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RESEARCH ARTICLE

Analysis of the ion mobility spectra of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol

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Abstract

Objectives. To determine the ion mobilities of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol; the structure of ions corresponding to characteristic signals; the detection limits of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol with the Kerber-T ion drift detector and the Segment automatic stationary gas detector.

Methods. Ion mobility spectrometry was used in order to determine the ion mobilities and detect analytes. The enthalpies of reactions of ion formation were calculated using the ORCA 4.1.1 software by means of the B3LYP density functional method with the 6-31G(d,p) basis set.

Results. The ion mobilities of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol were determined. A method for recording ion mobility spectra and their mathematical processing was developed. The dependencies of the change in ion mobility spectra on the analyte concentration were also studied. Possible mechanisms were proposed for the formation of the ion mobility spectra observed, in accordance with the ionization features of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol. The enthalpies of ion formation were calculated. The ionization schemes of the compounds were shown. The generalized results of experimental studies were presented, as were the features of compound identification taking into account the structure of the spectra, the concentrations of substances, and the detection conditions.

Conclusions. Characteristic signals of chloroacetophenone, tris(2-chloroethyl)amine, and methanethiol were identified. All studied hazardous substances can be detected with an ion mobility spectrometer at concentrations at the ppm level. The following detection limits of the substances were determined with the Segment gas detector: chloroacetophenone, 245 mg/m^3; tris(2-chloroethyl)amine, 0.01 mg/m^3; and methanethiol, 0.8 mg/m^3.

Keywords
ion mobility spectrometry, characteristic signal, ionization, detection, chloroacetophenone, methanethiol, tris(2-chloroethyl)amine

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НАУЧНАЯ СТАТЬЯ

Анализ спектров ионной подвижности хлорацетофенона, трис(2-хлорэтил)амина и метилмеркаптана

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Аннотация

Цели. Определить значения ионной подвижности хлорацетофенона, трис(2-хлорэтил)амин и метилмеркаптана; установить строение ионов, соответствующих характерным сигналам; определить предел обнаружения хлорацетофенона, метилмеркаптана и трис(2-хлорэтил)амина на ионно-дрейфовом детекторе «Кербер-Т» и автоматическом стационарном газосигнализаторе «Сегмент».

Методы. Метод спектрометрии ионной подвижности использован для определения значений ионной подвижности и детектирования аналитов. Энтальпии реакций образующихся ионов расчитаны в программе ORCA 4.1.1 методом функционала плотности B3LYP с набором базисных функций 6-31G(d,p).

Результаты. Определены значения ионной подвижности хлорацетофенона, трис(2-хлорэтил)амина и метилмеркаптана. Разработана методика получения спектров ионной подвижности и их математической обработки. Изучены зависимости изменения спектров ионной подвижности от концентрации аналита. Предложены возможные механизмы формирования наблюдаемых спектров ионной подвижности в соответствии с особенностями ионизации хлорацетофенона, метилмеркаптана и трис(2-хлорэтил)амина. Рассчитаны энтальпии образования ионов. Показаны схемы ионизации соединений. Приведены обобщенные результаты экспериментальных исследований, особенности идентификации соединений с учетом структуры спектров, концентраций веществ и условий детектирования.

Выводы. Выявлены характеристические сигналы хлорацетофенона, трис(2-хлорэтил)амина и метилмеркаптана. Все исследованные вещества группы аварийно-химически опасных веществ могут быть детектированы спектрометром ионной подвижности при аналитически значимых концентрациях на уровне 10^{-2} мг/м^3. Определены пределы обнаружения исследуемых веществ на газосигнализаторе «Сегмент». Предел обнаружения хлорацетофенона – 245 мг/м^3, трис(2-хлорэтил)амина – 0.01 мг/м^3 и метилмеркаптана – 0.8 мг/м^3.

Ключевые слова

спектрометрия ионной подвижности, характеристический сигнал, ионизация, детектирование, хлорацетофенон, метилмеркаптан, трис(2-хлорэтил)амин

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INTRODUCTION

Ion mobility devices currently use worldwide for the main purpose of detecting chemical warfare agents, drugs, and explosives [1, 2]. In addition, detectors based on ion mobility spectrometry have been successfully adapted for industrial, technological, and environmental studies, including food quality analysis and air composition monitoring [3–7].

The main advantage of devices based on ion mobility spectrometry, in comparison with those based on chromatography and mass spectrometry, is the speed of analysis. The average time to record a reliable profile of the ion mobility spectrum of the compound under study is from 3 to 10 s. The Kerber-T ion drift detector[1] (Kerber-T IDD) and the Segment automatic stationary gas detector[2] (Segment ASGD) (*Modus*, Russia) are portable, operate at atmospheric pressure, and do not incorporate large-sized systems for creating a vacuum.

This aim of this work is not to study the influence of interfering factors, including the presence of mechanical and other impurities in the air being analyzed. An important and practical matter is to optimize the design of the Segment ASGD enabling the use of the ion mobility spectrometer in a wide range of temperatures, including in winter at subzero temperatures. In order to remove dust and dirt particles, additional protection of the gas channel is provided, preventing air from blowing in with a coarse filter in the inlet sampling channel.

Currently, *Modus* is successfully working to achieve import substitution and develop devices for the rapid control of hazardous chemical substances, in order to prevent their use in terrorist activities. Also, increased requirements have recently been imposed on safety at industrial facilities, in the aims of monitoring air composition in the working area and in crowded places, thus requiring detection of a wider range of compounds.

The available literature describes the detection of a number of hazardous chemical substances. However, but the main attention of researchers is focused on organophosphorus compounds and mustard agents [8]. Expanding the database is the reason for carrying out this study.

All the objects under study are highly toxic and relatively available. Methanethiol is widely used in the organic synthesis of pesticides and herbicides and is used as an odorizing additive to natural gas. Tris-(2-chloroethyl)amine is a blister agent and is currently the only nitrogen mustard to retain its significance in chemical warfare. Chloroacetophenone is used in gas canisters as a riot control agent. Departments of the Ministry of Internal Affairs of the Russian Federation have at their disposal various types of aerosol sprays containing chloroacetophenone. These compounds need to be studied for the timely detection and elimination of the consequences of spraying these substances into the air and mixing them with water.

EXPERIMENTAL

The studies were carried out with the Kerber-T IDD and the Segment ASGD (*Modus*, Russia). Table 1 presents the specifications of the devices.

Kerber-T IDD is already widely used in the inspection equipment market. Segment ASGD is also intensively implemented by the Ministry of Internal Affairs, the Federal Security Service, and the Ministry of Defense of the Russian Federation, in order to detect hazardous chemical substances. Therefore, in order to expand the equipment database, comparative studies of the substances need to be performed on both devices.

The ion mobility spectra were recorded at atmospheric pressure with ambient air as a drift gas. The ability to record measurement results was provided by the device software. The result was a text file containing data on the target substances detected and drift time. These were used to construct an ion mobility spectrum.

For the purposes of this study, methanethiol with liquefied gas from a canister (*Merck*, Germany) and ethanethiol diluted in dry air from a cylinder (*GAZ-ANALITIK*, Russia) were used. Hydrogen sulfide was obtained by extracting aluminum sulfide from a freezer and decomposing it to hydrogen sulfide at a humidity of 20 to 55%. Tris(2-chloroethyl)amine was synthesized especially for the study. The purity of the reagent obtained was controlled by gas chromatography–mass spectrometry: a compound with a sample content of at least 99% was obtained. Chloroacetophenone, bromoacetophenone, and acetophenone (*Sigma-Aldrich*, USA) with a purity of at least 98% were also used in the study.

Samples for the preparation of solutions were weighed on an AND GR-120 scales (*A&D*, Japan) with a resolution of 0.0001 g.

A Lenpipet Light dispenser (*Thermo Scientific*, Russia) was used to prepare solutions and apply 1–10 µL of solutions of the required concentrations to a sampling cloth. The sampling cloth was made of a foil 11–15 µm thick, pre-annealed in the Kerber-T IDD furnace at 180°C.

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[1] Kerber-T portable ion drift detector. URL: http://www.analizator.ru/production/ims/kerber-t/. Accessed January 27, 2023.

[2] Segment automatic stationary gas detector. URL: https://www.analizator.ru/production/ims/segment/. Accessed January 27, 2023.

Table 1. Specifications of the Kerber-T IDD and Segment ASGD

Characteristic	Kerber-T IDD	Segment ASGD
Detection range of low-volatile organic substances for 2,4,6-trinitrotoluene (TNT), g	From $1.0 \cdot 10^{-11}$ to $2.0 \cdot 10^{-7}$	–
Detection limit of low-volatile organic substances for TNT – for solid particles, g – for vapor, g/cm^3	 No more than $1.0 \cdot 10^{-10}$ No more than $5.0 \cdot 10^{-13}$	–
Alarm threshold for controlled substances under normal climatic conditions, mg/m^3 – for sarin – for soman – for VX-type substance – for chlorine – for hydrogen sulfide	–	 $1.0 \cdot 10^{-2} \pm 30\%$ $1.0 \cdot 10^{-2} \pm 30\%$ $3.0 \cdot 10^{-3} \pm 30\%$ $1.0 \pm 30\%$ $10.0 \pm 30\%$
Ionization method	Pulsed corona discharge	Pulsed corona discharge
Drift tube temperature, °C	100	100
Time of detection and identification for all detectable substances, s	No more than 5	No more than 5
Probability of false alarm, %	No more than 1	No more than 1
Detector cleaning time in the event of contamination with target substances within detection range, min	No more than 3	No more than 3

The enthalpies of reactions were calculated using the ORCA 4.1.1 software (*FAccTs GmbH*, Germany) by the B3LYP[3] density functional method with the 6-31G(d,p) basis set.

Specifics of ion mobility spectrometry

The ion mobility spectrometry method is based on the ionization of molecules of the substance being studied at atmospheric pressure. First, reactant ions are formed in the discharge chamber, the concentration of which significantly exceeds the concentration of the substances to be determined. When the target substances enter the device, the reactant ions transfer a charge to the molecules by the mechanism of chemical ionization at atmospheric pressure [9].

Formation of ions in the ionization region

The formation of reactant ions in negative polarity under the influence of a corona discharge occurs as a result of resonant electron capture by neutral molecules, e.g., oxygen molecules. Ion–molecular reactions with sample molecules to form product ions can take place in accordance with the following scheme:

$$M + O_2^-(H_2O)_n \rightarrow MO_2^-(H_2O)_{n-x} + xH_2O,$$

wherein M is the sample, $O_2^-(H_2O)_n$ is the reactant ion, $MO_2^-(H_2O)_{n-x}$ is the product ion, and xH_2O is water.

This product ion may live long enough for the signal of its spectrum to manifest itself in the ion mobility spectrum, or it may undergo further transformations leading, e.g., to the ion M^-.

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[3] B3LYP is the Becke–3-parameter–Lee–Yang–Parr exchange–correlation functional.

When colliding with reactant ions in positive polarity, molecules of the substance being studied form cluster ions. These are transformed into more stable hydrated cluster ions by the elimination of water molecules:

$$M^+ + H^+(H_2O)_n \rightarrow MH^+(H_2O)_n \rightarrow$$
$$\rightarrow MH^+(H_2O)_{n-x} + xH_2O,$$

wherein M is the molecule of the substance being studied, $H^+(H_2O)_n$ is the reactant ion, $MH^+(H_2O)_n$ is the cluster ion, and $MH^+(H_2O)_{n-x}$ is the ion of the substance being studied.

The product ion formed in this process is called *protonated monomer*. The formation of a protonated dimer $M_2H^+(H_2O)_n$ and other molecular ions is possible. The number of water molecules in the cluster ranges from 1 to 3 depending on the nature of the compound [10, 11].

Ionized molecules of differing substances move in the drift chamber at different velocities depending on their charge, weight, and the effective cross-section of the formed ion. Molecular ions of differing compounds vary in drift time τ_d to the collector, enabling their nature to be determined. This time is proportional to the length L (cm) of the drift chamber, inversely proportional to the electric field gradient E, and calculated as:

$$\tau_d = \frac{1}{K} \cdot \frac{L}{E}, \quad (1)$$

wherein K is the ion mobility coefficient, cm^2/(V·s).

The ion mobility depends on temperature and pressure. In order to compare ion mobility values obtained under different conditions, the K values are converted to normal conditions:

$$K_0 = \frac{KP}{760} \cdot \frac{273}{T}, \quad (2)$$

wherein T and P are the temperature (K) and pressure (mm·Hg), respectively, in the gas atmosphere in which the ions move; and K_0 is called the reduced mobility (or reduced mobility coefficient). Reduced ion mobility is used in this work. The results are presented in the form of an ion mobility spectrum with the background spectrum subtracted.

Experimental procedure

In the course of work using Kerber-T IDD and Segment ASGD, a procedure for recording and determining the characteristic values of ion mobility was developed. A method for mathematical processing of the spectra was previously described in detail [12, 13].

Ion mobility spectra were recorded at atmospheric pressure with ambient air as a drift gas.

Tris(2-chloroethyl)amine was studied in various modifications: pure substance, hydrochloride, and a solution of the hydrochloride in water.

Using an Agilent microsyringe (*Agilent Technologies*, USA), 1, 2, 5, 8, and 12 μL of saturated vapor of pure tris(2-chloroethyl)amine were collected into 25-mL flasks.

Chloroacetophenone was detected by collecting saturated vapor and diluting it with ambient air. Using a two-component syringe, 2 to 10 mL of the saturated vapor of chloroacetophenone were collected into 35-mL flasks. The saturated vapor concentration in the gas phase was calculated using the ideal gas law:

$$pV = \frac{m}{M} \cdot RT, \quad (3)$$

wherein p is the saturated vapor pressure, V is the volume, m is the weight of the substance, M is the molecular weight, R is the universal gas constant, and T is room temperature in K.

Table 2 presents the concentrations of the analytes that were calculated using formula (3).

The sensitivity for the hydrochloride is lower than for the pure substance. Therefore, the hydrochloride was measured by heating the sampling cloth with

Table 2. Concentrations of tris(2-chloroethyl)amine in the gas phase

No.	Saturated vapor volume, μL	Flask volume, mL	Concentration, mg/m^3
1	1	25	0.005
2	2	25	0.01
3	5	25	0.025
4	8	25	0.04
5	12	25	0.06

the substance in the Kerber-T IDD. The analyte concentration C was calculated as:

$$C = \frac{C_{\mathrm{sv}} \cdot V_{\mathrm{sv}}}{V_{\mathrm{f}}}, \quad (4)$$

wherein C_{sv} is the saturated vapor concentration, V_{sv} is the saturated vapor volume, and V_{f} is the flask volume.

Table 3 presents the calculated concentrations of analytes for the Segment ASGD.

Kerber-T IDD monitored the sorption of the substance with passive sampling from the flask. Therefore, the sample was injected from a syringe, the substance then passed through the gas channel under pressure, and the peak of the substance was detected. The concentration was calculated under the assumption that the sample was diluted with an inlet air flow at a rate of $F = 500$ mL/min by the formula (5):

$$C = \frac{C_{\mathrm{sv}} \cdot V_{\mathrm{sv}}}{F \cdot t}, \quad (5)$$

wherein C is the concentration, C_{sv} is the saturated vapor concentration, V_{sv} is the saturated vapor volume, F is the inlet flow rate of the device, and t is the sample injection time.

Table 4 presents the concentrations of analytes for the Kerber-T IDD, calculated by formula (5).

Methanethiol measurements were performed as follows. The saturated methanethiol vapor was collected from a gas cylinder in 50-mL flask 1. The saturated vapor concentration was calculated using the ideal gas law. A 1-mL sample of the saturated vapor was collected in 500-mL flask 2; thus, the saturated vapor was diluted 500 times. The vapor from flask 2 was used to obtain the final concentrations.

Then 5 and 10 µL of the saturated vapor were taken with an Agilent microsyringe, and 0.1, 0.25, 0.5, and 1 mL of the saturated vapor were collected in 25-mL flasks using an insulin syringe.

Table 5 presents the concentrations of analytes, calculated using formula (5).

Table 3. Chloroacetophenone concentrations measured with the Segment ASGD in the gas phase

No.	Saturated vapor volume, µL	Flask volume, mL	Concentration, mg/m^3
1	4	35	485
2	5	35	600
3	6	35	725
4	8	35	970
5	10	35	1200

Table 4. Chloroacetophenone concentrations measured with the Kerber-T IDD in the gas phase

No.	Saturated vapor volume, µL	Sample injection time, s	Concentration, mg/m^3
1	3	5	300
2	4	5	400
3	5	5	500

Table 5. Methanethiol concentrations in the gas phase

No.	Saturated vapor volume in flask 2, µL	Flask volume, mL	Concentration, mg/m^3
1	5	25	0.8
2	10	25	1.6
3	100	25	16
4	250	25	40
5	500	25	80
6	1000	25	160

A glass flask containing an air mixture with a given concentration of the analyte was placed at the sampling channel of the ion mobility spectrometer for 5 s. The device automatically sampled the contents of the flask in the gas phase analysis mode.

Measurements were made after changing analyte concentration from 0.01 mg/m^3 to the concentration corresponding to the saturated vapor pressure of the analyte at a temperature of 20–25°C. The work presents spectra in the optimal range of detection concentrations.

RESULTS AND DISCUSSION

Study of chloroacetophenone

A series of chloroacetophenone spectra was recorded with the Kerber-T IDD at various concentrations, then mathematically processed to give an approximate estimation of the relative numbers of ions (Fig. 1). In negative polarity, the amplitude of one main peak of 2.709 cm^2/(V·s) increased with increasing concentration of the sample. In positive polarity, with increasing concentration, the amplitudes of all observed signals increase. However, the amplitude of the signal with a mobility of 1.475 cm^2/(V·s) is more stable, possible indicating the cluster nature of the ion structure.

Figure 2 shows a series of spectra of chloroacetophenone that were recorded with Segment ASGD.

According to these procedures and measurement conditions, the lower detection limit of chloroacetophenone for the Kerber-T IDD is 300 mg/m^3. For Segment ASGD it is 245 mg/m^3. Several peaks can be used to identify both polarities simultaneously: 1.708 and 1.475 cm^2/(V·s) with a deviation of 0.7% in positive polarity; and 2.650 cm^2/(V·s) with a deviation of 2.5% in negative polarity.

The ion mobility spectra of chloroacetophenone, acetophenone, and bromoacetophenone recorded with the Kerber-T IDD were compared, in order to determine the structures of the ions (Fig. 3).

In negative polarity, one peak can be observed for each of the halogen-containing compounds. The mobilities of the peaks of chloroacetophenone and bromoacetophenone correspond to the chloride ion (2.650 cm^2/(V·s)) and the bromide ion (2.485 cm^2/(V·s)), respectively. In positive polarity, there are three peaks for acetophenone: at 1.706, 1.578, and 1.300 cm^2/(V·s). These correspond in mobility to the peaks of chloro- and bromoacetophenone, indicating the same nature of protonation and, possibly, that the substances are ionized after the elimination of halogens. However, in the case of chloroacetophenone, two more peaks can be observed: at 1.776 and 1.478 cm^2/(V·s), probably related to protonated chlorine derivatives of ions. For bromoacetophenone, a peak at 1.397 cm^2/(V·s) is also detected, characterizing the protonated bromine derivative ion. The enthalpies of reactions of the resulting ions were calculated using the ORCA 4.1.1 program by means of the B3LYP

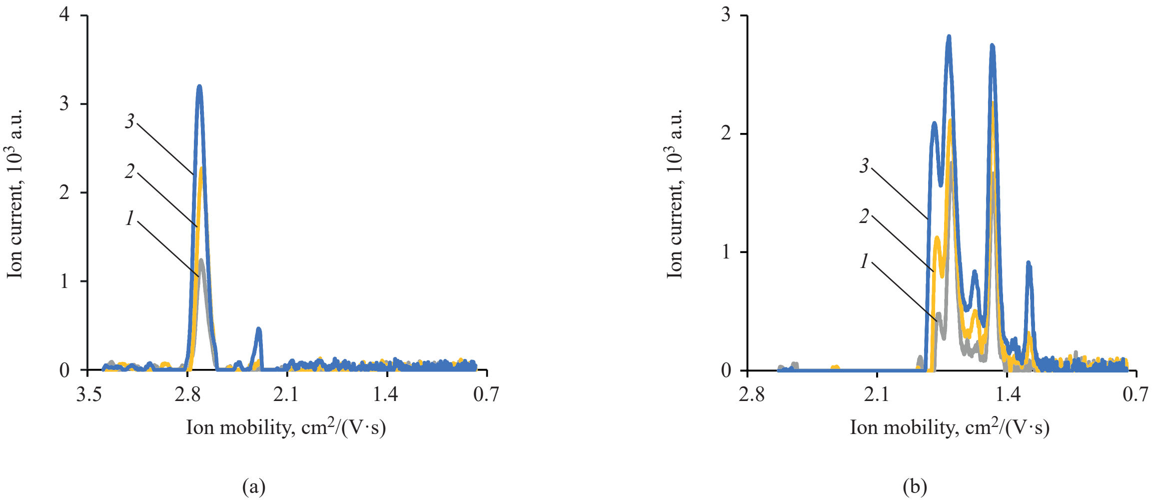
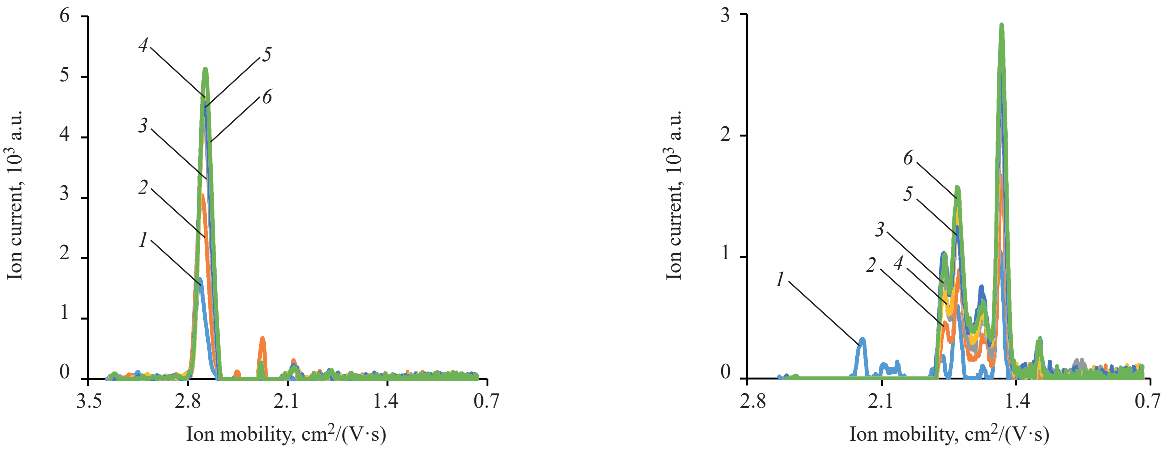


Fig. 1. Ion mobility spectra of chloroacetophenone recorded with Kerber-T IDD in
(a) negative and
(b) positive polarity
at concentrations of
(*1*) 300 mg/m^3 (grey line),
(*2*) 400 mg/m^3 (yellow line), and
(*3*) 500 mg/m^3 (dark blue line)



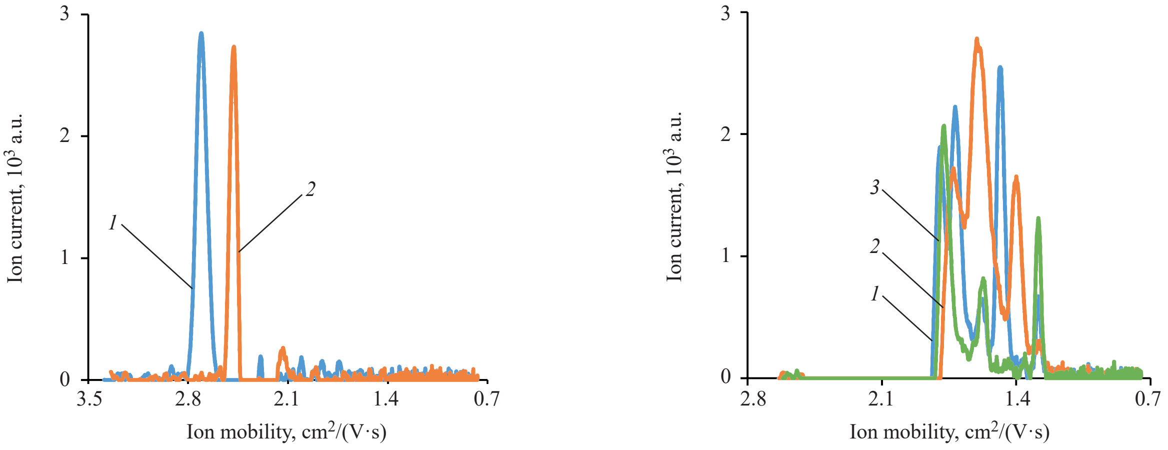
(a)

(b)

Fig. 2. Ion mobility spectra of chloroacetophenone recorded with the Segment ASGD in
(a) negative and
(b) positive polarity
at concentrations of
(*1*) 245 mg/m^3 (blue line),
(*2*) 485 mg/m^3 (orange line),
(*3*) 600 mg/m^3 (gray line),
(*4*) 725 mg/m^3 (yellow line),
(*5*) 970 mg/m^3 (dark blue line), and
(*6*) 1200 mg/m^3 (green line)

density functional method with the 6-31G(d,p) basis set (Table 6).

The most energetically favorable is the formation of a monomer ion with the elimination of a water molecule. However, the formation of an ion with a water molecule is also possible. The dimer of chloroacetophenone is easily formed. Trimers have a chain structure. According to calculations, they are unstable and easily dissociate into a dimer and a monomer upon collision with any molecule [12, 13]. Thus, the presence of signals of monomer and dimer ions in the ion mobility spectrum is most likely.

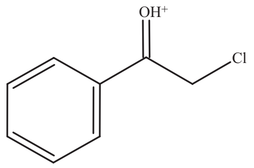
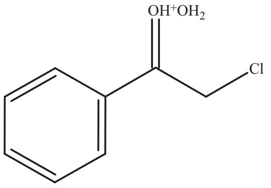
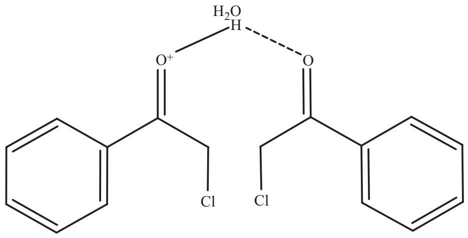


(a)

(b)

Fig. 3. Comparison of the ion mobility spectra of
(*1*) chloroacetophenone (blue line),
(*2*) bromoacetophenone (orange line), and
(*3*) acetophenone (green line) in (a) negative and (b) positive polarity

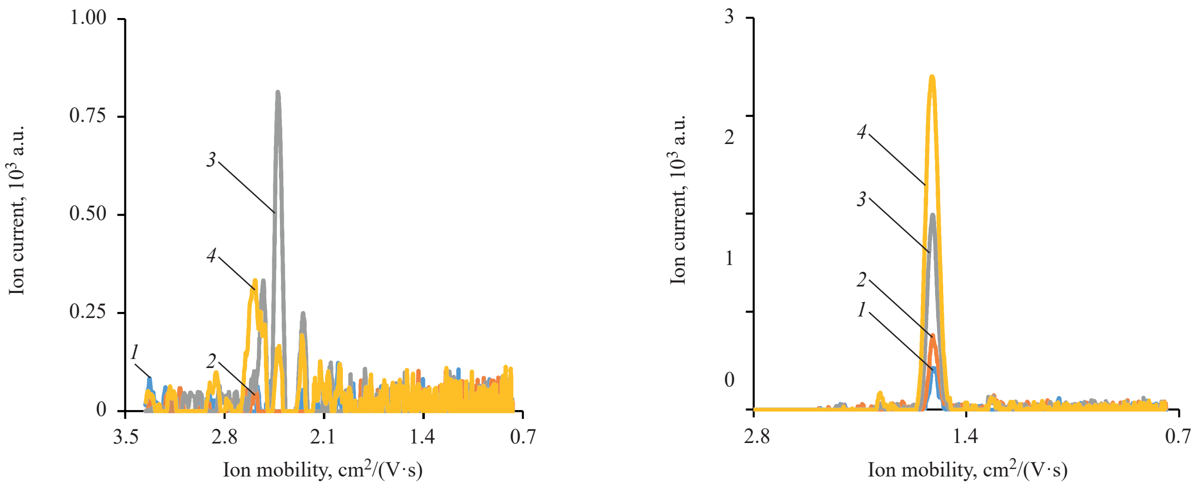
Table 6. Enthalpies of formation of chloroacetophenone ions

Structure of molecular ion	Enthalpy of formation, kJ/mol
	−148.9
	−85.2
	−88.3

Study of tris(2-chloroethyl)amine

Figure 4 shows the spectra of tris(2-chloroethyl)amine that were recorded with Kerber-T IDD.

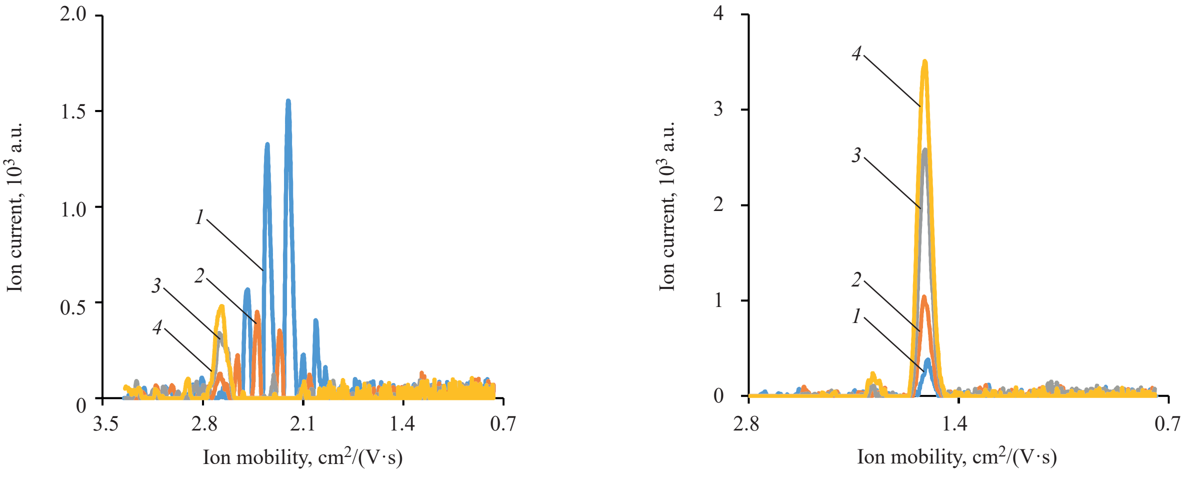
In negative polarity, instability of signals of the chloride ion can be observed. In positive polarity, there is a pronounced characteristic signal at a mobility of 1.512 $cm^2/(V·s)$ which is assigned to protonation at the nitrogen atom. As a result of the measurements, the optimal detection concentration was determined to be 0.04 mg/m^3.



(a)

(b)

Fig. 4. Ion mobility spectra of tris(2-chloroethyl)amine recorded with Kerber-T IDD in
(a) negative and
(b) positive polarity at concentrations of
(*1*) 0.01 mg/m^3 (blue line),
(*2*) 0.025 mg/m^3 (orange line),
(*3*) 0.04 mg/m^3 (gray line), and
(*4*) 0.06 mg/m^3 (yellow line)



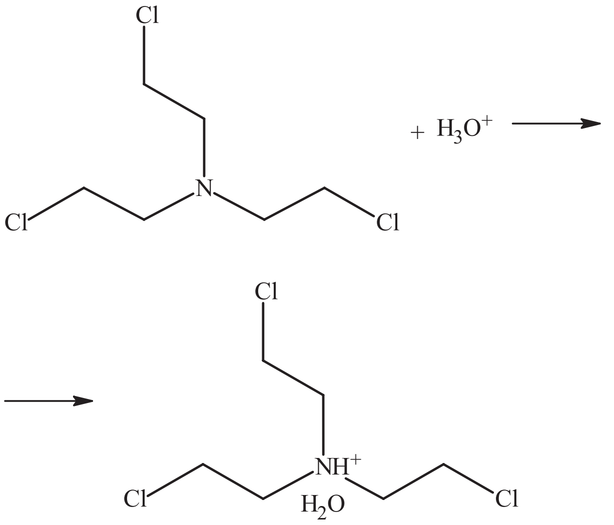
(a) (b)

Fig. 5. Ion mobility spectra of tris(2-chloroethyl)amine recorded with the Segment ASGD in
(a) negative and
(b) positive polarity at concentrations of
(*1*) 0.01 mg/m^3 (blue line),
(*2*) 0.025 mg/m^3 (orange line),
(*3*) 0.04 mg/m^3 (gray line), and
(*4*) 0.06 mg/m^3 (yellow line)

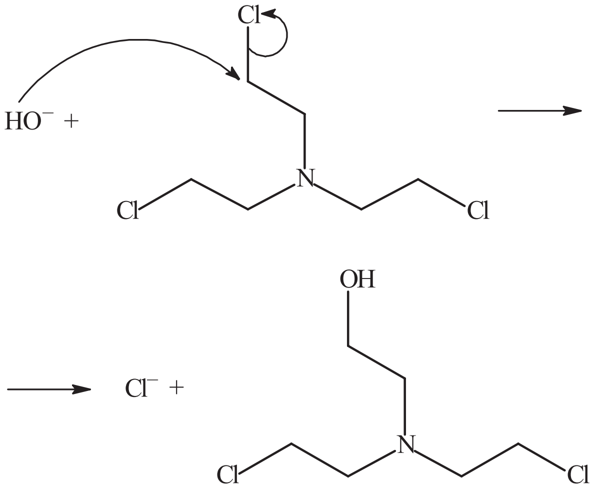
Figure 5 shows a series of spectra of tris(2-chloroethyl)amine samples recorded with Segment ASGD.

In negative polarity, with increasing concentration, there is an increase in the signal at a mobility of 2.650 $cm^2/(V·s)$, which can be attributed to the hydrogen chloride ion. Other chlorine signals and a deviation of the background peaks are also present, but are unstable. In positive polarity, there is a pronounced characteristic signal at a mobility of 1.512 $cm^2/(V·s)$, which corresponds to the signal of tris(2-chloroethyl)amine obtained recorded with the Kerber-T IDD.

Ionization in positive polarity is assumed to be at the nitrogen atom by the following mechanism:

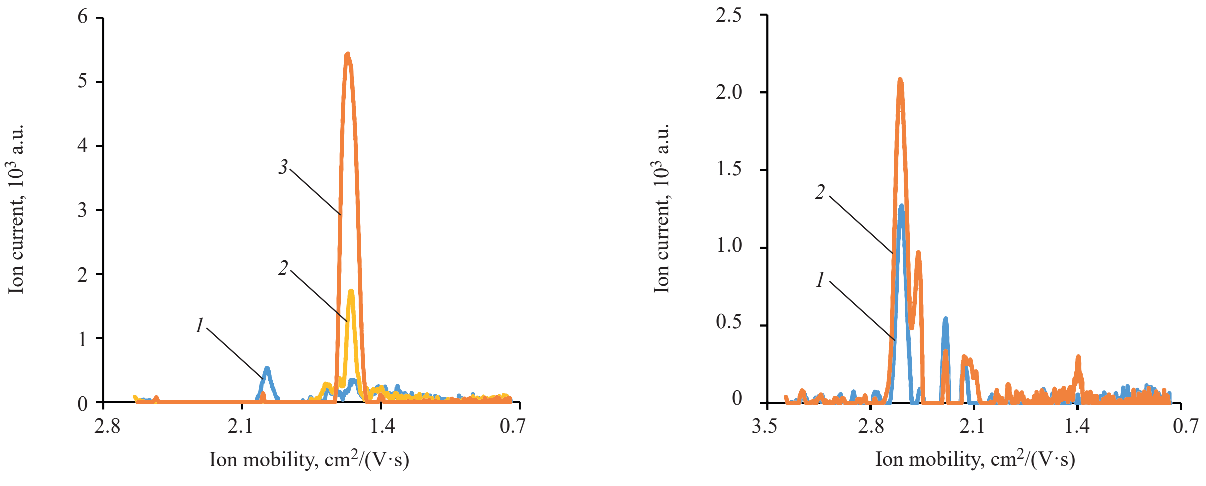


Ionization in negative polarity occurs at the chorine atom:



Formation of chlorine dimers and trimers is possible, and so is association with water molecules at the hydrogen atom.

Tris(2-chloroethyl)amine can be used by dissolving its hydrochloride in water and then introducing it into water supply systems. Therefore, aqueous hydrochloride solutions were studied using Kerber-T IDD (Fig. 6): 1 µL of the aqueous solution was applied to a sampling cloth. The cloth was left until water dried and then was placed in the device.



(a)

(b)

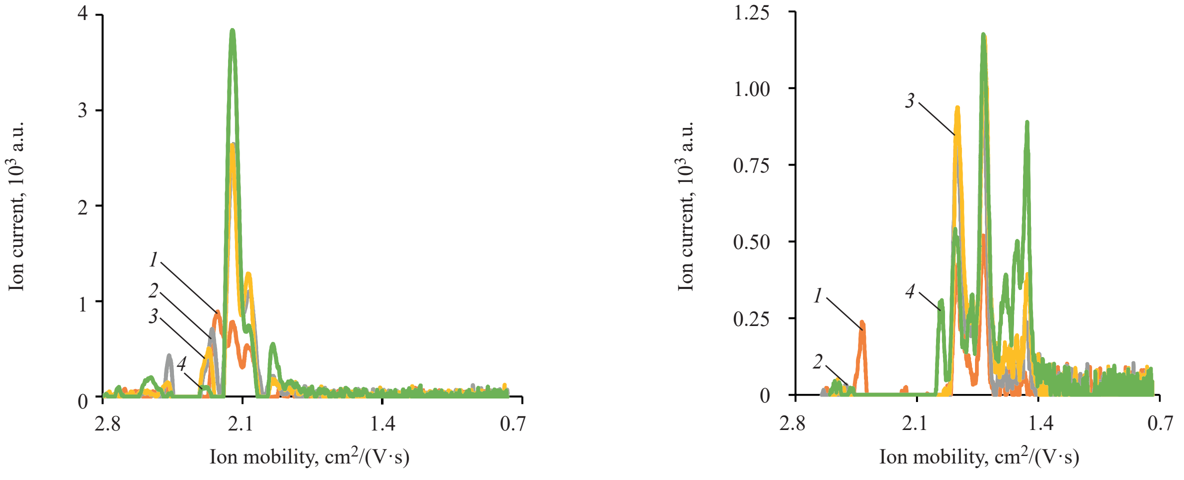
Fig. 6. Ion mobility spectra of tris(2-chloroethyl)amine recorded with the Kerber-T IDD in
(a) negative and
(b) positive polarity at weights of
(*1*) 2 ng (blue line),
(*2*) 70 ng (yelow line), and
(*3*) 200 ng (orange line)

The minimum detection limit on a sampling cloth is 2 ng. With an increase by an order of magnitude, the amplitude of the peaks reaches a maximum value and does not increase further. The minimum detection limit with an amplitude of 300 a.u. in the vapor above an aqueous solution is a solution concentration of 10^{-4} mol/L.

The ion mobilities in positive polarity for the substance, its hydrochloride, the vapor above an aqueous solution, and the sampling cloth are the same: 1.512 cm^2/(V·s).

Study of methanethiol

Figure 7 shows a series of methanethiol spectra recorded with Kerber-T IDD. In negative polarity, there is an increase in the amplitudes of two main peaks at



(a)

(b)

Fig. 7. Ion mobility spectra of methanethiol recorded with Kerber-T IDD in
(a) negative and
(b) positive polarity at concentrations of
(*1*) 1.6 mg/m^3 (orange line),
(*2*) 16 mg/m^3 (gray line),
(*3*) 40 mg/m^3 (yellow line), and
(*4*) 160 mg/m^3 (green line)

mobilities of 2.175 and 2.075 cm^2/(V·s) with an increase in the sample concentration. In positive polarity, up to a concentration of 40 mg/m^3, the signal at a mobility of 1.869 cm^2/(V·s) dominates. With an increase in concentration, signals at mobilities of 1.715 and 1.470 cm^2/(V·s) begin to dominate.

The lower detection limit of methanethiol using Kerber-T IDD is 1.6 mg/m^3. The signal at a mobility of 2.243 cm^2/(V·s) is insufficiently resolved. It merges with the peak at 2.175 cm^2/(V·s) to form a single peak. There is also a flow from the third background peak through 2.243 cm^2/(V·s) to the peak at 2.175 cm^2/(V·s). The complex dynamics of the spectrum makes it difficult to determine methanethiol only in negative polarity. Several peaks for identification in both polarities can be reasonably used simultaneously.

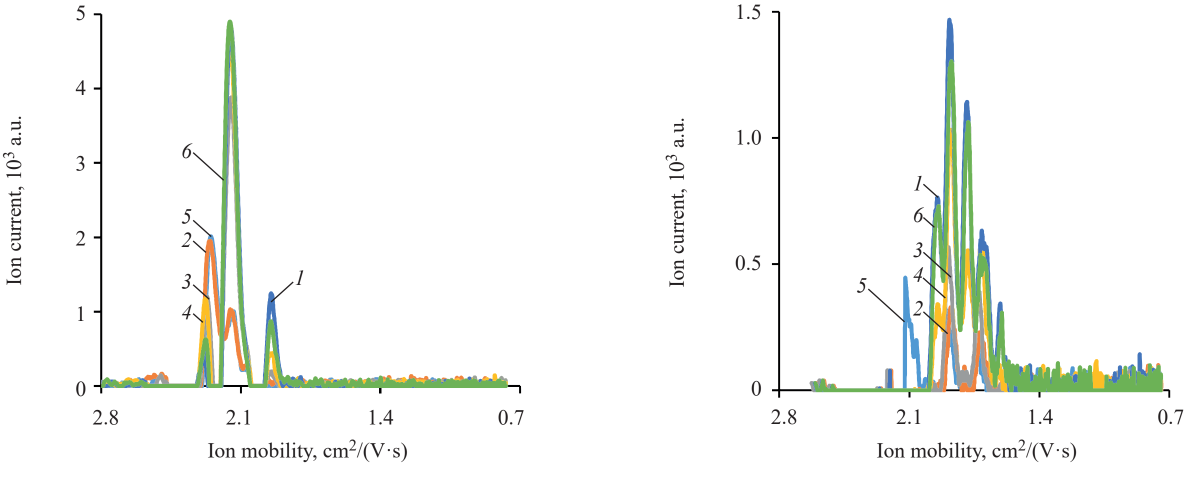
Figure 8 shows a series of methanethiol spectra recorded with Segment ASGD.

The measurements of methanethiol showed good convergence of signals in terms of mobility and peak amplitude. The ion mobility signal value of 2.150 cm^2/(V·s) with a deviation of 0.7% in negative polarity can be used, as well as signals at mobilities of 1.882 and 1.721 cm^2/(V·s) with a deviation of 0.7% in positive polarity. The signals at a mobility of 2.075 cm^2/(V·s) in negative polarity and 1.470 cm^2/(V·s) in positive polarity have small amplitudes, and therefore, they can be considered as additional analytical peaks.

The ion mobility spectra of hydrogen sulfide, methanethiol, and ethanethiol were compared to determine the structures of ions (Fig. 9).

In negative polarity, a separate peak at a mobility of 2.900 cm^2/(V·s) can be observed in the region of light ions, in which the formation of HS^- is most likely. There are also two converging peaks of methanethiol and hydrogen sulfide at mobilities of 2.243 and 2.150 cm^2/(V·s), as well as a separate peak of ethanethiol at a mobility of 2.020 cm^2/(V·s). The signal at a mobility of 2.243 cm^2/(V·s) can be due to the formation of an H–S–S– particle under the influence of a corona discharge.

Since the air in the cylinder is dry and the background of the room is more humid, the connection of the cylinder with the ethanethiol–air mixture to the device gives rise to a signal at a mobility of 2.030 cm^2/(V·s). Therefore, the first signal in positive polarity in the ethanethiol spectrum is not characteristic. The spectra of methanethiol and ethanethiol in positive polarity have a peak with at a mobility of 1.882 cm^2/(V·s), corresponding to hydrogen sulfide. In positive polarity, there are a number of peaks with approximately the same period of ion mobility changes. This forms the basis for the peaks to correspond to the monomer and dimer structure of the methanethiol and ethanethiol ions.



(a)

(b)

Fig. 8. Ion mobility spectra of methanethiol recorded with the Segment ASGD in
(a) negative and
(b) positive polarity at concentrations of
(*1*) 0.8 mg/m^3 (dark blue line),
(*2*) 1.6 mg/m^3 (orange line),
(*3*) 16 mg/m^3 (gray line),
(*4*) 40 mg/m^3 (yellow line),
(*5*) 80 mg/m^3 (blue line), and
(*6*) 160 mg/m^3 (green line)

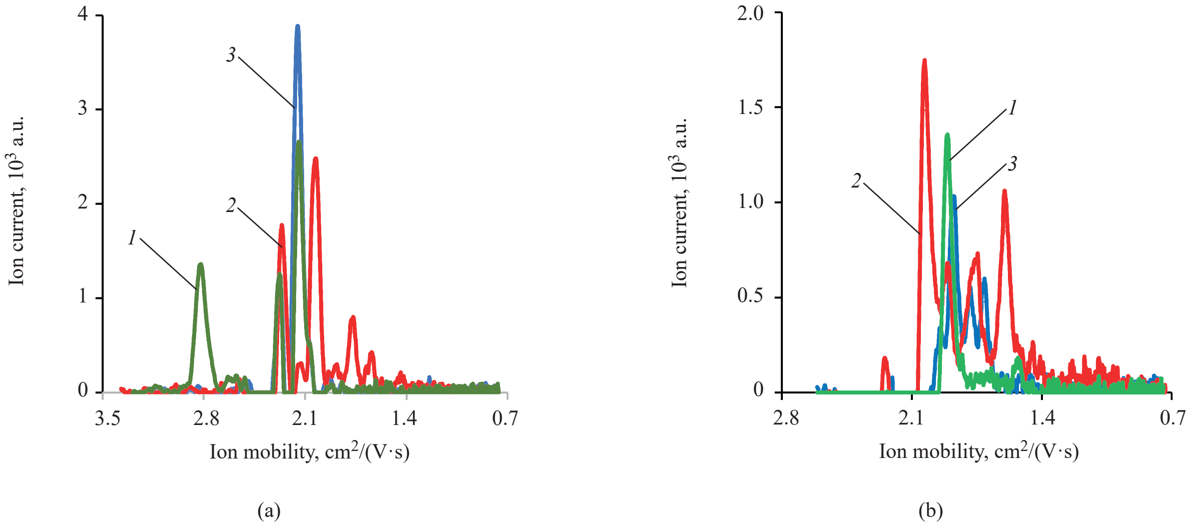


Fig. 9. Comparison of the ion mobility spectra of
(*1*) hydrogen sulfide (green line),
(*2*) ethanethiol (red line), and
(*3*) methanethiol (dark blue line) recorded with the Segment ASGD in
(a) negative and
(b) positive polarity

CONCLUSIONS

In this study, the ion mobility spectra of chloroacetophenone, methanethiol, and tris(2-chloroethyl)amine were recorded at various vapor concentrations in the gas phase. It was found that the ion mobility values determined by either Kerber-T IDD or Segment ASGD for each of the studied compounds are respectively the same, enabling both of these devices to be used identically for air control. The sensitivity of the Segment ASGD is higher, since the detection limit of substances is lower. All the hazardous chemical substances studied can be detected by ion mobility spectrometers at analytically significant concentrations at the ppm level. Recommendations were given for the use of signals in the Kerber-T IDD and Segment ASGD substance database. Ion mobility spectra and the determination of the ion structure were studied for the first time.

For chloroacetophenone, the ion mobility signal values of 2.650 cm^2/(V·s) with a deviation of 2.5% in negative polarity can be used, as well as signal values at mobilities of 1.706 and 1.478 cm^2/(V·s) with a deviation of 0.7% in positive polarity.

For tris(2-chloroethyl)amine, the ion mobility values can be set in positive polarity at 1.512 cm^2/(V·s) with a deviation of 0.7% and at 2.650 cm^2/(V·s) in negative polarity with a deviation of at least 2.5%. This is because the signal in this region of the spectrum strongly depends on external factors: temperature, humidity, and atmospheric pressure.

For methanethiol, the most characteristic signals are the ion mobility values of 2.150 cm^2/(V·s) with a deviation of 0.7% in negative polarity, and signals at mobilities of 1.882 and 1.721 cm^2/(V·s) with a deviation of 0.7% in positive polarity.

The signals obtained for the compounds allow detection to be set for several peaks simultaneously which can serve as a good filter for false positives.

This work may have practical significance in preventing terrorist attacks, monitoring the air in working areas at production sites, and averting other threats to human life and health. The introduction of new data on ion mobility values of the above substances into the Kerber-T IDD and the Segment ASGD of ion mobility spectrometers is favorable to the replacement of imported analogues of air monitoring devices.

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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 work concept, methodology development, writing and editing the text of the article.

E.S. Osinova—analysis of literary sources, methodology development.

L.A. Luzenina—conducting experiments, analysis of literary sources.

A.A. Kaplin—conducting experiments.

R.V. Yakushin—offering consultations on methodology and research.

A.E. Kovalenko—offering consultations on the results practical application and research.

G.V. Tsaplin—offering consultations on methodology, properties of organic substances, and organic synthesis.

Yu.B. Sinkevich—offering consultations on methodology, properties of organic substances, and organic synthesis.

A.A. Fenin—offering consultations on methodology and research, calculation of enthalpies of reactions.

Ju.R. Shaltaeva—offering consultations on methodology and research.

V.V. Belyakov—offering consultations on methodology and research.

A.O. Shablya—determination of research objects, provision of equipment, and consultation on the instrument base.

A.G. Sazonov—determination of research objects, provision of equipment, and consultation on the instrument base.

The authors declare no conflicts of interest.

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