

COMPARISON OF DRIFT TIMES OF DIFFERENT IMS

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Introduction

The comparison of spectra of different IMS as well as even spectra of the same device is some times considerably difficult. As description for the quantity to measure, in our case the speed of an ion in an electrical field, the mobility K [cm^2/Vs] is specified. In /1/ there is given an equation for the calculation of the mobility. However, mostly these parameters are not known or they are difficult to define. That's why the mobility mostly is determined experimentally.

The influence of pressure and temperature can be corrected. This gives the reduced mobility K_0 .

$$K_0 = K * (p / 1013 \text{ mbar}) * (273 \text{ K} / T).$$

In the following a value reciprocal to the reduced mobility is used, viz the reduced drift time t (standardized to 1013 mbar and 293 K). Further on a relative drift time t_r is defined which is based on the ratio between the drift time of the ion species to the reactant ions.

A comprehensive study of mobilities /2/ shows a contradictory picture. The values of various sources differ enormous. In this context reasons for this behaviour are described as well as a solution for comparability is suggested.

Possible influence parameters for the mobility of an ion species can be divided in two groups. Pressure, temperature and kind of drift gas determine the drift time directly. The residence

time in the drift tube and the reaction equilibrium during the ion production and drift define whether an ion species can be detected under the given circumstances.

Additionally the calculation of the mobility depends further on the mechanical and electrical parameters of the drift tube.

Influence of the drift gas

In fig. 1 the drift times of ethyl acetoacetate and an unknown impurity in helium, air and neon are plotted. The drift voltages vary, temperature and pressure are similar, but not measured. The result are three straight lines. The line of the noble gases crosses nearly the origin. The line of the drift times in air has an intercept. The reason /3/ for that is the different polarizability of the used gases. The tendency to cluster in noble gases is not so high. The resolution of the peaks changes hardly. The separation is in helium the best followed by neon.

The influence of the moisture of the drift gas

In tab. 1 there are shown the values of three different spectra of triethyl phosphate. The general conditions for these spectra are equal but not for acquisition date and moisture. The concentration moisture in drift gas and carrier gas for the both first spectra is constantly 3 ppm. The value in the third spectra is 650 ppm. The position of the dimer is stable for all spectra. RIP and monomer peak shift with increasing moisture enormously. The clustering is

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increasing (fig. 2) and the sharpness of the peaks reduces. The relative values are more stable than the reduced ones.

Comparing different spectra the influence of moisture has a not negligible importance.

The measurements of moisture by other devices needs more efforts and is very expensive.

The influence of temperature

Referring to the a.m. equation of reduced mobility the influence of temperature on all kinds of ions should be equal. But this is only correct for a small number of ions. There has been searched for a substance which is hardly influenced by temperature. As a reference standard for IMS 2,4-Lutidin $K_0=1,95$ was proposed and used in a whole string of papers /4-6/. Lutidin has to a large extent stable values for reduced mobility. In fig. 3 the reduced drift times of different ketone between 20 and 80 °C are plotted. In this range the course can be approximated by a straight line. Only the decanone dimer has a positive gradient. This kind of diagram is approved by the model of Tabrizchi /7/. It is possible to apply this to the relative drift times analogous. With help of this rule it is feasible to determine the temperature of other measured spectra.

An extended temperature corrected relative drift time can be described as follows:

$$t_{RT} = \alpha + \beta * t_R$$

R = relative to RIP
 T = extended temperature compensation
 α and β = factors to determine

Generally the rises (β) are low so that the error in this calculation is relatively high.

Comparison with other papers

In /8/ the monomer peaks of many VOC are listed. A RIP position is not given. Following preliminary investigations it is possible to argue that the spectra are collected at room temperature or some degrees higher. Acetone and the RIP have nearly the same drift times at that temperatures. In fig. 4 the values of the homologous series of 2-ketone are shown. The good correlation is obviously.

In reference /9/ the relative drift times of dimers are explicitly given (tab. 2). Because not all chemicals were available only some values are compared. Also in this case the correlation is well.

Conclusions and further research

This work is restricted to the positive mode. Generally for the negative mode are similar results obtainable. However the positive RIP is much more stable than the negative.

Relative drift time values compensate some difficult measurable factors better than absolute ones. These factors may result from varying mechanical or electrical parameters.

The comparison of different devices is enforced by relative values.

Aim of present research is the measurement of moisture and temperature of an IMS by suitable model substances.

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Date	27.11. 2001	23.01. 2002	02.02. 2002
Moisture C [ppm]	3	3	650
Temperature T [°C]	52,6	52,9	52,8
Pressure [mBar]	950	970	965
Red. drift time RIP	6,81	6,78	7,63
Red. drift time TEP monomer	9,20	9,16	9,71
Red. drift time TEP dimer	13,19	13,14	13,03
Rel. drift time TEP monomer	1,350	1,351	1,272
Rel. drift time TEP dimer	1,936	1,937	1,707

Tab.1: Drift times of TEP (Triethyl phosphate) at different dates and moisture

Compound	Referenz /9/	IUT-GSM T = 27 °C
Acetone	1,12	1,12
2-Propanol	1,25	1,24
2-Butanone	1,26	1,25
2-Butanol	1,35	1,35
n-Butylamine	1,38	1,38
Cyclohexanone	1,46	1,46
DMMP	1,46	1,47
4-Heptanone	1,59	1,60
n-Butylacetate	1,62	1,63

Tab. 2: Comparison of dimers

Fig. 1: Drift times of Ethyl acetoacetate (and some impurities) in Air, Helium and Neon

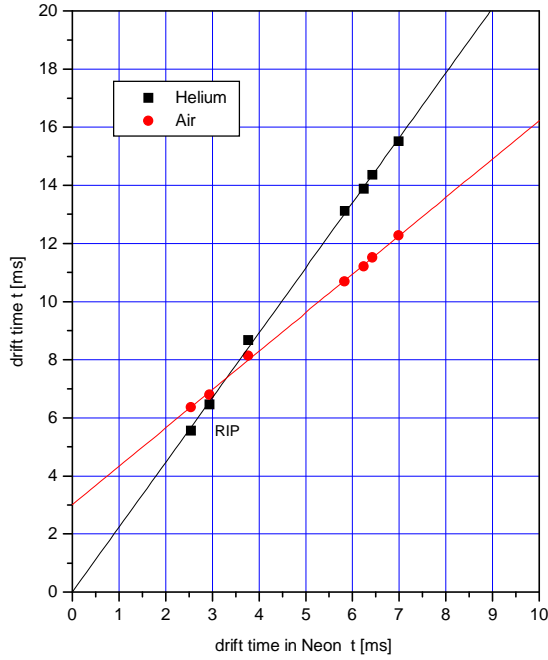


Fig. 3: Drift times of 2-Ketone in dependence of temperature

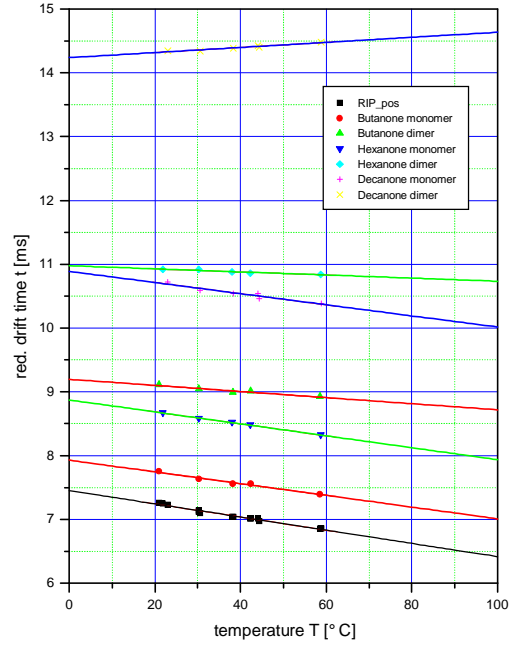


Fig.2: TEP spectra in dependence of moisture

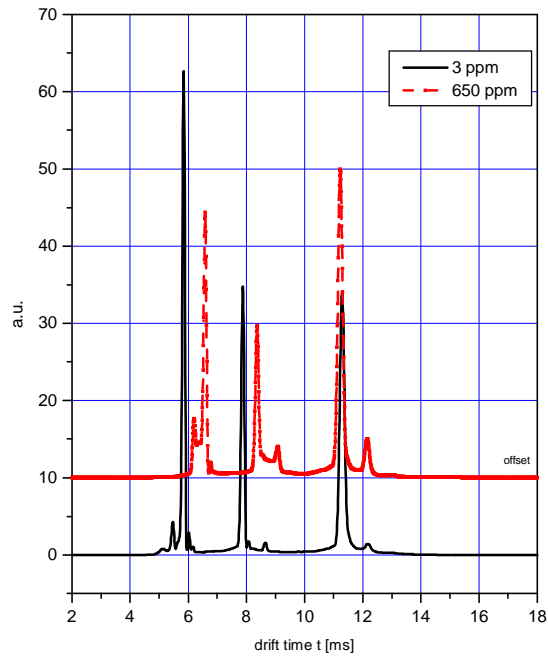


Fig. 4: Comparison of Monomer from Ref. 8 and IUT GSM (T = 30 °C)

