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Determination of Benzene, Toluene, and Xylene by means of an
Ion Mobility Spectrometer Device using Photoionization

J.W. Leonhardt¹, H. Bensch¹, D. Berger¹, M. Nolting², J.I.Baumbach³

¹ Institut für Umwelttechnologien, Berlin, Germany

² AUERGESELLSCHAFT/MSA, Berlin, Germany

³Institut für Spektrochemie und angewandte Spektroskopie,
Dortmund, Germany

ABSTRACT

The continuous monitoring of changes on the quality of ambient air is a field of advantage of ion mobility spectrometry. Benzene, Toluene, and Xylene are substances of special interest because of their toxicity. We present an optimised drift tube for ion mobility spectrometers, which uses photo-ionisation tubes to produce the ions to be analysed. The actual version of this drift tube has a length of 45 mm, an electric field strength established within the drift tube of about 180 V/cm and a shutter-opening-time of 400 μ s. With the hydrogen tube used for ionisation a mean flux of 10^{12} photons/cm²s was established for the experiments described.

We discuss the results of investigations on Benzene, Toluene, and Xylene in normal used gasoline SUPER. The detection limits obtained with the ion mobility spectrometer developed in co-operation are in the range of 10 ppbv in this case. Normally, charge transfer from Benzene ions to Toluene takes place. Nevertheless the simultaneous determination in mixtures is possible by a data evaluation procedure developed for this case. The interferences found between Xylene and others are rather weak. The ion mobility spectra of different concentrations of gasoline SUPER are attached as an example for the resolution and the detection limit of the instrument developed. Resolution and sensitivity of the system are well demonstrated. A hand-held portable device produced just now is to be tested for special environmental analytical problems in some industrial and scientific laboratories in Germany.

KEY WORDS

Benzene, gas analysis, gasoline, ion mobility spectrometry, Toluene, UV-ionisation, Xylene

INTRODUCTION

Ion mobility spectrometry is a very sensitive method that can be applied to monitoring of air pollutants at sub-parts per million concentrations in ambient air and at ambient pressure. An application tool is the continuous determination of cancer Benzene in air at work places and environmental protection. The addition of aromatics to petrol lies in the percent range. The dangerous risk follows immediately. Thus, a selective, portable and hand-held device must be able to detect the substances under control in the range of legal limit (in Germany called maximum permitted exposure level of pollution at the place of work [MAK]). In the case of Benzene, the instrument must be able to detect Benzene in an environment of Toluene and Xylene with MAK values 400 times higher than Benzene.

In this work, we present an UV-lamp supported ion mobility spectrometer to detect Benzene in such an environment and spectra of different gasolines.

EXPERIMENTAL SECTION.

The ion mobility measurements were carried out using a prototype of a UV-lamp supported drift tube. The schematic diagram of the experimental arrangement to detect Benzene, Toluene, and Xylene is given in Figure 1. Details of the geometrical parameters are summarised in figure 2. The parameters chosen for the instrumentation of the ion mobility spectrometer are presented in Table 1. In the ionisation range a H_2 -lamp was used as source for ionisation, and standard power supplies were employed to establish an electrostatic electric field in the drift region. At the

duplex-shutter ion swarms are created for time intervals less than 500 μs . Through this short gate time all ions start to travel in a plane of the drift field. The control unit for the shutter pulse drive circuit and the A/D-converter are on-line connected with a computer.

temperature	ambient (25°C)
pressure	ambient air
drift gas flow	500 ml/min
sample gas flow	50 ml/min
shutter	duplex-shutter
shutter open time	500 μs
amplifier	$5 \cdot 10^9$ V/A
ion source	H_2 - lamp, MgF-window
mean flux	10^{12} photons/cm ² s
interior diameter	30 mm
drift path	45 mm
electric field strength	170 - 230 V/cm
water content	≤ 50 ppmv

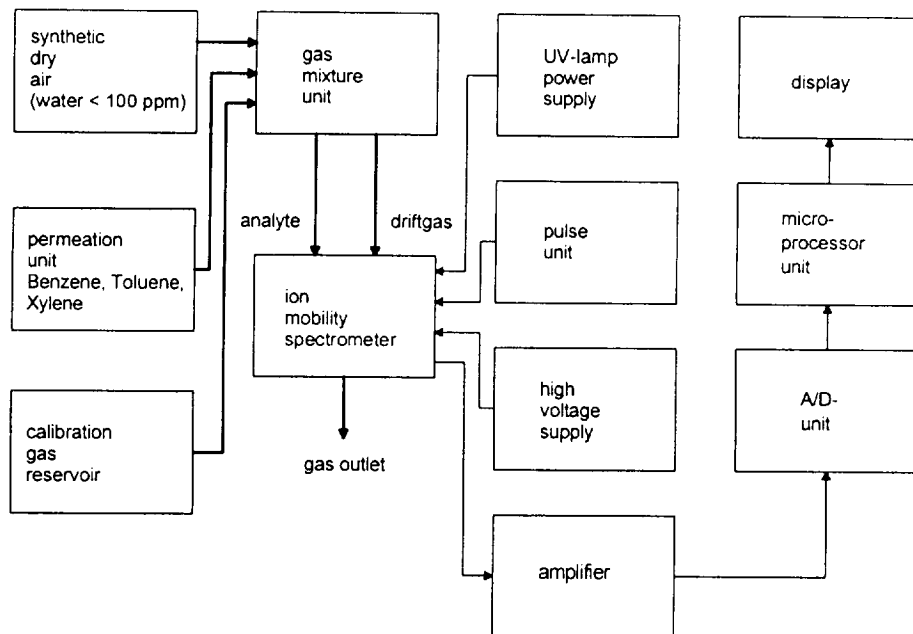


Figure 1:
Schematic diagram of the experimental arrangement to detect Benzene, Toluene, and Xylene using UV-ion mobility spectrometer

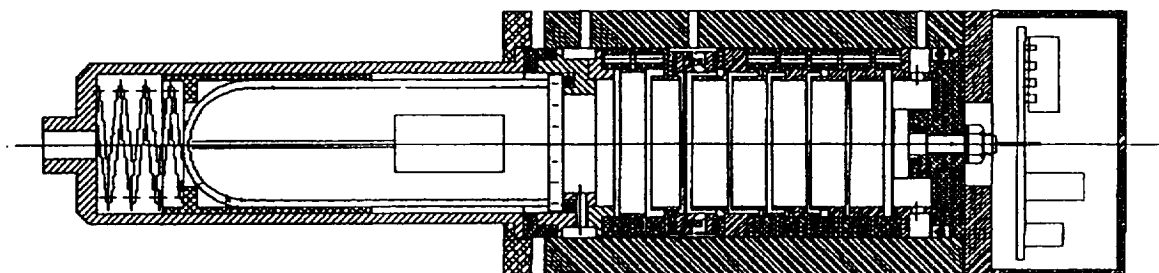


Figure 2:
Picture of the ion mobility spectrometer with UV-lamp, drift tube and data acquisition board (from left)

RESULTS AND DISCUSSION

The spectra of samples of different content of pure Benzene, Toluene, and Xylene are presented in figure 3, 4, and 5, respectively. In the case of Benzene we take 8 peaks, for Toluene 7 and Xylene 3. In Table 2 we consider these substances, the drift times correlated with different peaks and reduced mobility values belong to the drift times.

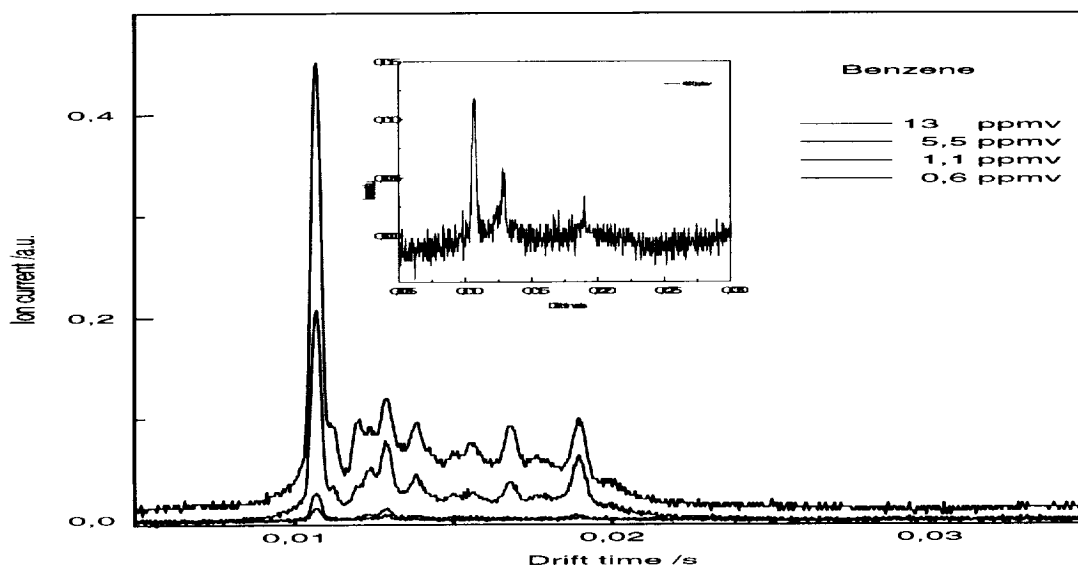


Figure 3:
Ion mobility spectra of different concentrations of pure Benzene

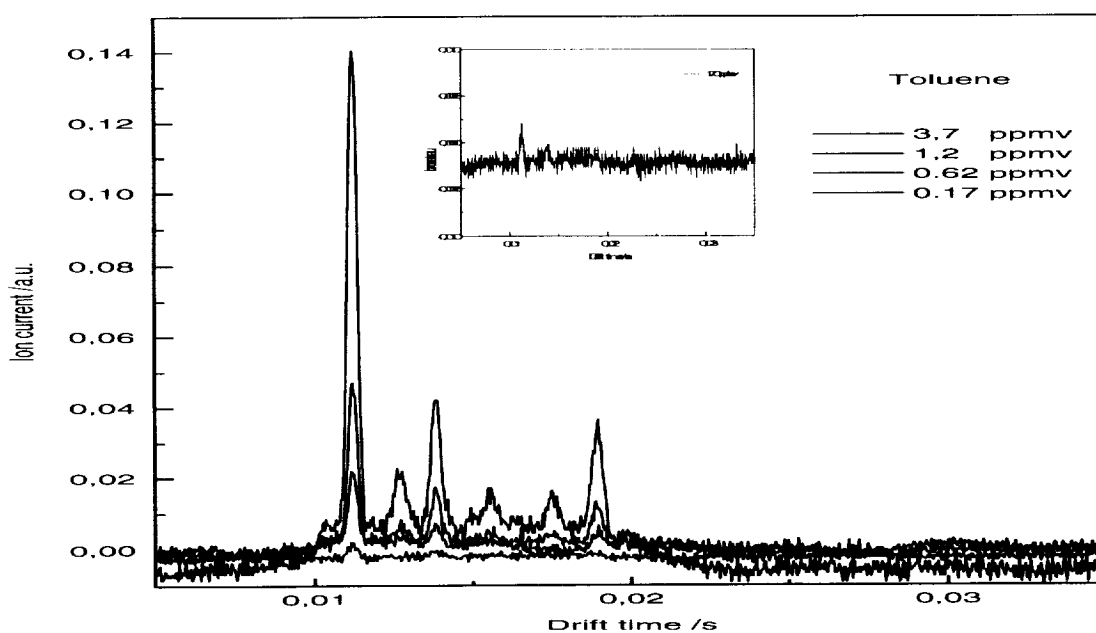


Figure 4:
Ion mobility spectra of different concentrations of pure Toluene

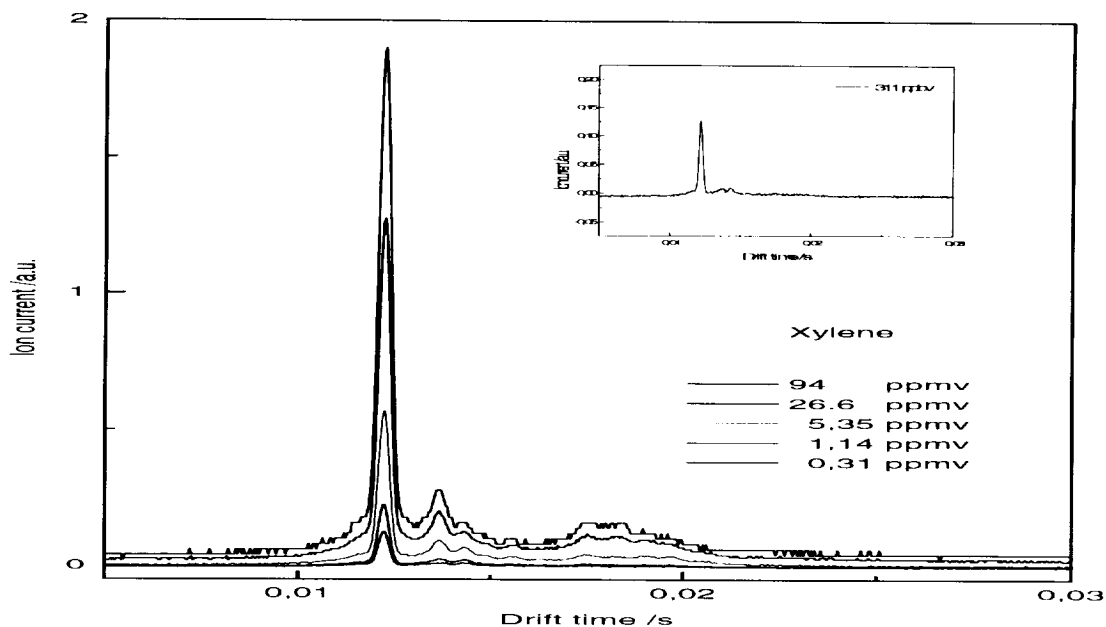


Figure 5:
Ion mobility spectra of different concentrations of pure Xylene

Table 2:
Correlation between measured drift times and reduced mobilities
in the case of pure Benzene, Toluene, and Xylene

Substance	Benzene		Toluene		Xylene	
	drift time	reduced mobility	drift time	reduced mobility	drift time	reduced mobility
	ms	cm ² /V s	ms	cm ² /V s	ms	cm ² /V s
1	10.66	2,27	10.04	2,33	11.81	2,96
2	11.20	2,16	11.20	2,16	13.18	1,84
3	11.96	2,03	12.72	1,91	13.85	1,75
4	12.88	1,88	13.82	1,75		
5	13.84	1,75	15.56	1,56		
6	15.56	1,56	17.50	1,39		
7	16.80	1,45	18.94	1,28		
8	18.96	1,28				

The spectra in the case of mixtures of Benzene and Toluene, as well as Benzene and Xylene are presented in Figure 6 and 7, respectively. It was observed an intensive charge transfer reaction between the positive charged Benzene ion and Toluene. The presence of Toluene is visible as increased peak height. In all cases a little peak of Benzene is present. This represents a short amount of Benzene in all cases is available as residual peak. It comes out, that in the

case of small concentrations of Toluene up to 1 ppmv the detection of Benzene can be realised in case of excess of Toluene quantitatively. In the case of very high concentrations of Toluene over 10 ppmv the detection of small amounts of Benzene the detection problem gets into difficulties. Thus, the simultaneous determination in the range of the MAK-value of Benzene and the MAK-value of Toluene needs further investigations and an optimal arrangement of the ionisation and the drift tube.

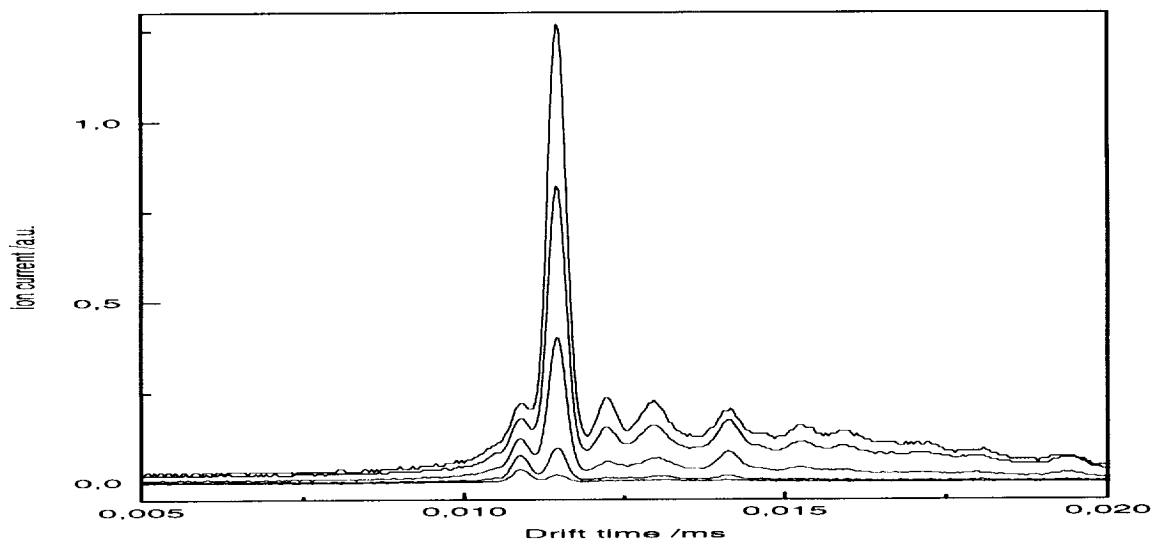


Figure 6:

Ion mobility spectra of different concentrations mixtures of Benzene and Toluene

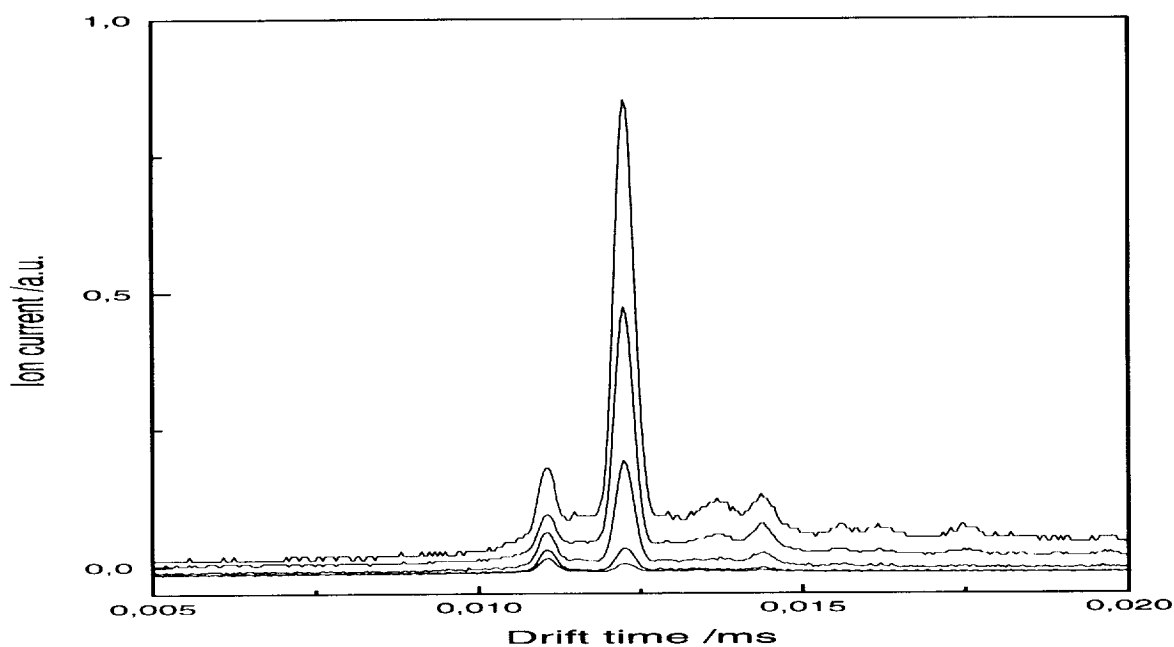


Figure 7:

Ion mobility spectra of different concentrations mixtures of Benzene and Xylene

The charge transfer rate between ions of Benzene and Xylene is lower than in the case of Benzene and Toluene. With regard of this fact a correction factor is useful.

In Figure 8 and 9 we present the first applications of the experimental device to detect gasoline SUPER UNLEADED and BENZIN UNLEADED available from a conventional petrol station in Germany.

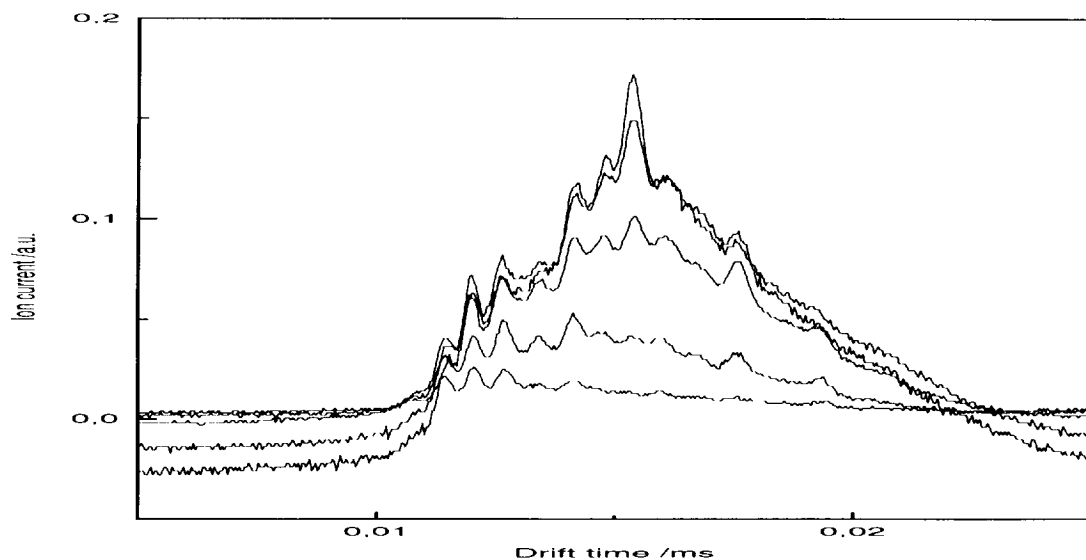


Figure 8:
Ion mobility spectra of gasoline SUPER UNLEADED.

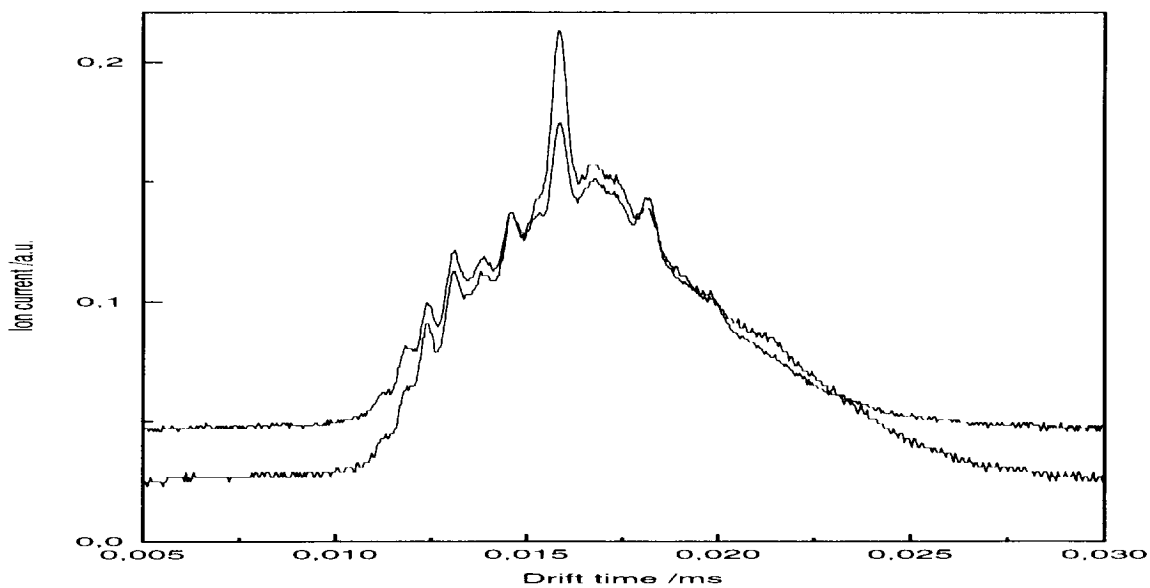


Figure 9:
Ion mobility spectra of gasoline BENZIN UNLEADED.

CONCLUSIONS

The main conclusions of the first experiments with Benzene, Toluene, and Xylene of the UV-lamp supported ion mobility spectrometer are the following:

- 1) A method for simultaneous determination of the concentrations of Toluene and Xylene is available.
- 2) The determination of Benzene in the range of the MAK-value is possible in the case of additional Xylene, also at higher Xylene concentrations.
- 3) The determination of Benzene in the case of additional Toluene is possible if the concentrations of both are lower than 1 ppmv.
- 4) The continuous monitoring of Benzene arising from petrol stations using UV-lamp supported ion mobility spectrometer is a new application field for the method presented.

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