Mobilities of halogenated compounds

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Introduction

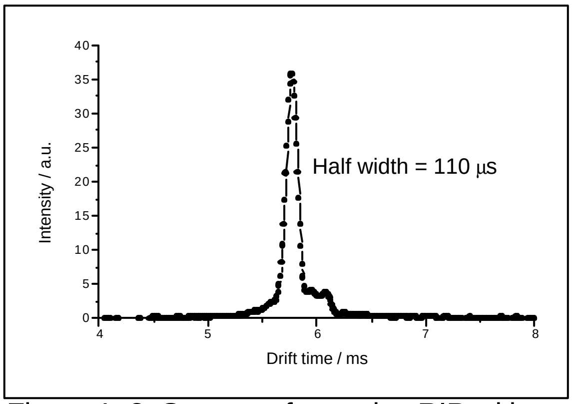
The detection of halogenated hydrocarbons and other compounds by means of an IMS is one of the most important problems in industrial use. Unfortunately many of halogenated compounds have the same mobilities and similar spectra. Therefore cross sensitivities take place and the detection of one compound like 1,2-dichloroethane or phosgene is rather difficult in presence of other halogenated compounds, which are used as solvents. Even in the case that the matrix compounds have lower sensitivities – at high concentrations they can affect the analytical result. So we started some studies of the mobilities of product ions of 16 compounds listed in table 1. Besides of the mobilities the half width of product ions were checked.

Method

The measurements were carried out by high resolution (see figures 1, 2) IUT-IMS type GSM for industrial use and by IUT GC-IMS.

Technical data of the IMS

Ionisation source	^{3}H, A < 50MBq
Drift length	54.5mm
Voltage	-2000V
Temperature of cell	315K
Spectra acquisition	30ms
Mode	sampling
Column	Restek MXT Q Plot



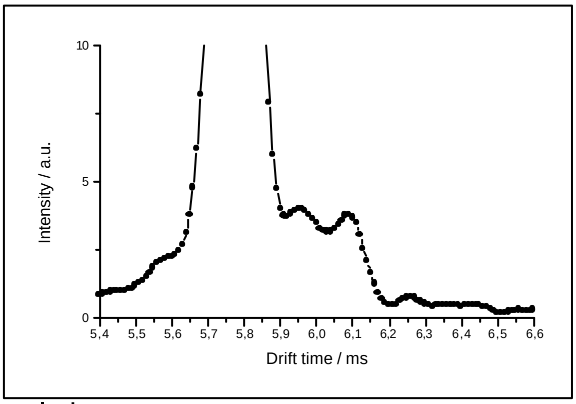


Figure 1, 2: Spectra of negative RIP without deconvolution

All spectra are recorded by oszilloscope and PC. The concentrations (0 – 4 ppm) of the used chemicals at purity of > 99% was produced by diffusion tubes.

Results

In table 1 are listed all measured compounds, the reduced mobilities of their negative product ions and the half widths of the peaks.

Compound	red. mobility [cm^2/Vs]		half width [µs]	
Negative Product Ions	1	2	1	2
Phosgene	2.625		79	
Chlorodimethylether	2.638	2.388	71	51
Dichloromethane	2.625		78	
1,2-Dichloroethane	2.625		77	
Trichloromethane	2.459	2.395	51	
Trichloroethene	2.625	2.392	76	48
2,2,2-Trichloroethanol	1.866	1.518	60	72
Tetrachloromethane	2.625		76	
Tetrachloroethene	2.625		73	
Dichlorodifluoromethane	2.600		71	
Trifluoroethanol	1.863	1.523	61	
Dibromomethane	2.447	1.779	49	57
1,2-Dibromoethane	2.455		51	
1,3-Dibromopropane	2.459		48	
1,4-Dibromobutane	2.459		48	
Methyliodine	2.388		47	
Chlorine	2.388		48	

Table 1: Measured compounds and their properties

As examples the typical spectra of some compounds are given in figures 3 - 7.

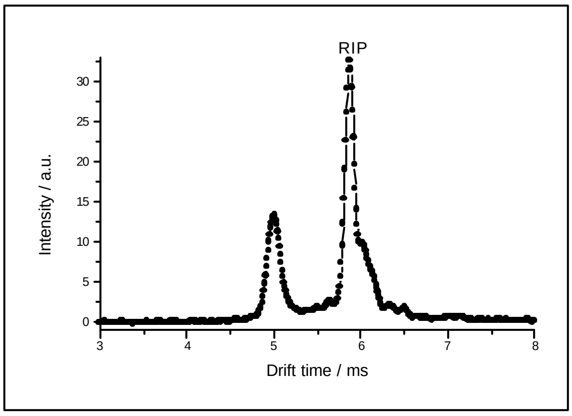


Figure 3: Spectrum of tetrachloromethane

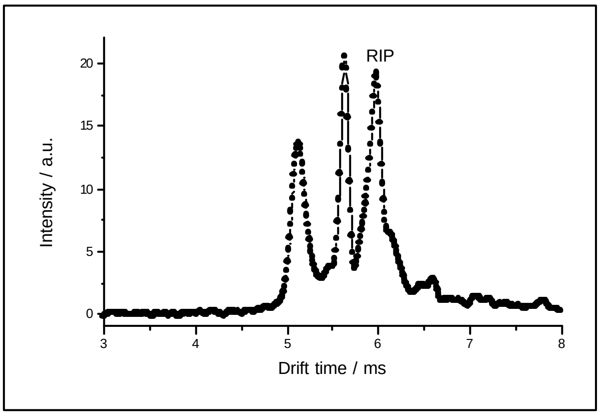


Figure 4: Spectrum of trichloroethene

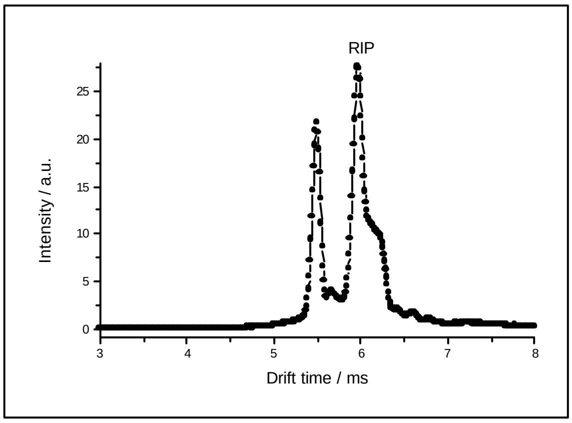


Figure 5: Spectrum of 1,3-dibromopropane

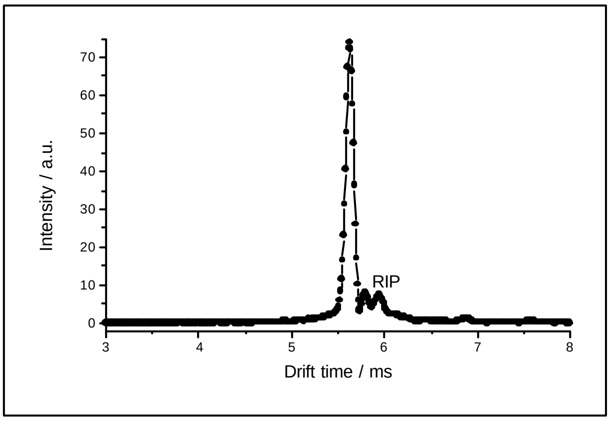


Figure 6: Spectrum of methyliodine

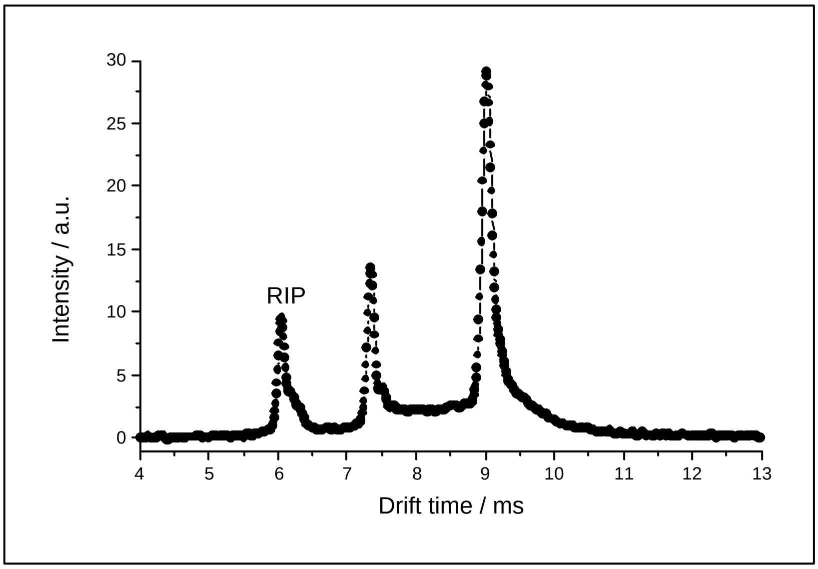


Figure 7: Spectrum of trifluoroethanol

Discussion

(1) As shown in the table there are 6 chlorinated carbons, which have product ion mobilities of (2.620 $\pm$ 0.025) cm^2/Vs. There is no chance to separate them at given resolution in mixtures.

(2) The half width of this 6 product ions is equal to (75 $\pm$ 4) µs, which is relatively broad in comparison with all other peaks.

(3) Chlorodimethylether, trichloromethane, trichloroethene, 2,2,2-trichloroethanol, trifluoroethanol and dibromomethane produce 2 product ion peaks. The first 3 of them have a second ion with the same mobility as chlorine. This matter of fact will help by identification of them.

(4) Compounds with 2 or 4 haloatoms produce 1 product ion only. There may be some symmetry effect.

(5) As expected iodine- and bromine substituted compounds have somewhat lower mobilities as the chlorinated compounds.

(6) The resolution of the used IMS is better than 50. In complex mixtures we also meet often the problem of interrecombination or quenching of product ions. Therefore correct analysis is possible in defined matrixes only. This is one of the reasons that GC-preseparation is necessary for halogenated compounds analysis.

Conclusions

In conclusion of point (6) in the discussion and also in respect of the limited number of reactions ions in the ion source the GSM is equipped by an GC-entrance port without carrier gas. The improved analysis of 1,2-dichloroethane in presence of dichloromethane and trichloroethene, compounds with big differences in sensitivity, is demonstrated in figure 8.

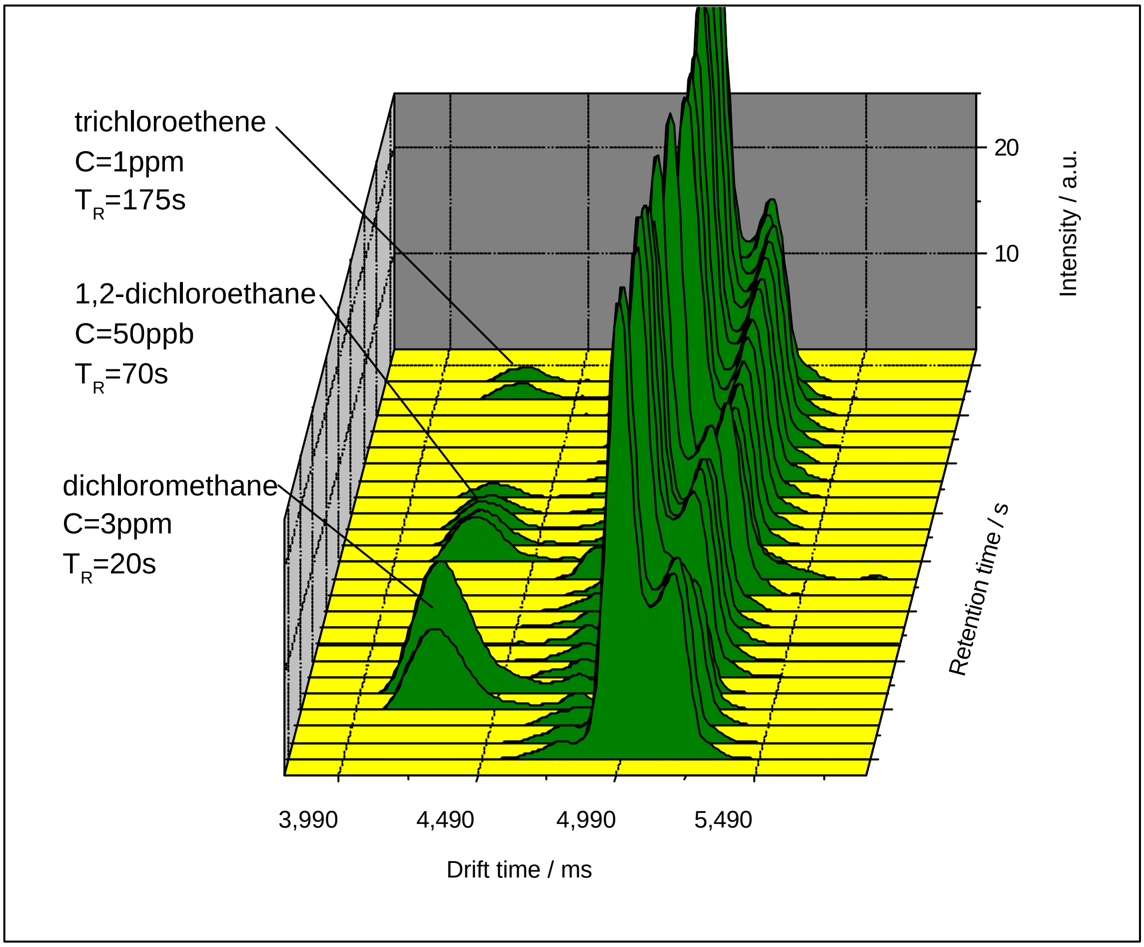


Figure 8: GC-spectrum of a mixture of 50ppb 1,2-dichloroethane, dichloromethane and trichloroethene in the ppm range

References

[1] Z. Karpas, Y.-F. Wang, G. A. Eiceman, Qualitative and quantitative response characteristic of a capillary gas chromatograph/ion mobility spectrometer to halogenated compounds, Anal. Chem. Acta, 282, 19-31, 1993

[2] J.W. Leonhardt, W. Rohrbeck, H. Bensch, A high resolution IMS for environmental studies, Fourth International Workshop on Ion Mobility Spectrometry, 16.8.-9.8.1995, Cambrigde, U.K.

[3] H.H. Hill, W.F. Siems, R.H. St.Louis, D.G. McKinn, “Ion mobility spectrometry“ Anal. Chem. 62, 1201A-1209A, 1990

[4] J.E. Roehl, “Environmental and Process Applications for Ion Mobility Spectrometry“ Appl. Spectrosc. Rev. 26, 1-57, 1991

[5] S. Sielemann, J.I. Baumbach, P. Pilzecker, G. Walendzik, Detection of trans-1,2-dichlorethene, trichloroethene and tetrachloroethene using Multi-Capillary Columns Coupled to Ion Mobility Spectrometers with UV-Ionisation Sources, journal of ISIMS, 1999