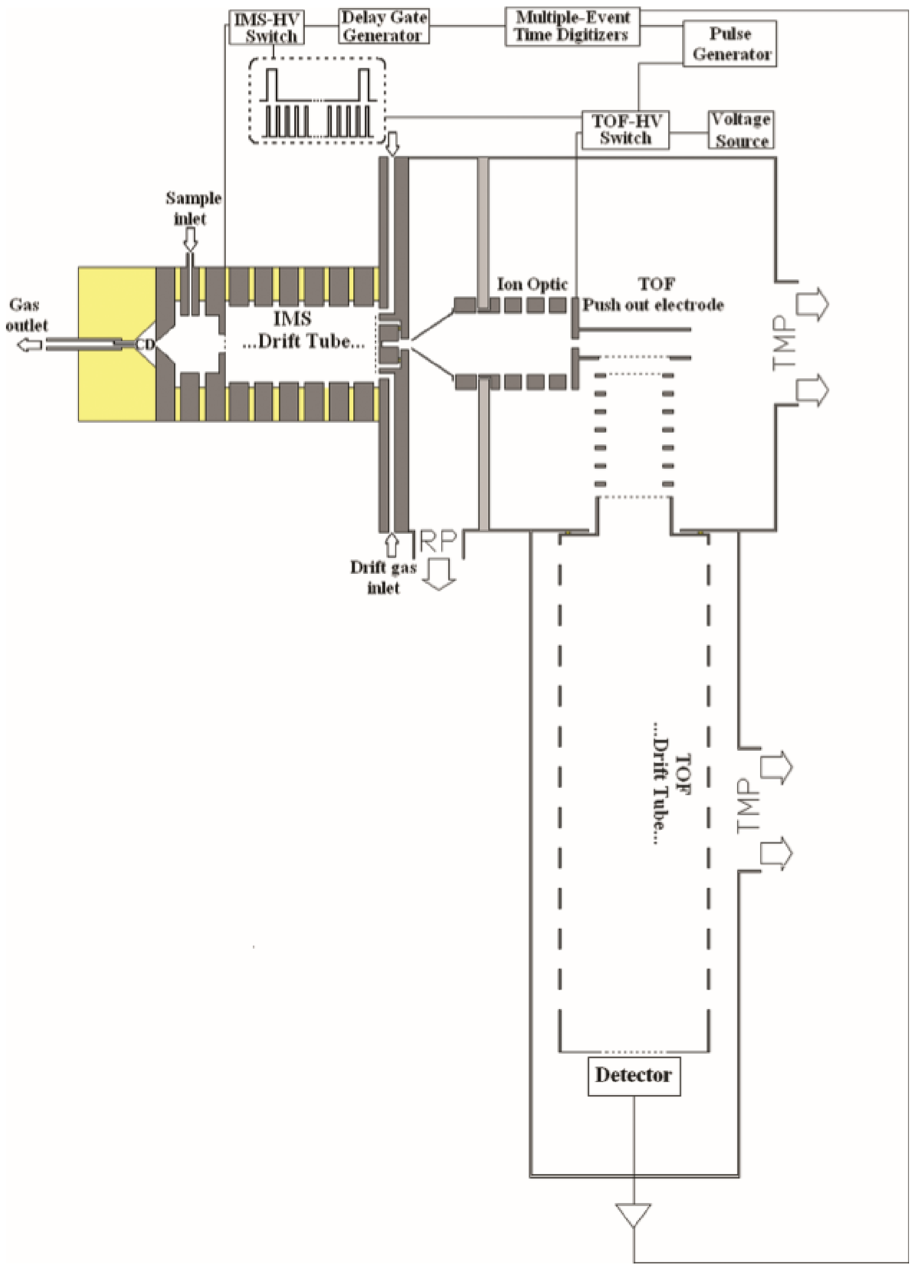

Figure 2. Schematic view of CD-IMS-oa-TOF instrument

6. Results

Next chapters are dedicated to the results which were obtain by the means of ion mobility spectrometry – mass spectrometry. Results were divided into different subsections. Each of subsection deals with different research project.

7. Fast Quantification of Whisky Lactone in Oak Wood by Ion Mobility Spectrometer

Ageing of the distilled beverages is an important process influencing the final quality of the beverages. Many of them (e.g. whiskies and brandies) mature in the oak casks, which contribute to the final taste and aroma of the beverages. Spirits maturation in oak casks and the resulting olfactory perception depends on the content of volatile extractive compounds in the oak [15, 16, 17]. The changes in the spirits are due to changes in the composition and concentration of the compounds influencing the taste and aroma. The content of these substances in the oak wood depends on the natural factors such as climate, topography, soil and dendrology [18]. Different oak species differ in the composition of volatile substances, such as the β-methyl-γ-octolactone (whisky lactone or WL), which is an important ingredient in the whisky [19]. In Europe the most abundant oak species are *Quercus petraea* and *Quercus robur*. WL has been found to be more abundant in *Q. petraea* than in *Q. robur* [20]. However, in *Q. petraea* wood exists high natural variability of WL concentration within and between individual trees [21]. For this reason, it is important to find an ideal method to detect WL in the oak wood, a method which will be cheap, fast and efficient.

In this study a new, fast, sensitive and simple method of whisky lactone detection based on the Ion Mobility Spectrometry (IMS) is presented. IMS is spectrometric method based on the separation of ions in homogenous electric field at atmospheric pressure [22, 23, 24, 25]. This technique is widely used in the fields of security (detection of explosives, drugs and harmful substances) [8, 26], however, more and more industrial applications of IMS technique appear. An IMS apparatus equipped with Atmospheric Pressure Chemical Ionisation (APCI) for direct detection of the whisky lactone from the oak wood have been applied. Prior the analysis of oak samples, laboratory studies with WL standard (Sigma Aldrich) using IMS and IMS combined with oaTOF MS have been applied. IMS-oaTOF MS technique allowed us to determine the m/z of the ions within ion mobility peaks. The laboratory study with the WL standard was followed by IMS study of the oak wood samples of different *Q. petraea* trees. In the IMS spectra of different oak wood samples the WL peaks were identified and their intensity was proportional to the WL concentration.

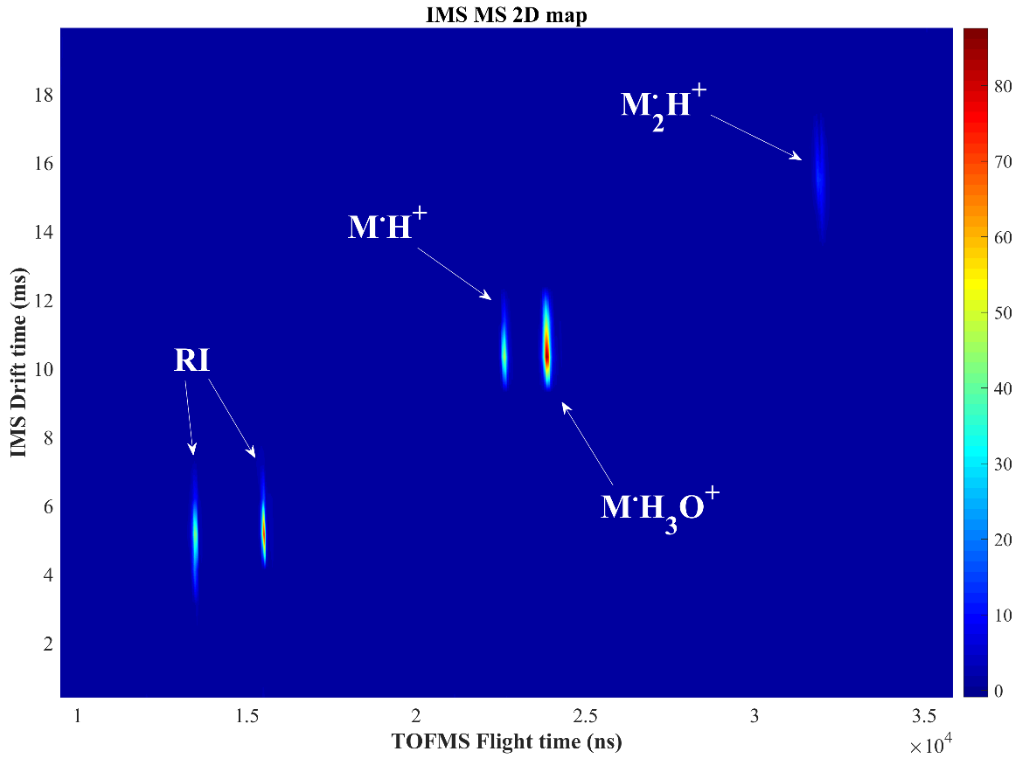

Figure 3. Two dimensional IMS-MS map of whisky lactone. The monomer IMS peak consist of ($M{\cdot}H^+{\cdot}(H_2O)_{0,1}$) and the dimer peak of $M_2{\cdot}H^+$ ions.

7.1. Investigation of selected volatile organic compounds (VOCs) solvents by Atmospheric Chemical Ionization Ion Mobility Spectrometry coupled with orthogonal accelerated Time of Flight Mass spectrometry

VOCs are widely used in the chemical synthesis and chemical industry. In analytical chemistry, VOCs solvents are used in the processes of sample preparation and in different chromatographic techniques. Traces of the VOCs are thus very often present in the laboratory environment and in the analytical samples. In the case of hyphenated technique, such as thin layer chromatography (TLC) with IMS (TLC-IMS), we deal with the problem of the presence of the solvents VOCs contaminants in the IMS spectra. For this reason, we have carried out a study focused on the identification of the solvents present in the TLC samples. In addition, we have tried to understand the processes of ion formation from VOCs in IMS as they may interact with the analytes and influence the response of the system[27, 28, 29]. In present study we have selected six VOCs – solvents (methanol, ethanol, propan-2-ol, acetone, diethylamine and ethyl acetate) and we have recorded their IMS spectra in positive polarity Atmospheric Pressure Chemical Ionisation Ion Mobility Spectrometry (APCI-IMS) and by the Ion Mobility Spectrometry-orthogonal acceleration Time Of Flight Mass Spectrometry technique (IMS – oaTOF MS).

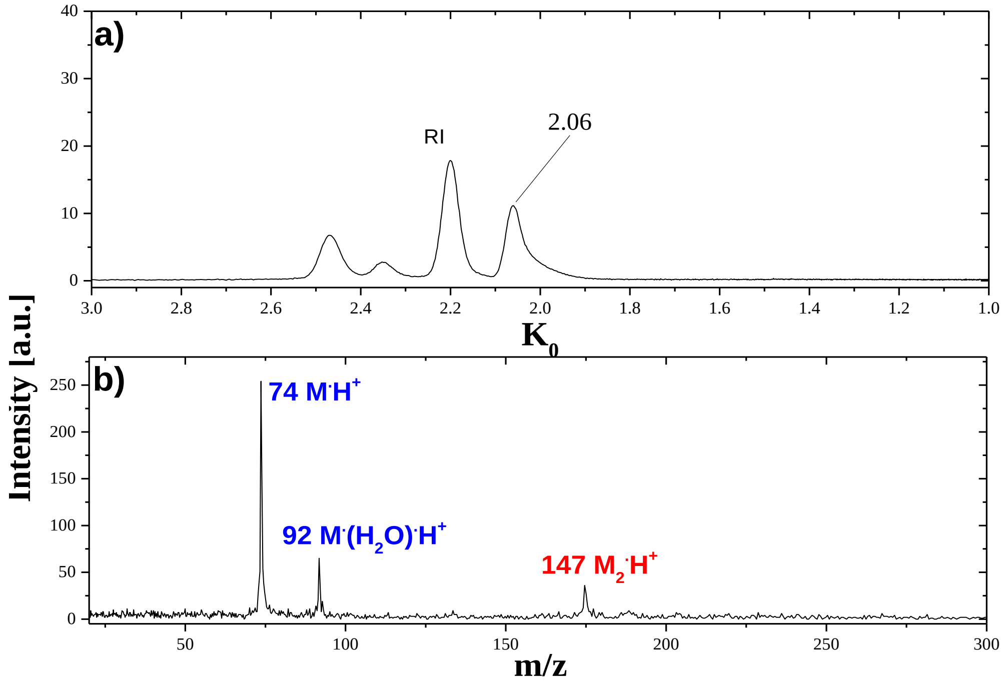

Figure 4. IMS (a) and MS (b) spectra for diethylamine at 370 K and 700 mbar and concentration 0.1 ppm.

8. Phthalates

In recent years phthalates have been accused of showing negative impact on human health. Breast cancer in females or mental and motor development in children can be caused by long term exposure on phthalates [31]. So, it is important to have a fast, sensitive and high-resolution technique for their detection. The most common techniques for detection of phthalate esters are gas chromatography coupled with mass spectrometry (GC-MS) and high-performance liquid chromatography (HPLC) [30][31].

Corona Discharge Ion Mobility Spectrometry (CD-IMS) combined with orthogonal acceleration Time of Flight Mass Spectrometry technique (IMS-oaTOF) [12] is a powerful tool with high resolution separation of complex samples and isomeric compounds. This technique was applied for studies of phthalates.

In this part three isomers or dimethyl phthalate (dimethyl phthalate –DMP (ortho - isomer), dimethyl isophthalate – DMIP (meta) and dimethyl terephthalate – DMTP (para)) using the IMS-oaTOF technique have been investigated. The ionisation of the phthalates was on the basis of Atmospheric Pressure Chemical Ionisation. The IMS – oaTOF spectra consisted of clusters ions $M{\cdot}H^+ \cdot(H_2O)_n$ with different degree of hydration (n=0,1,2,3) for different isomers. In the case of DMP isomer almost exclusive formation of $M{\cdot}H^+$ by proton transfer ionisation is observed, while in case of DMIP and DMTP hydrated ions $M{\cdot}H^+ \cdot(H_2O)_n$ (n=1,2,3) respectively $M{\cdot}H^+ \cdot(H_2O)_n$ (n=0,1,2) were detected, formed via adduct formation reaction. This behaviour can be explained by different ionisation mechanism. DFT calculations have been carried out to elucidate the ionisation processes

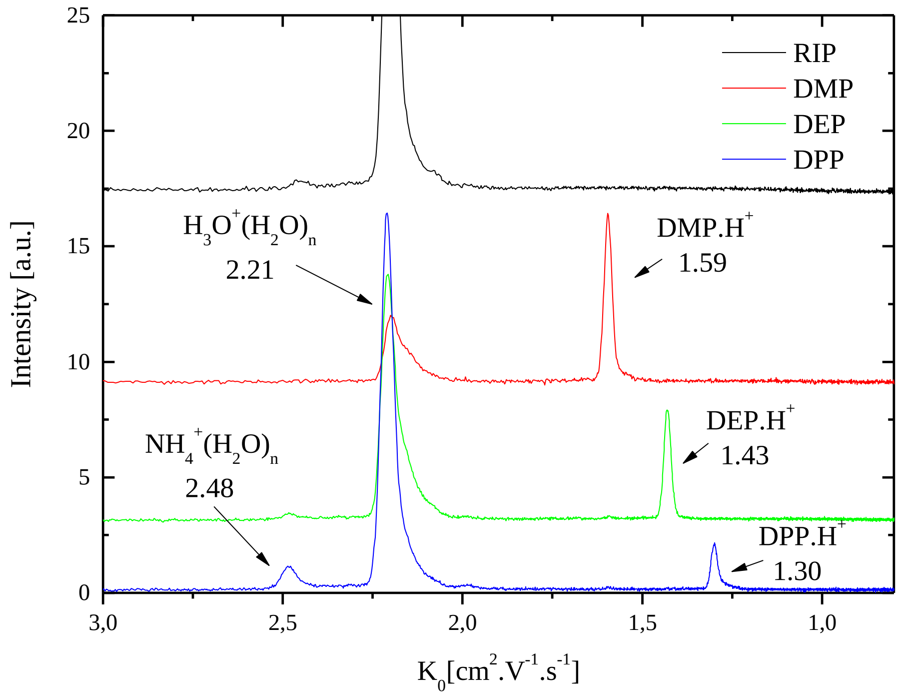

Figure 5. Ion mobility spectra for investigated phthalates.

8.1. *Study of Atmospheric Pressure Chemical Ionization Mechanism in Corona Discharge Ion Source with and without NH¬3 Dopant by Ion Mobility Spectrometry combined with Mass Spectrometry: A Theoretical and Experimental Study*

In Ion Mobility Spectrometry with Atmospheric Pressure Chemical Ionization due to the relative high water concentration in drift gas dominantly as a reactant ions (RI) exist clusters of hydronium ion with different number of hydration $H_3O^+(H_2O)_n$. But it is an advantage of IMS that by adding some admixtures to the drift gas it is possible to manipulate with the reactant ions, these admixtures are called dopants. In positive polarity operating IMS the most common used dopant is ammonia, which instead of $H_3O^+(H_2O)_n$ produces $NH_4^+(H_2O)_n$ ions which participate in ionisation process.

In this part, ionisation of several volatile organic compounds (VOCs) i.e. 2-nonanone, cyclopentanone, acetophenone, pyridine and di-tert-butylpyridine with and without NH_3 as a dopant was studied by IMS-oaTOF-MS and supported by theoretical calculations. In absence of ammonia the ionization proceeds via $H^+(H_2O)_n$ attachment to the VOC followed by partial dehydration and formation of $MH^+(H_2O)_x$ product ions. In the presence of NH_3 as a dopant, hydrated ammonium ($NH_4^+(H_2O)_n$) is attached to the analyte and an intermediate $[MNH_4^+(H_2O)_n]^*$ is formed. Subsequently, this intermediate can lose water molecule to produce $MNH_4^+(H_2O)_x$ product ion or lose both water and ammonia molecule to produce $MH^+(H_2O)_x$ as product ion.

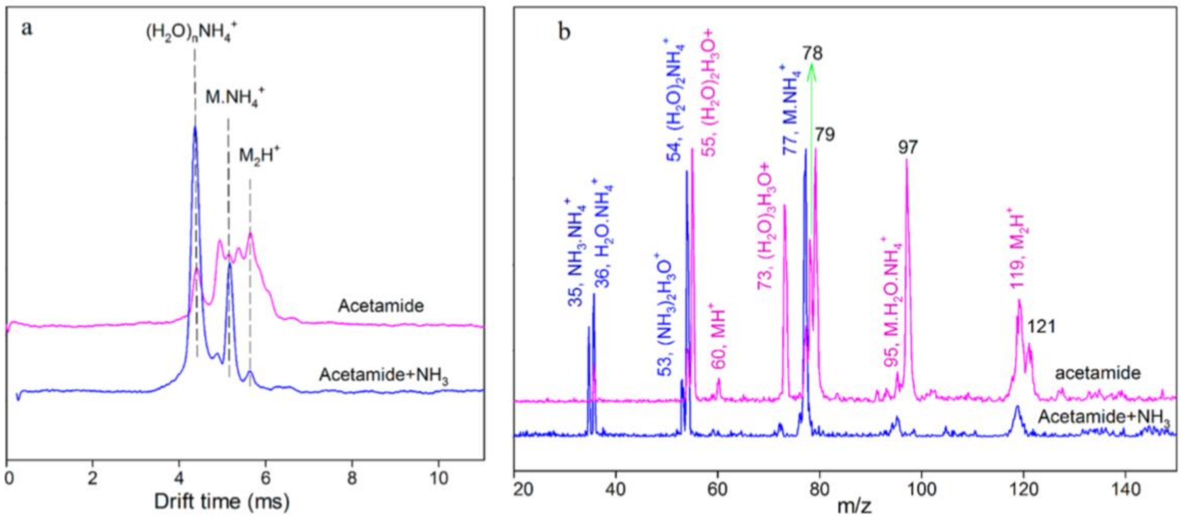

Figure 6. Comparison of the (a) IMS and (b) MS spectra of acetamide with and without NH3 dopant.

To explain how molecule will be ionised, its basicity can be helpful. For molecules with low basicity, $MNH_4^+(H_2O)_x$ is formed as product ion due to strong $MH^+{-}NH_3$ interaction. On the other hand, for molecules with high basicity the $M{-}H^+$ interaction is stronger than the $H^+{-}NH_3$ thus the $M{-}H^+{-}NH_3$ loses ammonia, and $MH^+(H_2O)_x$ is formed as product ions. Therefore, in the presence of the ammonia with $NH_4^+(H_2O)_n$ as RI, the product ions depend on the basicity of analyte (M) while in absence of ammonia when $H^+(H_2O)_n$ is a dominant reactant ion, the product ions are always $MH^+(H_2O)_n$.

8.2. Effect of Basicity and Structure on the Hydration of Protonated Molecules, Proton-Bound Dimer and Cluster Formation: An ion Mobility- Time of Flight Mass Spectrometry and Theoretical Study

Atmospheric pressure chemical ionisation sources (APCI) applied in IMS like corona discharge (CD) are commonly used but mechanism of ionisation in such source is not fully described. There exist many factors which can affect that process i.e. temperature, pressure, composition of the drift gas and humidity. Also, different molecules with diverse properties act differently during ionisation.

In this work effect of basicity and structure of ammonia, formaldehyde, formic acid, acetone, butanone, 2-ocatanone, 2-nonanone, acetophenone, ethanol, pyridine on the protonation, hydration and cluster formation was studied by IMS-oaTOF-MS setup with corona discharge ion source. Experiment was also supported by DFT calculations.

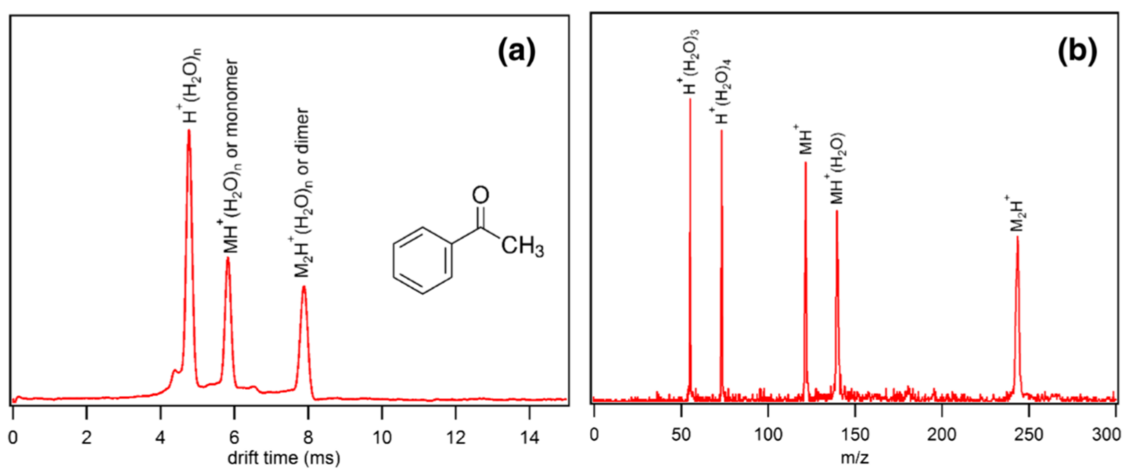

Figure 7. Comparison of (a) IMS and (b) MS spectra of 10 µL of head space of acetophenone in an IMS-MS with drift tube temperature and pressure of 110 °C and 0.75 bar, respectively

Results showed that degree of hydration of MH+ decreases as the proton affinity of analyte (M) increases thus more basic compounds form smaller MH+(H2O)n clusters. The same behaviour was observed in case of proton-bound dimers (M2H+), trimers (M3H+), and tetramers (M4H+) formation, it means that the molecules with higher basicity show lower tendency to form dimer, trimer or tetramer. Another factor which can influence the hydration degree is M and MH+ structure. Ammonia has high basicity but easily forms large clusters like NH4+(H2O)3. It can be explained by the fact that in NH4+ all hydrogen atoms are identical and can create hydrogen bonds. Furthermore, for asymmetric proton-bounded dimers like MH+N was found that these are more likely to be formed for molecules (M and N) with similar basicity.

9. *General conclusions*

This thesis dealt with the detection of several interesting molecules using Corona Discharge Ion Mobility Spectrometry (CD-IMS) and Ion Mobility Spectrometry coupled with orthogonally accelerated Time Of Flight Mass Spectrometry (IMS-oaTOF-MS).

First compound which was investigated is whisky lactone (β-methyl-γ-octalactone). It has been proven that IMS is suitable to detect whisky lactone in oak wood samples and to estimate concentration of it. This knowledge is important for manufacturers of wooden barrels as they can predict concentration of whisky lactone in final product. This is an example of potential of Ion Mobility Spectrometry in industry.

Another studied compounds were methanol, ethanol, propan-2-ol, acetone, ethyl acetate and diethylamine. These volatile organic compounds (VOCs) are commonly present in environment and trace amounts of these can be also found in analytical samples or final products. Using IMS technique we succeeded to detect these chemicals and IMS-MS experiment gave insight into nature of ions formed in the ionisation region.

IMS-MS was also applied for investigating dimethyl phthalate isomers. Obtained results proved that this technique is isomer and conformer selective. IMS and IMS-oaTOF mass spectra for investigated isomers showed differences in ion mobilities and in the ions formed in IMS. Dimethyl phthalate formation of MH^+ was observed while in case of dimethyl isophthalate and dimethyl terephthalate hydrated ions $MH^+(H_2O)_n$ (n = 1, 2, 3) and $MH^+(H_2O)_n$ (n = 0, 1, 2) respectively were observed.

Changing composition of drift gas by adding dopant gas can influence ionisation mechanism thus generated ions differ. 2-nonanone, cyclopentanone, acetophenone, pyridine and di-tert-butylpyridine were studied by IMS-MS technique with and without NH_3 as a dopant and different behaviour for different molecules have been observed. Generally, without ammonia the ionization proceeds via $H^+(H_2O)_n$ attachment to the sample while NH_3 is present, hydrated ammonium ($NH_4^+(H_2O)_n$) is attached to the analyte. We attribute this phenomenon to the basicity of a molecule.

Finally, effect of basicity and structure of ammonia, formaldehyde, formic acid, acetone, butanone, 2-ocatanone, 2-nonanone, acetophenone, ethanol, pyridine on the protonation, hydration and cluster formation was studied. Results showed that when proton affinity of analyte is higher, degree of hydration of MH^+ decreasing and smaller $MH^+(H_2O)_n$ clusters are formed. In case of ammonia and formaldehyde also structure influences the hydration degree. Furthermore, for asymmetric proton-bounded dimers like MH^+N was found that these are more likely to be formed for molecules (M and N) with similar basicity.

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1. *Author's publications*

1. B. Michalczuk, L. Moravský, P. Papp, P. Mach, M. Sabo, and Š. Matejčík, 'Isomer and conformer selective atmospheric pressure chemical ionisation of dimethyl phthalate', Phys. Chem. Chem. Phys., vol. 21, no. 25, pp. 13679–13685, Jun. 2019.

2. B. Michalczuk, M. Sabo, K. Jatzová, L. Moravský, M. Gregorová, Š.Matejčík, Fast quantification of whisky lactone in oak wood by ion mobility spectrometer, Talanta (2019),doi: https://doi.org/10.1016/j.talanta.2019.120567 (not yet registered in UK library)

3. Y. Valadbeigi, V. Ilbeigi, B. Michalczuk, M. Sabo, and S. Matejcik, 'Study of Atmospheric Pressure Chemical Ionization Mechanism in Corona Discharge Ion Source with and without NH 3 Dopant by Ion Mobility Spectrometry combined with Mass Spectrometry: A Theoretical and Experimental Study', J. Phys. Chem. A, vol. 123, no. 1, pp. 313–322, Jan. 2019.

4. Y. Valadbeigi, V. Ilbeigi, B. Michalczuk, M. Sabo, and S. Matejcik, 'Effect of Basicity and Structure on the Hydration of Protonated Molecules, Proton-Bound Dimer and Cluster Formation: An Ion Mobility-Time of Flight Mass Spectrometry and Theoretical Study', J. Am. Soc. Mass Spectrom., May 2019.

UNIVERZITA KOMENSKÉHO
FAKULTA MATEMATIKY, FYZIKY A INFORMATIKY
Zoznam publikačnej činnosti 2016-2019
Mgr. Bartosz Michalczuk

ADC Vedecké práce v zahraničných karentovaných časopisoch

ADC01 Michalczuk, Bartosz [UKOMFKEF] (40%) - Moravský, Ladislav [UKOMFKEF] (30%) - Papp, Peter [UKOMFKEF] (10%) - Mach, Pavel [UKOMFKJFB] (5%) - Sabo, Martin (5%) - Matejčík, Štefan [UKOMFKEF] (10%): Isomer and conformer selective atmospheric pressurechemical ionisation of dimethyl phthalate
Lit.: 31 zázn.
In: Physical Chemistry Chemical Physics. - Roč. 21, č. 25 (2019), s. 13679-13685. - ISSN (print) 1463-9076
Registrované v: scopus
Registrované v: wos
Indikátor časopisu:
IF (JCR) 2016=4,123
IF (JCR) 2017=3,906

ADC02 Valadbeigi, Younes (10%) - Ilbeigi, Vahideh (10%) - Michalczuk, Bartosz [UKOMFKEF] (50%) - Sabo, Martin (15%) - Matejčík, Štefan [UKOMFKEF] (15%): Study of atmospheric pressure chemical ionization mechanism in corona discharge ion source with andwithout NH3 dopant by ion mobility spectrometry combined with mass spectrometry: A theoretical and experimental study
Lit.: 36 zázn.
In: The Journal of Physical Chemistry A. - Roč. 123, č. 1 (2019), s. 313-322. - ISSN (print) 1089-5639
Registrované v: scopus
Registrované v: wos
Indikátor časopisu:
IF (JCR) 2016=2,847
IF (JCR) 2017=2,836

ADC03 Valadbeigi, Younes (10%) - Ilbeigi, Vahideh (10%) - Michalczuk, Bartosz [UKOMFKEF] (60%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Effect of basicity and structure on the hydration of protonated molecules, proton-bound dimer andcluster formation: an ion mobility-time of flight mass spectrometry and theoretical study
Lit.: 47 zázn.
In: Journal of the American Society for Mass Spectrometry. - Roč. 30, č. 7 (2019), s. 1242-1253. - ISSN (print) 1044-0305
Registrované v: scopus
Registrované v: wos

AFD Publikované príspevky na domácich vedeckých konferenciách

AFD01 Hrdá, Jana (30%) - Moravský, Ladislav [UKOMFKEF] (30%) - Michalczuk, Bartosz [UKOMFKEF] (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Detection of phthalates by atmospheric pressure chemical ionisation ion mobility spectrometry
Lit.: 6 zázn.
In: 22nd Symposium on Application of Plasma Processes and 11th EU-Japan Joint Symposium on Plasma Processing : Book of Contributed Papers. - Bratislava : Katedra experimentálnej fyziky, 2019. - S. 282-286. - ISBN 978-80-8147-089-9
[SAPP 2019 : Symposium on Application of Plasma Processes. 22, Štrbské Pleso, 18.01.2019 - 24.03.2019]
[EU-Japan JSPP 2019 : EU-Japan Joint Symposium on Plasma Processing. 11, Štrbské Pleso, 18.01.2019 - 24.01.2019]
URL:
http://neon.dpp.fmph.uniba.sk/sappxxii/download/SAPP_XXII_JSPP_XI_Book_of_Contributed_Papers.pdf

AFD02 Michalczuk, Bartosz [UKOMFKEF] (60%) - Sabo, Martin (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Detection of alkanes using ion mobility spectrometry
Lit. 7 zázn., 1 obr.
In: 21st Symposium on Application of Plasma Processes SAPP. - Bratislava : Department of Experimental Physics FMFI UK, 2017. - S. 197-198. - ISBN 978-80-8147-076-9
[SAPP 2017 : Symposium on Application of Plasma Processes. 21st, Štrbské Pleso, 13.-18.1.2017]

AFD03 Michalczuk, Bartosz [UKOMFKEF] (40%) - Moravský, Ladislav [UKOMFKEF] (40%) - Matejčík, Štefan [UKOMFKEF] (20%): Ion mobility spectrometry for rapid quantative analysis of whisky lactone in oak wood
Lit.: 6 zázn.
In: 22nd Symposium on Application of Plasma Processes and 11th EU-Japan Joint Symposium on Plasma Processing : Book of Contributed Papers. - Bratislava : Katedra experimentálnej fyziky, 2019. - S. 287-289. - ISBN 978-80-8147-089-9
[SAPP 2019 : Symposium on Application of Plasma Processes. 22, Štrbské Pleso, 18.01.2019 - 24.03.2019]
[EU-Japan JSPP 2019 : EU-Japan Joint Symposium on Plasma Processing. 11, Štrbské Pleso, 18.01.2019 - 24.01.2019]
URL:
http://neon.dpp.fmph.uniba.sk/sappxxii/download/SAPP_XXII_JSPP_XI_Book_of_Contributed_Papers.pdf

AFD04 Moravský, Ladislav [UKOMFKEF] (40%) - Michalczuk, Bartosz [UKOMFKEF] (40%) - Matejčík, Štefan [UKOMFKEF] (20%): Ion mobility spectrometry monitoring of decomposition of dimethyl phthalate by positive corona discharge
Lit.: 6 zázn.
In: 22nd Symposium on Application of Plasma Processes and 11th EU-Japan Joint Symposium on Plasma Processing : Book of Contributed Papers. - Bratislava : Katedra experimentálnej fyziky, 2019. - S. 131-134. - ISBN 978-80-8147-089-9
[SAPP 2019 : Symposium on Application of Plasma Processes. 22, Štrbské Pleso, 18.01.2019 - 24.03.2019]
[EU-Japan JSPP 2019 : EU-Japan Joint Symposium on Plasma Processing. 11, Štrbské Pleso, 18.01.2019 - 24.01.2019]
URL:
http://neon.dpp.fmph.uniba.sk/sappxxii/download/SAPP_XXII_JSPP_XI_Book_of_Contributed_Papers.pdf

AFG Abstrakty príspevkov zo zahraničných vedeckých konferencií

AFG01 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Ion mobility spectrometry monitoring of phtalate degradation by

atmospheric pressure discharges
Lit. 3 zázn.
In: ICPL 2017 : International Conference on Plasmas with Liquids. - Praha : Institute of Plasma Physics CAS, 2017. - S. 67. - ISBN 978-80-87026-07-6
[ICPL 2017 : International Conference on Plasmas with Liquids. Praha, 5.-9.3.2017]

BEE Odborné práce v zahraničných zborníkoch (konferenčných aj nekonferenčných)

BEE01 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Isomers detection by ion mobility spectrometry- mass spectrometry [elektronický dokument]
Lit.: 7 zázn.
In: 21st Symposium on Atomic, Cluster and Surface Physics 2018 (SASP 2018) [elektronický dokument] : Contributions. - Innsbruck : Universität Innsbruck, 2018. - S. 159-161 [online]
[SASP 2018 : Symposium on Atomic, Cluster and Surface Physics. 21, Obergurgl, 11.02.2018 - 16.02.2018]
URL: https://www.uibk.ac.at/sasp/sasp18/sasp2018_boa_interim.pdf

BEE02 Moravský, Ladislav [UKOMFKEF] (50%) - Michalczuk, Bartosz [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Ion Mobility Spectrometry monitoring of degradation of organic compounds by plasma jet [elektronický dokument]
Lit.: 10 zázn.
In: 21st Symposium on Atomic, Cluster and Surface Physics 2018 (SASP 2018) [elektronický dokument] : Contributions. - Innsbruck : Universität Innsbruck, 2018. - S. 74-77 [online]
[SASP 2018 : Symposium on Atomic, Cluster and Surface Physics. 21, Obergurgl, 11.02.2018 - 16.02.2018]
URL: https://www.uibk.ac.at/sasp/sasp18/sasp2018_boa_interim.pdf

BEE03 Moravský, Ladislav [UKOMFKEF] (50%) - Michalczuk, Bartosz [UKOMFKEF] (25%) - Matejčík, Štefan [UKOMFKEF] (25%): Ion mobility spectrometry monitoring of decomposition of phthalates by corona discharge
Nové výsledky výskumu
Lit.: 5 zázn.
In: 34 ICPIG and ICRP-10. - Sapporo : [s.n.], 2019. - S. 1-2, Art. No. PO18AM-069
[ICPIG 2019 : International Conference of Phenomena in Ionized Gases. 34, Sapporo, 14.07.2019 - 19.07.2019]
[ICRP 2019 : International Conference on Reactive Plasmas. 10, Sapporo, 14.07.2019 - 19.07.2019]

BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie, ...)

BFA01 Matejčík, Štefan [UKOMFKEF] (50%) - Michalczuk, Bartosz [UKOMFKEF] (20%) - Moravský, Ladislav [UKOMFKEF] (20%) - Sabo, Martin (10%): APCI ionisation of phthalates studein bylon Mobility Spectrometry - Mass Spectrometry
Lit.: 4 zázn.
In: ISIMS 27th Annual Conference. - Calgary : International Society for Ion Mobility Spectrometry, 2018. - S. 52-53
[ISIMS 2018 : International Society for Ion Mobility Spectrometry. 27, Calgary, 22.07.2018 - 27.07.2018]

BFA02 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (20%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (20%): Corona discharge ion mobility spectrometry as a good technique for phthalates detection
Popis urobený 4.12.2017
Lit. 4 zázn., 1 obr.
In: First International Conference of Soft Chemical Ionisation Mass Spectrometry and Applications to Trace Gas. - [Dornbirn] : [FH Vorarlberg, University of Applied Sciences], 2017. - S. 29
[Soft Chemical Ionisation Mass Spectrometry and Applications to Trace Gas 2017 : International Conference. 1st, Dornbirn, 18.-20.9.2017]
URL: https://homepages.fhv.at/ku/CSCIMS_abstracts.pdf

BFA03 Michalczuk, Bartosz [UKOMFKEF] (60%) - Moravský, Ladislav [UKOMFKEF] (20%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Detection of phthalate esters using corona discharge ion mobility spectrometry
Lit. 5 zázn.
In: ISIMS 2017 : 26th Annual Conference : Conference Materials. - [S.l.] : [ISMIS], 2017. - S. 64
[ISIMS 2017 : Annual Conference on Ion Mobility Spectrometry. 26th, Warszawa, 23.-27.7.2017]

BFA04 Michalczuk, Bartosz [UKOMFKEF] (40%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (20%): Tracking degradation of phthalate, by atmospheric pressure discharge, by Ion Mobility Spectrometry
Lit. 4 zázn.
In: The 10th EU-Japan Joint Symposium on Plasma Processing (JSPP2017). - [Osaka] : [Osaka University], 2017. - Nestr. [2 s.]
[JSPP 2017 : Plasma Processing : EU-Japan Joint Symposium. Nago, 4.-7.12.2017]

BFA05 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Monitoring of environmental pollutans degradation using Ion Mobility Spectrometry
Lit.: 7 zázn.
In: ISIMS 27th Annual Conference. - Calgary : International Society for Ion Mobility Spectrometry, 2018. - S. 58-59
[ISIMS 2018 : International Society for Ion Mobility Spectrometry. 27, Calgary, 22.07.2018 - 27.07.2018]

BFA06 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Ion Mobility Spectrometry - Mass Spectrometry as a good tool for monitoring trace amounts of phthalates
Lit.: 5 zázn.
In: ISIMS 27th Annual Conference. - Calgary : International Society for Ion Mobility Spectrometry, 2018. - S. 60-61
[ISIMS 2018 : International Society for Ion Mobility Spectrometry. 27, Calgary, 22.07.2018 - 27.07.2018]

BFA07 Michalczuk, Bartosz [UKOMFKEF] (50%) - Moravský, Ladislav [UKOMFKEF] (30%) - Sabo, Martin (5%) - Matejčík, Štefan [UKOMFKEF] (15%): Ultrasensitive method of monitoring of VOC s decomposition in corona discharge based on Ion Mobility Spectrometry
Lit.: 6 zázn.
In: HAKONE 16 : 16th International Symposium on High Pressure Low Temperature Plasma Chemistry. - Peking : Tsinghua University, 2018. - S. 1-2, nestr.
[HAKONE 2018 : High Pressure Low Temperature Plasma Chemistry : International Symposium. 16, Peking, 02.09.2018 - 07.09.2018]

BFA08 Michalczuk, Bartosz [UKOMFKEF] (45%) - Moravský, Ladislav [UKOMFKEF] (45%) - Matejčík, Štefan [UKOMFKEF] (10%): Rapid quantitative analysis of volatiles in oak wood by Ion Mobility Spectrometry [elektronický dokument]
Lit.: 2 zázn.
In: Spectrometry for Security Applications [elektronický dokument] : First International Workshop. - Cambridge : Chemical Sciences Security Group, 2019. - S. 31-31 [online]
[Spectrometry for Security Applications. 1, Dornbirn, 10.02.2019 - 13.02.2019]
URL: https://homepages.fhv.at/ku/SfSAbstracts.pdf

BFA09 Moravský, Ladislav [UKOMFKEF] (40%) - Michalczuk, Bartosz [UKOMFKEF] (30%) - Matejčík, Štefan [UKOMFKEF] (30%): Ion mobility spectrometry monitoring of phthalate degradation by atmospheric corona discharge
Lit. 6 zázn.
In: The 10th EU-Japan Joint Symposium on Plasma Processing (JSPP2017). - [Osaka] : [Osaka University], 2017. - Nestr. [2 s.]
[JSPP 2017 : Plasma Processing : EU-Japan Joint Symposium. Nago, 4.-7.12.2017]

BFA10 Moravský, Ladislav [UKOMFKEF] (40%) - Michalczuk, Bartosz [UKOMFKEF] (40%) - Matejčík, Štefan [UKOMFKEF] (20%): Monitoring decomposition of phthalates by corona discharge based on ion mobility spectrometry [elektronický dokument]
In: GEM 20 : The 20th Gaseous Electronics Meeting [elektronický dokument]. - Cairns : James Cook University, 2018. - S. 1-1, nestr. [USB-key]
[GEM 2018 : Gaseous Electronics Meeting. 20, Magnetic Island, 21.06.2018 - 24.06.2018]

BFA11 Moravský, Ladislav [UKOMFKEF] (60%) - Michalczuk, Bartosz [UKOMFKEF] (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Ion Mobility Spectrometry monitoring of decomposition of Phthalates by Corona Discharge [elektronický dokument]
Lit.: 6 zázn.

In: ESCAMPIG 24 [elektronický dokument] : Abstracts. - Glasgow : University of Glasgow, 2018. - S. 208-209 [USB-key]
[ESCAMPIG 2018 : Europhysics Conference on Atomic and Molecular Physics of Ionised Gases. 24, Glasgow, 07.07.2018 - 21.07.2018]

BFA12 Moravský, Ladislav [UKOMFKEF] (40%) - Michalczuk, Bartosz [UKOMFKEF] (40%) - Hrdá, Jana (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Phthalate detection by APCI ion mobility spectrometry [elektronický dokument]
Lit.: 2 zázn.
In: Spectrometry for Security Applications [elektronický dokument] : First International Workshop. - Cambridge : Chemical Sciences Security Group, 2019. - S. 30-30 [online]
[Spectrometry for Security Applications 2019 : International Workshop. 1, Dornbirn, 10.02.2019 - 13.02.2019]
URL: https://homepages.fhv.at/ku/SfSAbstracts.pdf

BFB Abstrakty odborných prác z domácich podujatí (konferencie, ...)

BFB01 Ilbeigi, Vahideh (10%) - Michalczuk, Bartosz [UKOMFKEF] (30%) - Moravský, Ladislav [UKOMFKEF] (30%) - Matejčík, Štefan [UKOMFKEF] (30%): Mechanism of corona discharge (CD) atmospheric pressure chemical ionization (APCI) with and without NH3 dopantstudied by ion mobility spectrometry combined with mass spectrometry
Lit.: 3 zázn.
In: Book of Abstracts: The Seminar on Trends in Plasma Physics. - Bratislava : Katedra experimentálnej fyziky, 2018. - S. 11-11
[New Trends in Plasma Physics 2018 : Seminár BB. Doľany, 04.10.2018]

BFB02 Moravský, Ladislav [UKOMFKEF] (34%) - Michalczuk, Bartosz [UKOMFKEF] (33%) - Matejčík, Štefan [UKOMFKEF] (33%): Ion mobility spectrometry monitoring of phthalate isomers
In: Book of Abstracts: The Seminar on Trends in Plasma Physics. - Bratislava : Katedra experimentálnej fyziky, 2018. - S. 12-12
[New Trends in Plasma Physics 2018 : Seminár BB. Doľany, 04.10.2018]

Štatistika kategórií (Záznamov spolu: 25):
ADC Vedecké práce v zahraničných karentovaných časopisoch (3)
AFD Publikované príspevky na domácich vedeckých konferenciách (4)
AFG Abstrakty príspevkov zo zahraničných vedeckých konferencií (1)
BEE Odborné práce v zahraničných zborníkoch (konferenčných aj nekonferenčných) (3)
BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie, ...) (12)
BFB Abstrakty odborných prác z domácich podujatí (konferencie, ...) (2)

9.12.2019