

Effect of Temperature on Separation of Sarin (GB) Ions in Differential Mobility Spectrometry

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ABSTRACT

Different environmental conditions in which, equipment based on differential ion mobility spectrometry must operate, forced designers and engineers to analyze the impact of, among other things, external factors on their performance and efficiency. These devices, thanks to the DMS technology, can identify and characterize the ions contained in the gaseous state. However, many areas of this technique remain undiscovered, which should be examined in more detail. One such aspect is the influence of the temperature of gaseous medium, containing tested analyte. The research presented in this article shows why temperature is an important factor on the distribution of generated peaks. The results are shown for different spectra generated carrier gas temperatures (50°C - 80°C) in which ions were toxic warfare agents. Based on those graphs, it can be stated that increase of the temperature allows for better separation of the peaks from the background. Because of the similar ion mobility of the analyte and background ions for high and low electric field, DMS device can send false alarms, due to the poor interpretations of passing a signal to them. So to be able to accurately assess the level of risk due to the presence of substances BST in air, the test medium was added to isobutanol and isopropanol additives. They help better analyze and separate measured ions.

Keywords: DMS; Spectrometry; Ion Mobility

1. Introduction

Current knowledge of the DMS method has been described in various publications, however, this article will present the basic phenomena that took part in the examinations. Method of differential ion spectrometry has been recognized as a powerful tool for the separation and characterization of ions present in the gas phase. Ion mobility spectrometry (IMS) is now one of the best techniques for chemical warfare agent's detection [1-4] especially differential mobility spectrometry (DMS) [5-10]. In the past, DMS was called field asymmetric waveform ion mobility spectrometry (FAIMS) [11,12]. DMS is a special method used in ion separation based on difference in ion mobility in high and low electric field under atmospheric pressure [13]. Relation between mobility of ions and electric field may be described by Equation (1):

$$K(E/N) = K_0 \cdot [1 + \alpha(E/N)] \quad (1)$$

where:

K —ion mobility, $\text{cm}^2/\text{V}\cdot\text{s}$,
 E —electric field strength, V/cm ,
 K_0 —reduced mobility [$\text{cm}^2/\text{V}\cdot\text{s}$],
 E/N —electric field expressed in units of Townsend, [Td], ($1 \text{ Td} = 1 \cdot 10^{-17} \text{ V}\cdot\text{cm}^2$),
 $\alpha(E/N)$ —function characterized by mobility field.

Mobility of the ions depends on mass and charge of the ion and flow rate of carrier gas. The schema of ion transfer in the DMS chamber is presented in the **Figure 1**. Under alternating electric field applied to the electrodes, some of the ions in the chamber are intercepted. Changing values of compensated electric field, it may be used as specific ion filter [14,15].

Stability and repeatability of spectra obtained by DMS have a great meaning in chemical analysis. Pressure and temperature of carrier gas have an influence on the ion mobility and peak shifts on the spectra. The main goal of this work was investigation of influence of temperature on the resolution and separation of the ions chemical warfare agents on the example of sarin (GB).

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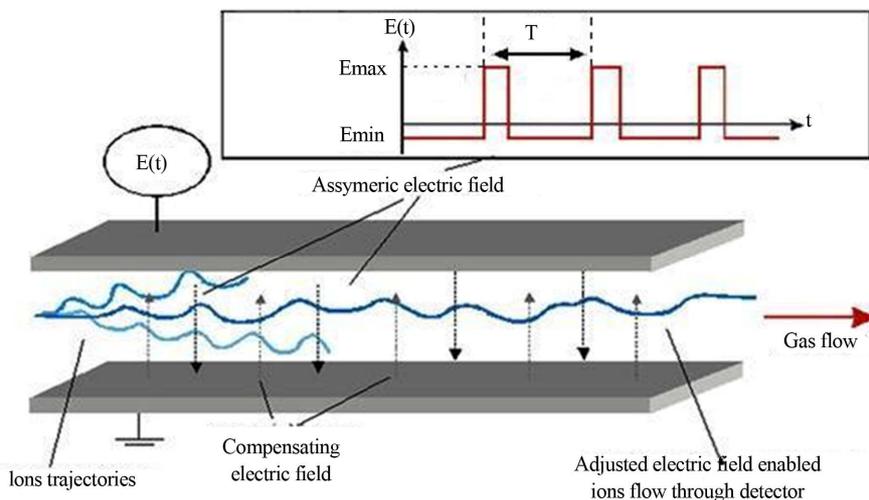


Figure 1. Scheme of ions flow through DMS spectrometer.

2. Experimental

2.1. Analyte

In the studies was used sarin synthesized in WICHIR in Laboratory of Chemicals Synthesis Covered by the Convention on the Prohibition of Chemical Weapons. WICHIR has the authority to work with toxic warfare agents under the Concession No. B-007/2004. The concentration of sarin in the air was 60 mg/m^3 .

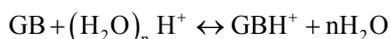
2.2. Apparatus and Measurement Conditions

Measurements were carried out using ceramic DMS whose diagram is shown in **Figure 2**.

Measurements were carried out using air as a carrier gas, isopropanol and isobutanol as a dopant carrier gas ($c = 8 \text{ mg/m}^3$), the temperature of ambient gas: 50°C , 60°C , 70°C and 80°C , and ions $(\text{H}_2\text{O})^+ \text{nH}^+$ (for positive ions) and $\text{O}_2\text{-(H}_2\text{O)}^- \text{n}$ (for negative ions) as a reactive ions RIP (reactant ion peak) generator voltage electric field HSV (high separation voltage) 890 V .

3. Results

In the presence of sarin, the proton affinity of the connection is greater than the water in the proton transfer reaction is formed protonated monomer GBH^+ . If the concentration of the sample is large, then the protonated monomer reacts with another molecule to form a dimer of sarin $(\text{GB})_2\text{H}^+$.



Sample response graphs for sarin DMS obtained for two carrier gas temperatures without additives is shown in **Figures 3** and **4**. The spectral peaks are visible ions

derived from the reaction, the monomer and dimer of the sample.

With increasing of the temperature there is a shift of the peaks from the dimer and monomer of sarin towards higher compensation voltage CV. In all cases, only the peak from a dimer of sarin $(\text{GB})_2\text{H}^+$ can be observed for high voltage of HSV. The monomer peak GBH^+ is not shown above 950 V voltage HSV with carrier gas at a temperature of 70°C or above 900 V for a temperature of 80°C . Different results were obtained with sarin, when the carrier gas contained additional small amount of isopropanol (**Figures 5** and **6**).

On the spectrum of DMS (**Figure 5**) is a clear peak of the monomer and dimer of sarin, while isopropanol peak is barely visible. The increase in temperature causes a slight shift of the peaks towards higher voltage CV (**Figure 6**). The high temperature peak from isopropanol is absent above 750 V HSV. The biggest shifts were observed when carrier gas was doped with isobutanol. (**Figures 7** and **8**).

Dependence of CV on the temperature for the monomer and dimer of sarin is presented on **Figure 9**. Greatest influence of the temperature was noticed when carrier gas contained isobutanol. The peaks shift was observed from value -6.8 V for monomer and -4 V for dimer (temperature 50°C) up to value -2.3 V for monomer and -0.6 V for dimer (temperature 80°C). Curve obtained for the soman dimer is very interesting at many aspects. In the absence of additive in the carrier gas, dimer peak occurs at the positive voltage CV. After the introduction of dopants into a carrier gas there is a shift towards the negative peak voltage CV.

Shift of the peaks in the positive voltage CV is associated with the formation of clusters. Declusterization of ions causes movement in the direction of the negative peak voltage CV.

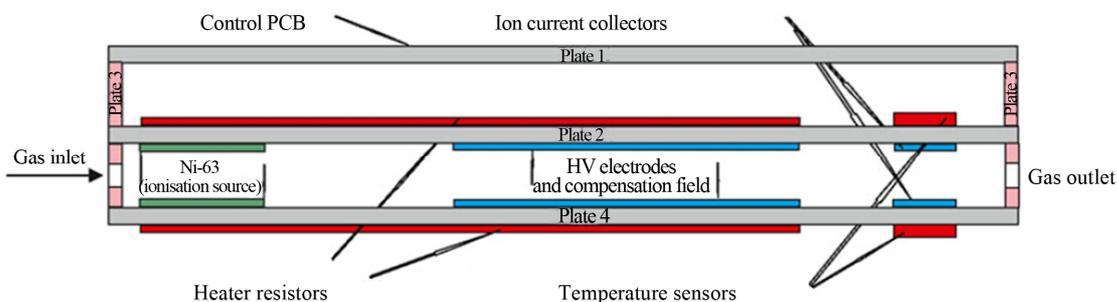


Figure 2. Scheme of DMS spectrometer.

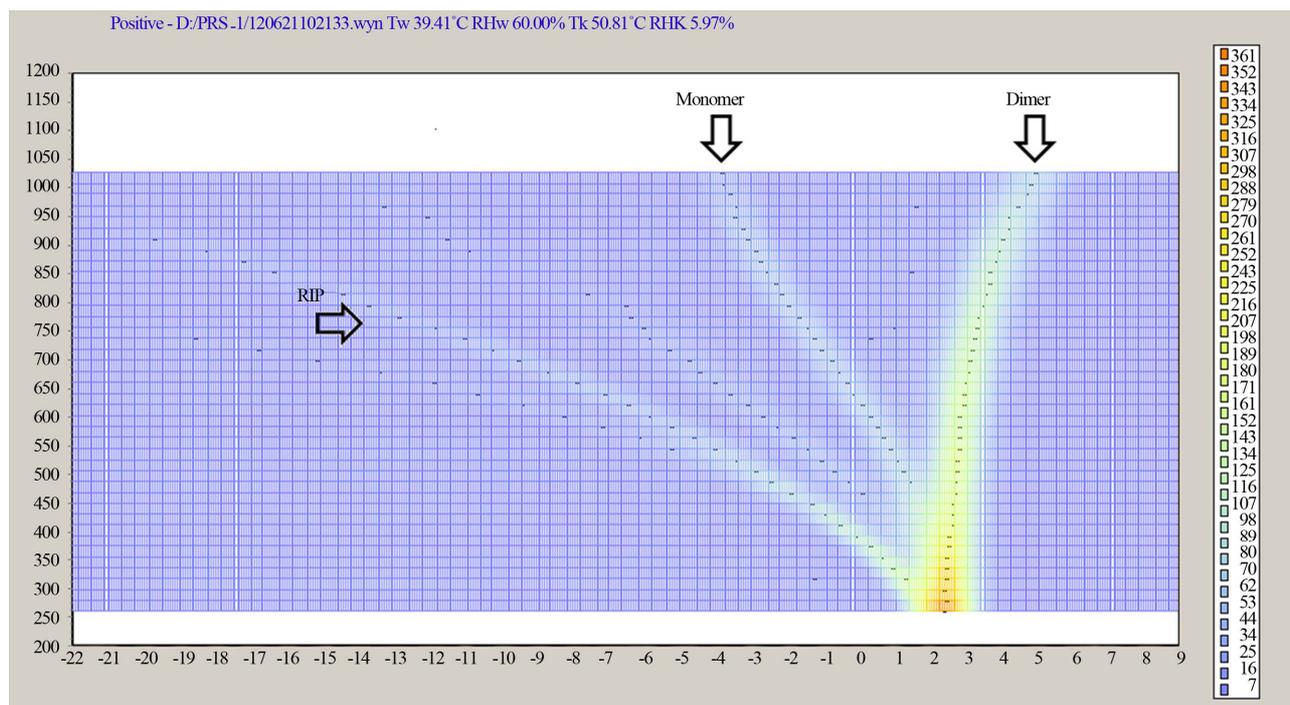
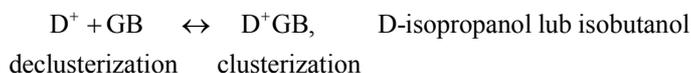


Figure 3. Differential mobility spectra of sarin, gas temperature 50°C, without dopant.



Differential ion spectrometry is well suited to present the shape of the ion—if it is asymmetrical, such as water molecule (dipole shape) then the coefficient α is changed to a greater extent (greater shift to higher negative voltage) through an increase in the ion temperature is generally asymmetric ion reduction process, and the higher asymmetry allows the use of dopants. Furthermore, an additional request for a differential ion spectrometry is not a classic application of the theory of the effect of temperature on the position of the peak $K = K_0 * T/273$ because in this case there is explored m/z but the degree

of asymmetry of the ion, hence the effect of temperature for different ions should be described individually and may be another parameter describing the type of ions.

4. Conclusions

Our studies have confirmed that the chamber construction DMS allows achieving better performance compared with the classical IMS. DMS advantage is the ability to get a better resolution, higher sensitivity, and reduction of the number of false signals. As these parameters could be reached, it was necessary to examine how changing weather conditions will affect the performance of the spectrometer. One of the factors affecting the per-

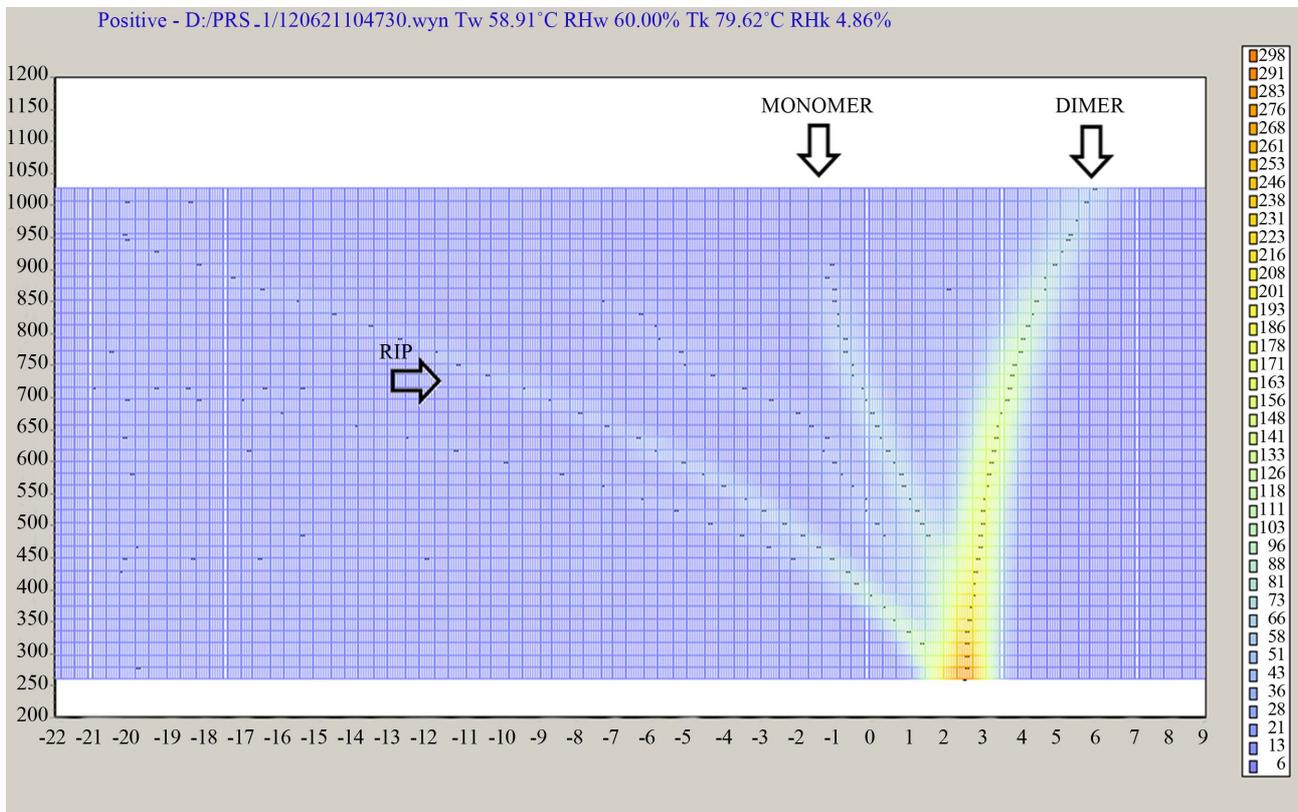


Figure 4. Differential mobility spectra of sarin, gas temperature 80°C, without dopant.

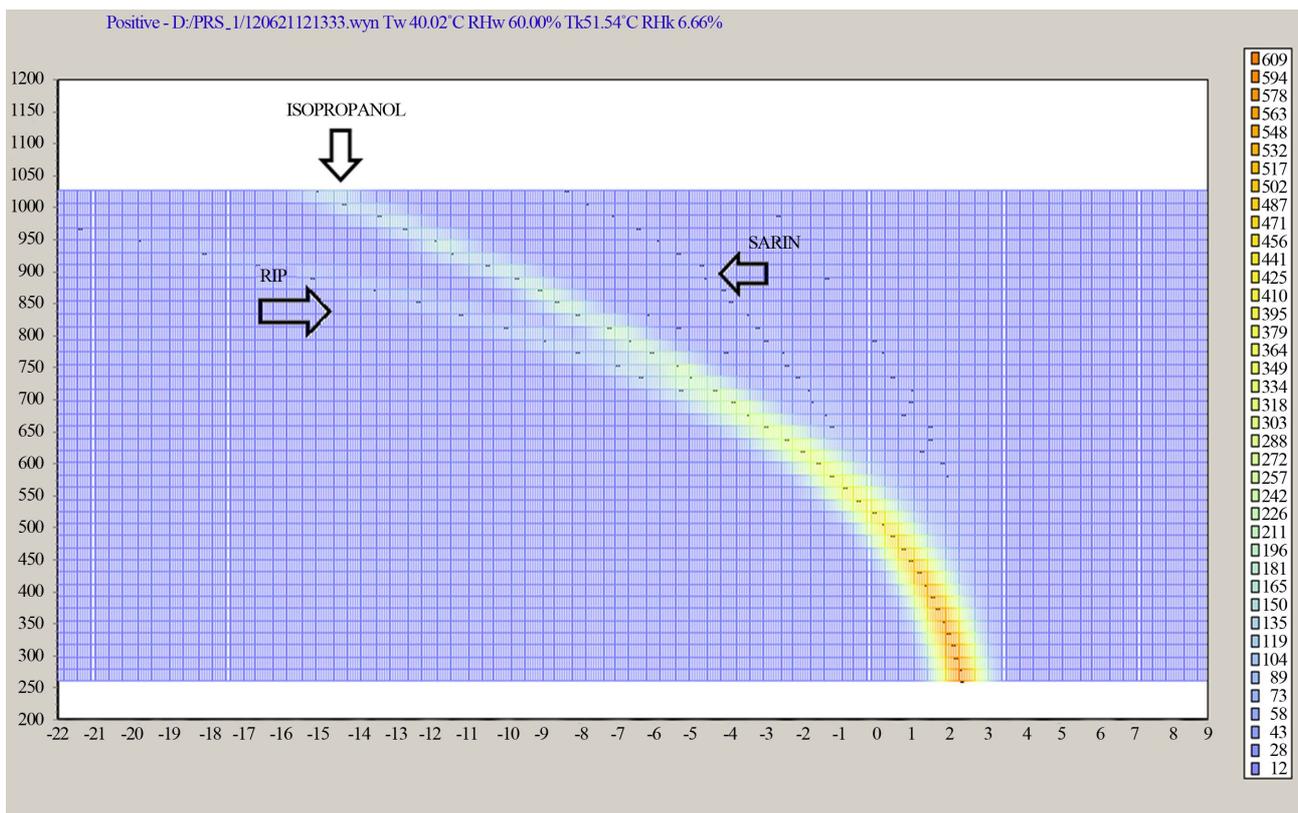


Figure 5. Differential mobility spectra of sarin, gas temperature 50°C, dopant isopropanol.

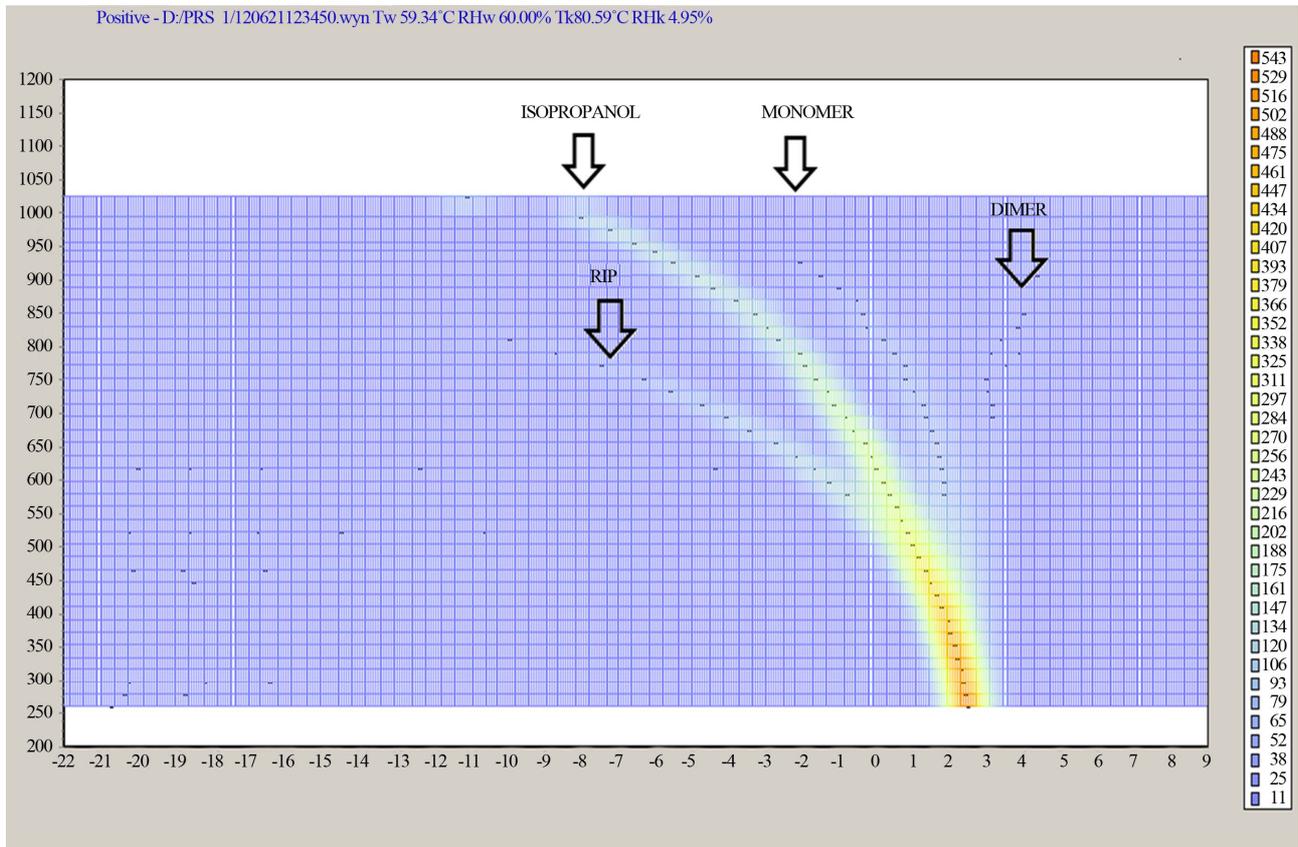


Figure 6. Differential mobility spectra of sarin, gas temperature 80°C, dopant isopropanol.

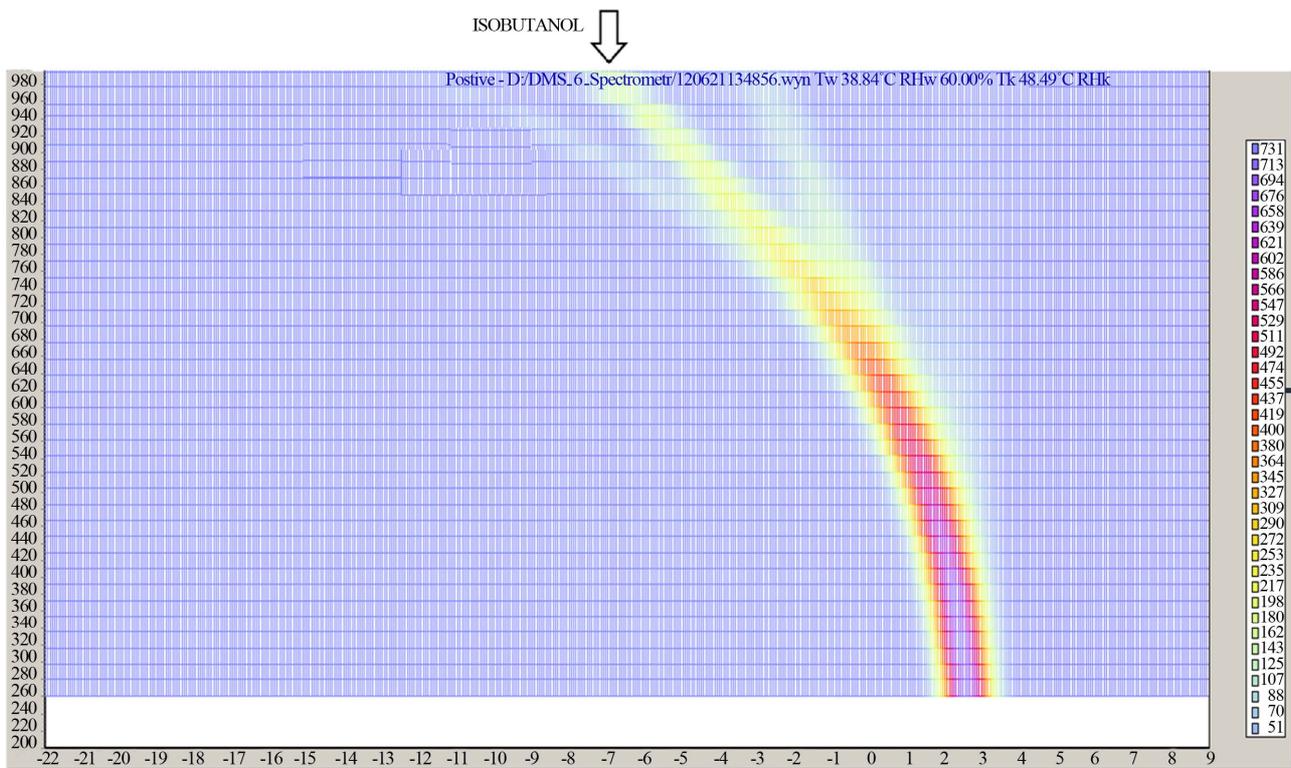


Figure 7. Differential mobility spectra of sarin, gas temperature 50°C, dopant isobutanol.

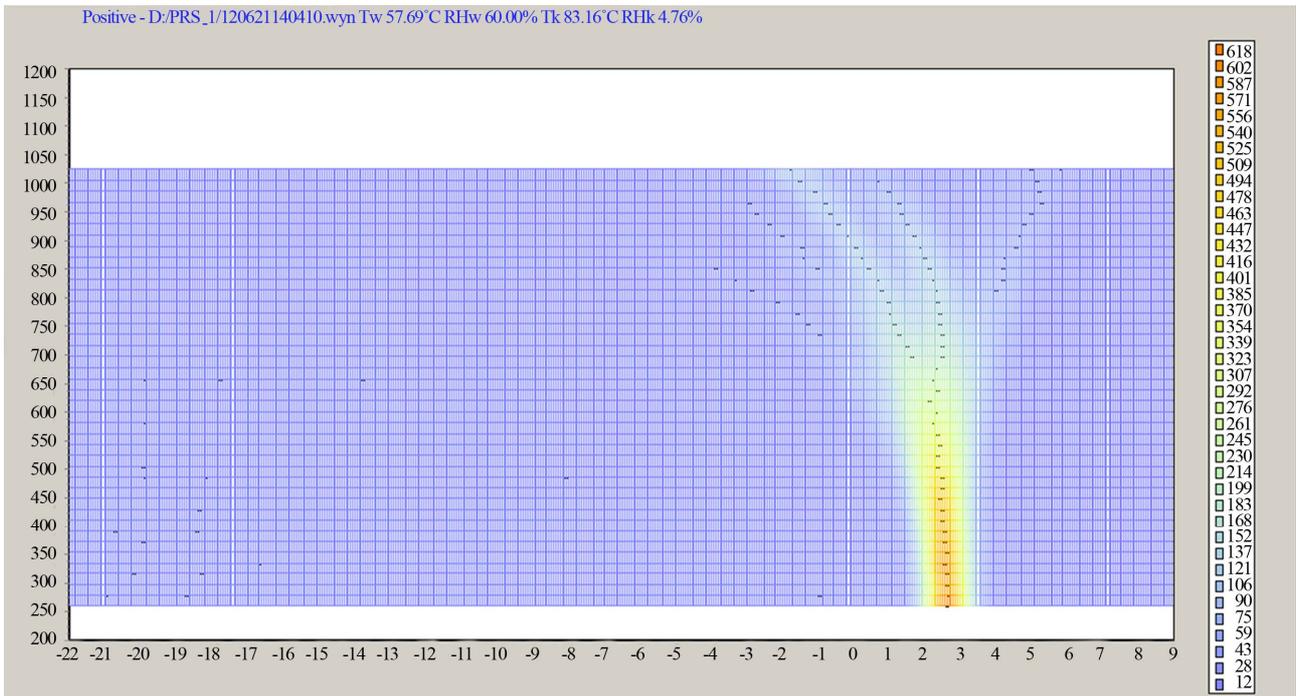


Figure 8. Differential mobility spectra of sarin, gas temperature 80°C, dopant isobutanol.

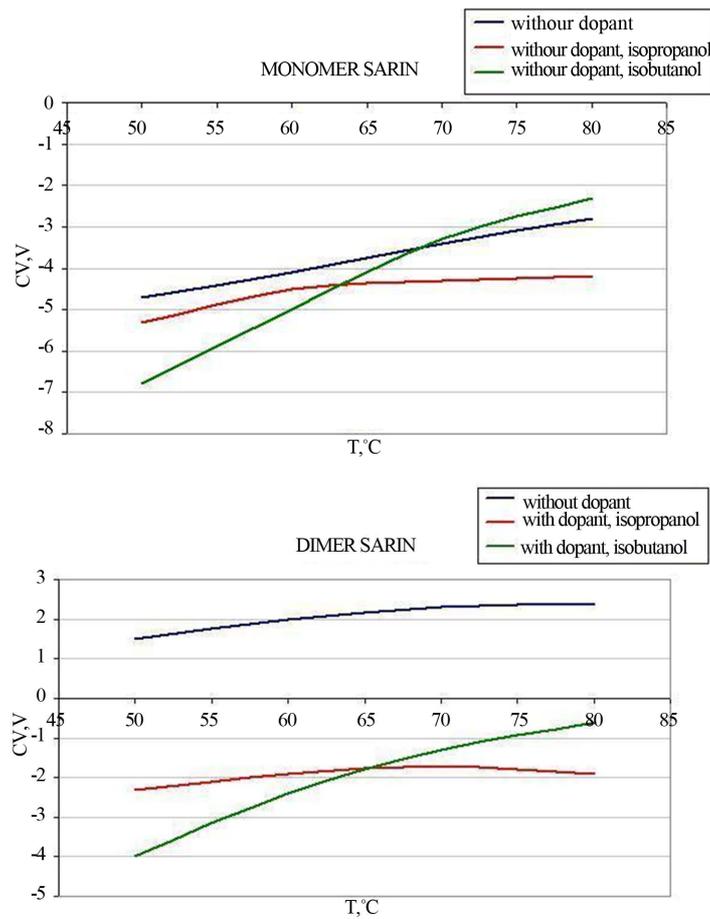


Figure 9. Compension voltage CV as a function of gas temperature.

formance of the device is the temperature outside.

Based on the survey, it found a significant effect of temperature on the position of the carrier gas ion peaks BST on the example of sarin. The results indicate that the recorded spectra and related parameters to describe ions at different temperatures have different values and allow better identification of the compound (less likelihood of false alarm).

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