ANALYTICAL METHODS IN CHEMISTRY
AND CHEMICAL TECHNOLOGY

АНАЛИТИЧЕСКИЕ МЕТОДЫ
В ХИМИИ И ХИМИЧЕСКОЙ ТЕХНОЛОГИИ

ISSN 2686-7575 (Online)

https://doi.org/10.32362/2410-6593-2021-16-6-512-525

UDC 535.33/34:547.77

RESEARCH ARTICLE

Ion mobility spectrometry of *N*-methylimidazole and possibilities of its determination

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Abstract

Objectives. *To determine the ion mobility of N-methylimidazole, establish the structure of ions corresponding to characteristic signals, and determine the detection limit of N-methylimidazole on the ion-drift detector Kerber.*
Methods. *Ion mobility spectrometry was used to study the ionization processes. The enthalpies of the reactions of monomer and dimer ions were calculated in the ORCA 4.1.1 software by the B3LYP density functional method with a set of basic functions 6-31G (d, p).*
Results. *The drift time and ion mobility values of N-methylimidazole were determined. A method for mathematical processing of spectra and a program for its implementation was developed. The changing peculiarities of the ion mobility spectrum during measurement at a given time were studied. According to the interpretation of the spectrum signals, the structure of the generated ions was proposed, and the enthalpies of ion formation were determined.*
Conclusions. *The characteristic signal of the N-methylimidazole ion protonated at the nitrogen atom of the pyridine type was revealed. It was found that two signals in the ion mobility spectra of N-methylimidazole correspond to the presence of the monomer and dimer ions. The detection limit of N-methylimidazole on the ion-drift detector Kerber was determined, amounting to 3 pg.*

Keywords: *ion mobility spectrometry (IMS), characteristic signal, protonation, heterocyclic nitrogen compounds, pyridine, imidazole, N-methylimidazole*

For citation: Aleksandrova D.A., Melamed T.B., Baberkina E.P., Fenin A.A., Osinova E.S., Kovalenko A.E., Yakushin R.V., Shaltaeva Yu.R., Belyakov V.V., Zykova D.I. Ion mobility spectrometry of *N*-methylimidazole and possibilities of its determination. *Tonk. Khim. Tekhnol. = Fine Chem. Technol*. 2021;16(6):512–525 (Russ., Eng.). https://doi.org/10.32362/2410-6593-2021-16-6-512-525

НАУЧНАЯ СТАТЬЯ

Спектрометрия ионной подвижности *N*-метилимидазола и возможности его определения

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Аннотация

Цели. *Определение значений ионной подвижности N-метилимидазола. Установление строения ионов, соответствующих характерным сигналам. Определение предела обнаружения N-метилимидазола на ионно-дрейфовом детекторе Кербер.*

Методы. *Метод спектрометрии ионной подвижности был использован для исследования процессов ионизации. Энтальпии реакций мономерных и димерных ионов расчитаны в программе ORCA 4.1.1 методом функционала плотности B3LYP с набором базисных функций 6-31G(d,p).*

Результаты. *Определены значения времени дрейфа и ионной подвижности N-метилимидазола. Разработана методика математической обработки спектров и программа для ее реализации. Изучены особенности изменения характера спектра ионной подвижности в процессе измерения в данный момент времени. Предложено строение генерируемых ионов в соответствии с интерпретацией сигналов спектра. Определены энтальпии образования ионов.*

Выводы. *Выявлен характеристический сигнал иона N-метилимидазола, протонированного по атому азота пиридинового типа. Установлено, что два сигнала в спектрах ионной подвижности N-метилимидазола соответствуют наличию мономерной и димерной формы ионов. Определен предел обнаружения N-метилимидазола на ионно-дрейфовом детекторе Кербер, составляющий 3 пг.*

Ключевые слова: *спектрометрия ионной подвижности, характеристический сигнал, протонирование, гетероциклические соединения азота, пиридин, имидазол, N-метилимидазол*

Для цитирования: Александрова Д.А., Меламед Т.Б., Баберкина Е.П., Фенин А.А., Осинова Е.С., Коваленко А.Е., Якушин Р.В., Шалтаева Ю.Р., Беляков В.В., Зыкова Д.И. Спектрометрия ионной подвижности *N*-метилимидазола и возможности его определения. *Тонкие химические технологии*. 2021;16(6):512–525. https://doi.org/10.32362/2410-6593-2021-16-6-512-525

INTRODUCTION

Ion mobility spectrometry is a promising fast modern method for analyzing chemical compounds in the gas phase [1, 2]. The method is promising for solving a wide range of analytical problems because of its speed, high sensitivity, lack of vacuum systems, and portability [3–9]. However, a large number of possible ion-molecular reactions take place in the drift space of an ion mobility spectrometer, as well as an incompletely studied mechanism of ion formation complicate the reliable interpretation of ion mobility spectra. Expanding the capabilities of the method is of great theoretical and practical interest.

Recently, the so-called “designer drugs” have become popular. Small changes in the chemical structure of legally controlled substances (homologs and small newly introduced functional groups) make it possible to circumvent existing bans and sell potentially hazardous substances disguised as legal drugs. Often the consequences of exposure to modified substances on the body cause the rapid development of physical and psychological dependence (addiction) to them, which turns out to be far more dangerous than the original drugs. Such compounds are difficult to detect because they are not included in the major databases of analytical instruments.

As a result, determining the characteristic signal of a whole class of compounds becomes important for detecting synthetic cannabinoids [10, 11].

Earlier, to develop conditions for the detection of synthetic cannabinoids based on imidazole by ion mobility spectrometry, a research on the behavior of imidazole was conducted on the ion-drift detector Kerber, which is already used by the Ministry of Internal Affairs, Federal Security Service, Ministry of Emergency Situations, and Federal Customs Service of the Russian Federation to detect main drugs and explosives [12–15]. It was discovered that the spectrum of the ion mobility of imidazole always contains two signals with ion mobility of 2.100 $cm^2/(V \cdot s)$ and 1.700 $cm^2/(V \cdot s)$, corresponding to the monomer and dimer ions, respectively. The effect of concentrations on the characteristics of the spectrum is investigated. An assumption was made about the structure of the dimer, and it was demonstrated that the interconversion of the monomer–dimer forms occurs during measurement, depending on the concentration of the sample.

According to the published data, imidazole can form dimers as well as long chains associated with water [16, 17]. However, in the range of spectrum registration, a multitude of signals of oligomeric chains was not recorded; instead only one signal of the dimer was recorded, therefore, it was assumed that it was this signal that was formed. Its structure was proposed considering the formation of a complex with water [1].

The results of the study of *N*-methylimidazole, which is not prone to the formation of stable dimer forms, are presented in this paper to obtain additional data on the nature of the ion mobility spectra of imidazole derivatives.

The goal of this work is to determine the characteristic signals of *N*-methylimidazole using ion mobility spectrometry, thereby confirming the proposed structure of ions formed during corona discharge ionization.

EXPERIMENTAL

The studies were conducted on an ion-drift detector (IDD) Kerber[1] manufactured by *Yuzhpolimetal-Holding Group of Companies* (Russia). The characteristics of the device are given in Table 1.

Ion mobility spectra were obtained at atmospheric pressure using ambient air as the drift gas. Target

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[1] Yuzhpolymetal Holding. Kerber-T portable ion-drift detector. http://www.analizator.ru/production/ims/kerber-t/. Accessed September 16, 2021.

Table 1. Specifications of IDD Kerber

Characteristic	IDD Kerber value
Detection range of low-volatile organic substances by 2,4,6-trinitrotoluene (TNT), g	from 1.0×10^{-11} to 2.0×10^{-7}
Low-volatile organic matter detection limit for 2,4,6-trinitrotoluene (TNT) – for solid particles, g – in pairs, g/cm^3	 no more 1.0×10^{-11} no more 1.0×10^{-14}
Ionization method	Pulsed corona discharge
Drift tube temperature, °C	100
Time of detection and identification for all detectable substances, s	no more 5
The probability of a false alarm, %	no more 1
Detector cleaning time in case of contamination with target substances within the detection range, s	no more 180

substances were registered using the software IDD Kerber in the "Spectrum" format. The measurement results were text files containing information about the parameters of the system, the detected target substances and the drift time. Ionograms were constructed according to the indicated data.

A sample of *N*-methylimidazole produced by *Acros Organics* (USA) with a purity of 99% was selected for the study.

We used a balance of the brand A&D GR-120 (*AND*, Japan) with a discreteness of 0.0001 g.

A Lenpipet Light 1–10 µL dispenser (*Thermo Scientific*, USA) was used to prepare solutions of the required concentrations and to apply the substance to a sampling napkin. The sampling napkin is an aluminum foil with dimensions of 120 × 60 mm and a thickness of 11–16 µm.

The enthalpies of reactions were calculated using the ORCA 4.1.1 program of the Max Planck Institute for Energy Conversion Chemistry (Germany) by the density functional method B3LYP with a set of basic functions 6-31G (d, p).

POSITIVE ION FORMATION BY CORONA DISCHARGE

The method of ion mobility spectrometry is based on the ionization of the molecules of the investigated substance at atmospheric pressure. First, reactant ions $H^+(H_2O)_n$ are formed in the discharge chamber, whose concentration significantly exceeds that of the substances to be detected.

Reactant ions transfer charge to molecules of the target substances by the mechanism of chemical ionization presented below:

$$M^+ + H^+(H_2O)_n \rightarrow MH^+(H_2O)_n \rightarrow MH^+(H_2O)_{(n-x)} + x\,H_2O \quad (1)$$

where M—test compound molecule, $H^+(H_2O)_n$—reactant ion, $MH^+(H_2O)_n$—cluster ion, $MH^+(H_2O)_{(n-x)}$—test compound ion.

In the process, product monomer and dimer ions can be formed, $M_2H^+(H_2O)_n$, as well as other molecular ions. Product ions are associated with water molecules. Depending on the nature of the compound, the number of water molecules in the resulting cluster can vary from one to three [1, 2].

The drift time τ_d (the arrival time of ions to the collector) is determined by the charge, mass, and effective cross-section of the formed ion. The drift time is proportional to the length of the drift chamber L(cm) and inversely proportional to the electric field gradient E:

$$\tau_d = 1/K \times L/E \quad (2)$$

where K—mobility coefficient, $cm^2/(V \cdot s)$. Ion mobility depends on temperature and atmospheric pressure. To compare the values of ion mobility, the values of K obtained under different conditions lead to normal conditions and obtain the reduced mobility K_0 (or reduced coefficient of mobility):

$$K_0 = (K \times P)/101325 \times 273/T \quad (3)$$

where T—temperature (Kelvin) and P—pressure (Pascal) of the gas atmosphere in which the ions move [2]. This work shows the values of the reduced ion mobility.

The results are presented in the form of a "spectrum" of ion mobility (ionograms).

METHODS

The spectrum of ion mobility of *N*-methylimidazole was obtained while passing through the drift chamber's ionized molecules.The analyte sample was collected either at room temperature 22°C or after heating the substrate to 100°C for some seconds. The spectrum was captured at a frequency of 1 s. This approach to the analysis of spectra made it possible to determine both the ion mobility of characteristic signals and the redistribution of their intensities, which characterizes the formation and interconversion of ions in the drift chamber of an ion-drift detector.

It was discovered that the ion mobility of *N*-methylimidazole is unaffected by temperature of the analyte sample. As a result, the sampling was carried out by heating to 100ºC to obtain a signal with a high value of the ion current.

For mathematical data processing, a program was developed that allows obtaining data and processing a large number of ion mobility spectra for the purpose of their subsequent study and analysis. The interpreted programming language Python 3.3 was used to create the program.

In general, the operation of the program can be described as follows. The program consists of three scripts, each with a specific task. In the first step, the list of source files is sorted alphabetically, as the os.walk() function returns filenames in no particular order. This operation is necessary in order to accurately reproduce the order of recording spectra on the Kerber IDD.

The presence of substance signals is considered relative to background signals, since the air always contains a certain amount of ions (impurities), and the spectrum of the background signal may change depending on the current concentrations of impurities in the air. Therefore, it is imperative that a "zero" or "background" measurement is performed first. Background data is also required when determining the detection limit of a sample.

IDD Kerber of Classic and Next series saves spectra files in .dat and .spe formats, respectively. Depending on the format of the files in the directory, the program calls the corresponding function from the imported local modules imp_spe and imp_dat. Further processing is carried out by procedures described in the imp_dat and imp_spe modules. The reduced ion mobility is calculated at each moment of time, considering the conversion factor, which contains the values of temperature and atmospheric pressure during the measurement.

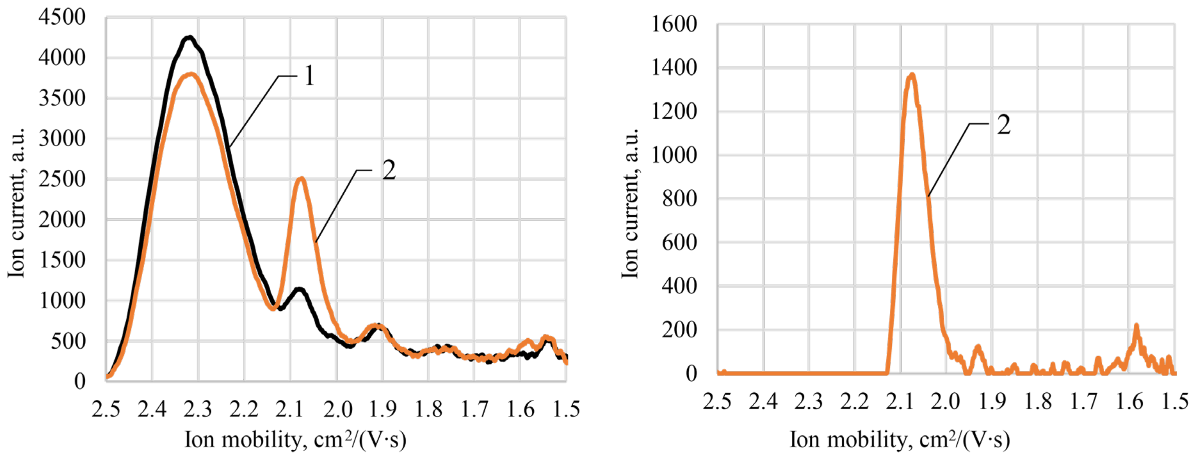
Next, the program requests data to remove noise signals. During the subsequent processing of the spectra, the values of the ion current signals of the ambient air background are subtracted from the values of the ion current signals of the sample, which increases the visibility of the spectrum. Before this operation is performed, the initial signal of the device is stored in adjacent columns; if necessary, it is possible to construct a spectrum with the initial data.

Further investigation of the ionization processes requires the calculation of the peak areas of the sample characteristic signal. In terms of mathematical analysis, all signals on the ionogram are curved trapezoids. Therefore, to obtain additional data on the structure and interconversion of analyte ions, the area of a curved trapezoid was calculated using the method of middle rectangles. The length of the rectangle was taken as 1/2 the sum of the values between the corresponding points along the ion current axis. The spectrum was used to determine the boundaries of the signal of the substance (along the abscissa) and the area of the peak (curvilinear trapezoid) was calculated by summing the corresponding values. The boundaries of the array to be summed for the formula =SUM(number1; [number2]; ...) were determined manually or using the formula =MATCH(search_value; lookup_array; [match_type]). Further, depending on the tasks of the user and the nature of the investigated substance, one can compare the intensity of signals, their changes, similarities and differences.

As a result of the mathematical processing, an Excel file was created that included all the selected data in both the positive and negative ionization regions.

Figure 1 illustrates the processing of the ion mobility spectrum using the program.

To determine the limit of detection of *N*-methylimidazole on the Kerber IDD, a method of serial dilution of the solution was developed. For this, a solution of *N*-methylimidazole in diethyl ether with a concentration of 0.0003 g/cm^3 was used. One mm^3



a

b

Fig. 1. Ion mobility spectrum of *N*-methylimidazole before (a) and after (b) mathematical processing. (1) Background and (2) *N*-methylimidazole.

of the solution was applied with a dispenser onto a sampling tissue. After evaporation of the solvent, a sample weighing $3 \cdot 10^{-7}$ g was taken with heating for 5 s. As a result, a spectrum was obtained with an amplitude of 5000 analog-to-digital conversion units (a.u.). Then the analyte solution was diluted in order to decrease the concentration of the solution by one order of magnitude by adding a solvent, until a signal of the sample with a mass of 3 pg with an amplitude of 800 a.u. was obtained. The signal of the substance did not exceed the noise values with a decrease in the concentration of the solution by one more order of magnitude.

RESULTS AND DISCUSSION

Heterocyclic nitrogen compounds that have basic properties and an sp^2-hybrid nitrogen atom of the pyridine type were selected for the studies. As a result of the research, a series of *N*-methylimidazole, imidazole, and pyridine spectra were obtained. They were mathematically processed to identify the characteristic signals of ions (Fig. 2).

As seen from Fig. 2, in all spectra of ion mobility, a characteristic signal is observed in the range of 2.1 cm^2/(V·s), previously assigned to the protonated form of the monomer at the pyridine nitrogen atom, which is consistent with preliminary studies of other heterocyclic compounds [12, 14, 15]. This signal is the only characteristic in the spectrum of ion mobility of pyridine. The spectra of imidazole and *N*-methylimidazole (Fig. 1) also show stable signals with ion mobility of 1.7 and 1.6 cm^2/(V·s), respectively, preliminarily assigned to the protonated forms of their dimers. It should be noted that the nature of the spectra of imidazole and *N*-methylimidazole is identical in the number of signals obtained, which suggests the formation of an *N*-methylimidazole dimer, despite the presence of a methyl substituent on the pyrrole nitrogen atom.

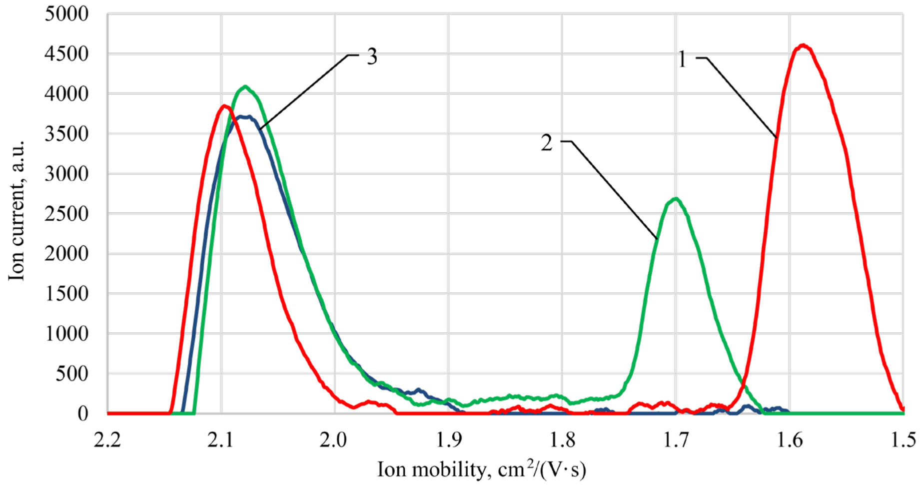


Fig. 2. Ionogram of *N*-methylimidazole (1), imidazole (2), and pyridine (3).

To establish the structure of generated ions, we calculated the enthalpies of specific reactions occurring during the formation of analyte ions (Table 2).

There have been several proposed structures for monomer and dimer analyte ions. The enthalpies of reactions were calculated in the ORCA 4.1.1 program using the B3LYP density functional method with a set of basis functions 6-31G (d, p). Based on the obtained data, the most probable structures of imidazole and *N*-methylimidazole ions were proposed. The structure of the monomers of the ions of imidazole No. 2 and *N*-methylimidazole No. 4 coincides, as evidenced by the enthalpies of the reaction processes and close values of the ion mobility. The presence of a water molecule in the structure of an analyte ion is in complete agreement with the data on the formation of ions during a corona discharge in the form of associates with water [1].

Table 2. Monomeric ion reaction enthalpies of imidazole and *N*-methylimidazole

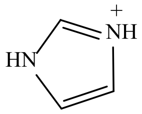
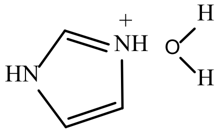
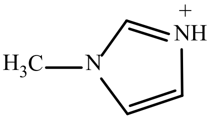
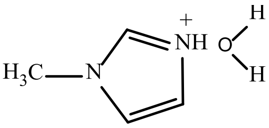
No.	Ion structure	Reaction enthalpy, kJ/mol
1		−247
2		−331
3		−265
4		−346

Table 3. Reaction enthalpies of dimeric and trimeric ions of imidazole and *N*-methylimidazole

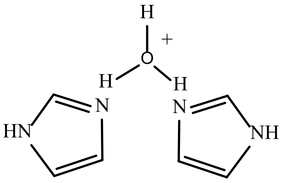
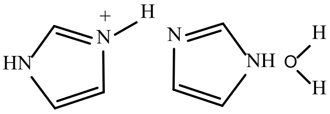
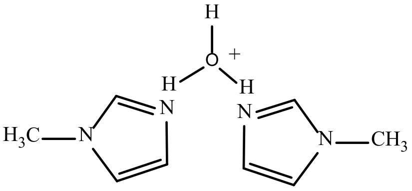
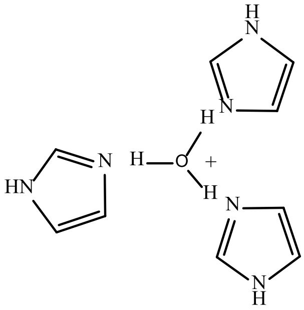
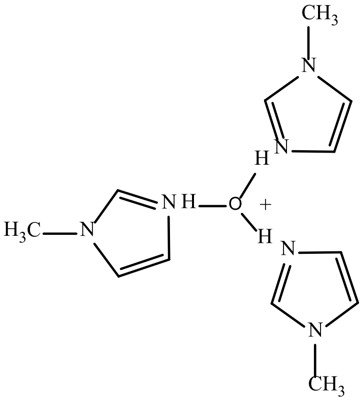
No.	Ion structure	Reaction enthalpy, kJ/mol
1		−96.4
2		−112
3		−97.6

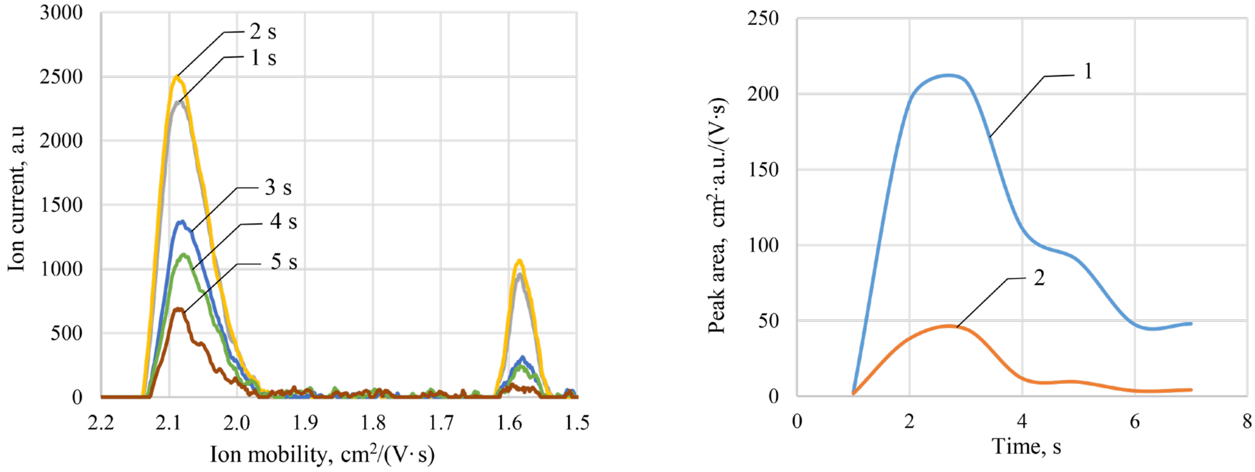
Table 3. Continued

No.	Ion structure	Reaction enthalpy, kJ/mol
4		−85.4
5		−84.1

Various structures were proposed for dimer ions (Table 3).

Since imidazole tends to form chains under normal conditions and the enthalpy of formation of such a dimer is lower, the formation of dimer No. 2 is most likely. For *N*-methylimidazole, such a structure is impossible due to the substituent at the first atom; therefore, dimer No. 3 is formed. Signals corresponding to oligomer forms of ions were not observed in the spectrum.

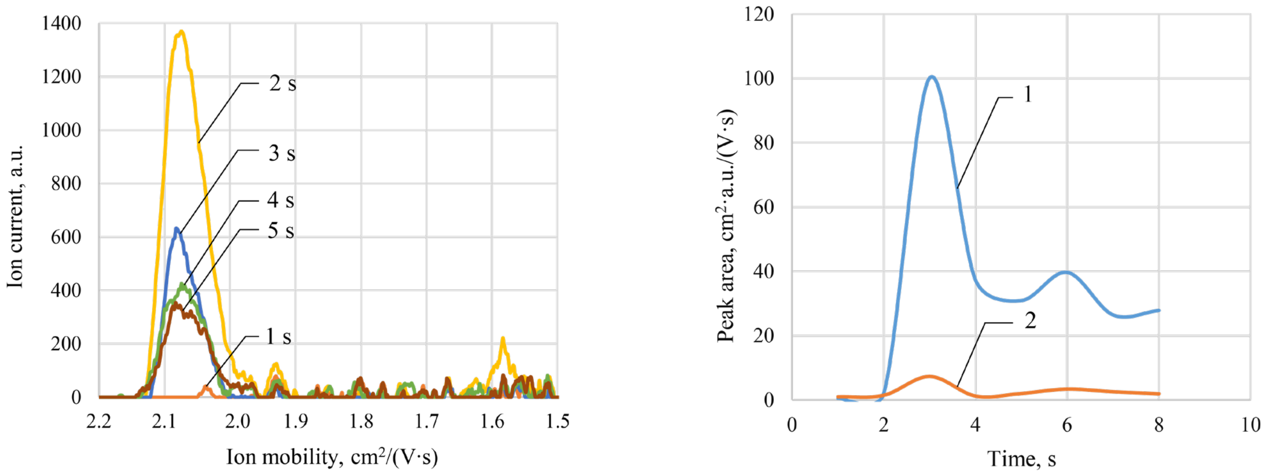
To establish the limit of detection of *N*-methylimidazole, the ion mobility spectra were studied at various concentrations. The corresponding ionograms are shown in Figs. 3 and 4.



a

b

Fig. 3. Ion mobility spectrum of *N*-methylimidazole with a mass of 3 ng and time dependence of the signal intensity: (a) dependence of the ion current on the ion mobility of *N*-methylimidazole (spectra were taken every 1 s after the start of measurement); (b) ion mobility change in the spectrum of *N*-methylimidazole: (1) monomer ion and (2) dimer ion.



a

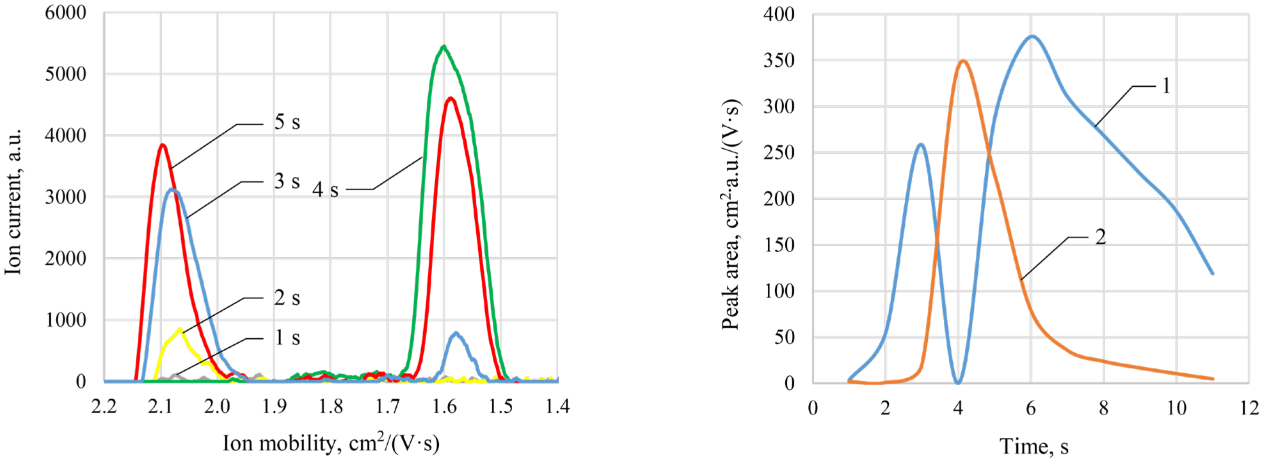
b

Fig. 4. Ion mobility spectrum of *N*-methylimidazole with a mass of 0.3 ng and time dependence of the signal intensity: (a) dependence of the ion current on the ion mobility of *N*-methylimidazole (spectra were taken every 1 s after the start of measurement); (b) ion mobility change in the spectrum of *N*-methylimidazole: (1) monomer ion and (2) dimer ion.

The change in the peak areas completely correlates with the signal intensity and indicates the simultaneous presence of two ions. A simultaneous increase and then a decrease in the intensity of the signals of both peaks was observed, with the monomer peak having a higher amplitude than the dimer peak (Fig. 3).

With a decrease in the mass of the sample, the following changes occur in the spectrum (Fig. 4).

The ion mobility of the monomer signal corresponds to the mobility of the 3-ng *N*-methylimidazole sample (Fig. 3). And the dimer peak is practically absent. With a decrease in the concentration of *N*-methylimidazole in the sample in the ion mobility spectrometer, the destruction of the dimer begins due to collision with gas molecules in the drift chamber, which is reflected in the ion mobility spectrum.



a

b

Fig. 5. Ion mobility spectrum of *N*-methylimidazole in water solution and time dependence of the signal intensity: (a) dependence of the ion current on the ion mobility of *N*-methylimidazole (spectra were taken every 1 s after the start of measurement); (b) ion mobility change in the spectrum of *N*-methylimidazole: (1) monomer ion and (2) dimer ion.

The analysis of the ion mobility spectra of *N*-methylimidazole water solution is below. The obtained ionogram and the corresponding dependence of the change in signal intensity on time are shown in Fig. 5.

The dimer ion of *N*-methylimidazole shows non-stability and degrades within 4 s after the start of the measurement, while the monomer concentration decreases gradually. Due to the destruction of the dimer ion, the monomer concentration begins to increase again. Similar processes were observed for unsubstituted imidazole, which is demonstrated in Fig. 6.

For the limiting detection value of *N*-methylimidazole with a mass of 3 pcg, a decrease in the intensity of the signal with an ion mobility of 2.1 to 800 a.u. and a complete disappearance of the signal with a lower ion mobility attributed to the signal of the dimer ion are observed (Fig. 7). The nature of the ionogram is identical to the spectrum shown

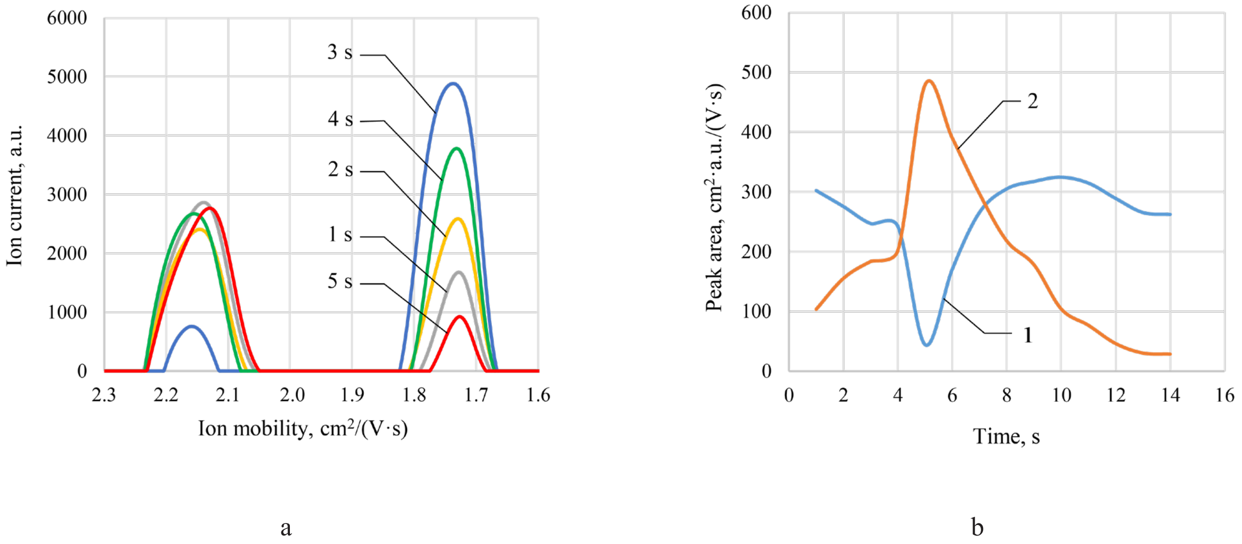


Fig. 6. Ion mobility spectrum of imidazole in water solution and time dependence of the signal intensity: (a) dependence of the ion current on the ion mobility of imidazole (spectra were taken every 1 s after the start of measurement); (b) ion mobility change in the spectrum of imidazole: (1) monomer ion and (2) dimer ion.

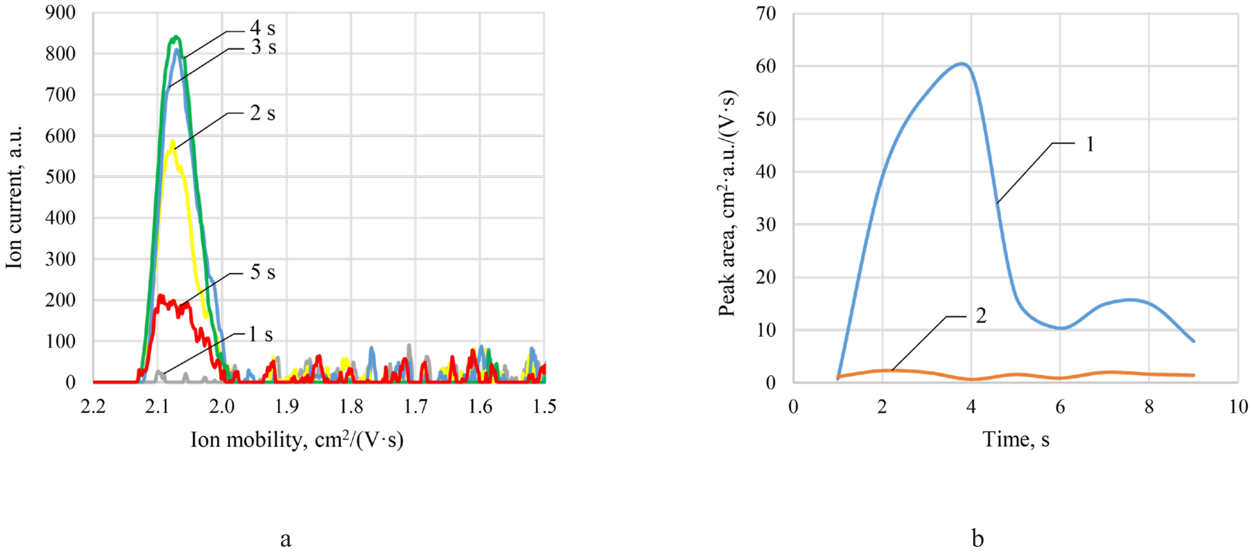


Fig. 7. Ion mobility spectrum of *N*-methylimidazole with a mass of 0.3 pg and time dependence of the signal intensity: (a) dependence of the ion current on the ion mobility of *N*-methylimidazole (spectra were taken every 1 s after the start of measurement); (b) ion mobility change in the spectrum of *N*-methylimidazole: (1) monomer ion and (2) dimer ion.

for a sample weighing 0.3 ng. It is noteworthy that the detection limit for imidazole is 0.3 ng. The difference can be explained by the higher volatility of *N*-methylimidazole.

CONCLUSIONS

It was discovered that the two signals in the ion mobility spectra of *N*-methylimidazole correspond to the presence of protonated monomer and dimer ions. It was also discovered that there was no redistribution of peak intensities as the analyte ions pass through the drift chamber. Nevertheless, the spectrum of the ion mobility of a solution of *N*-methylimidazole in water was characterized by an increase in the monomer concentration due to the decomposition of dimer ions. When the spectra of monomer ions were compared to the spectra of imidazole, it was discovered that the values of the ion mobility of monomer ions appear in a relatively narrow range.

The ion protonated at the pyridine nitrogen atom signal corresponds to ion mobility of 2.1 ± 0.7% $\text{cm}^2/(\text{V}\cdot\text{s})$ and can be used to identify the pyridine nitrogen atom in the molecule. Moreover, the stability of dimer ions and the detection limits of compounds differ. The dimer ion is more stable for imidazole. The detection limit of *N*-methylimidazole was determined to be 0.3 pg.

Authors' contributions

D.A. Aleksandrova – methodology development, conducting experiments, analysis of literary sources, writing and editing the text of the article;

T.B. Melamed – methodology development, conducting experiments, processing experimental data, writing and editing the text of the article;

E.P. Baberkina – developing the scientific concept, methodology development, writing and editing the text of the article;

A.A. Fenin – offering consultations on methodology and research, calculations of enthalpies of reactions;

E.S. Osinova – analysis of literary sources, methodology development;

A.E. Kovalenko – offering consultations on methodology and research;

R.V. Yakushin – offering consultations on methodology and research;

Yu.R. Shaltaeva – offering consultations on methodology and research;

V.V. Belyakov – offering consultations on methodology and research;

D.I. Zykova – development of a program for processing ion mobility spectra.

The authors declare no conflicts of interest.

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[Russian Original Text: Aleksandrova D.A., Melamed T.B., Baberkina E.P., Kovalenko A.E., Kuznetsov Vl.Vit., Kuznetsov Vit. Vl., Fenin A.A., Shaltaeva Yu.R., Belyakov V.V. Ion Mobility Spectrometry of Imidazole and Possibilities of its Determination. *Zhurnal Analiticheskoi Khimii.* 2021;76(11):989–996 (in Russ.). https://doi.org/10.31857/S0044450221110025]

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The article was submitted: November 01; approved after reviewing: November 26, 2021; accepted for publication: December 04, 2021.

Translated from Russian into English by H. Moshkov
Edited for English language and spelling by Enago, an editing brand of Crimson Interactive Inc.