Electronic Supplementary Material (ESI) for Analytical Methods.

- Supplementary Information -

Analysis of hazardous chemicals by "stand alone" drift tube ion mobility spectrometry: A review

S. Armenta [a]*, F.A. Esteve-Turrillas [a], M. Alcalà [b]

[a] Analytical Chemistry Department, University of Valencia, 50th Dr. Moliner St., 46100 Burjassot, Spain

[b] Department of Chemistry, Faculty of Sciences, Universitat Autònoma de Barcelona, Bellaterra, Barcelona 08193, Spain

Table S1. Mobility constant values for pesticides analysed in Reference. [1]

Analyte	K_0 ($cm^2 V^{-1} s^{-1}$)
Isocarbophos	1.421 ± 0.01
Omethoate	1.591 ± 0.01
Monocrotophos	1.507 ± 0.01
Phosphamidon	1.368 ± 0.01
Methamidophos	1.786 ± 0.01
	1.424 ± 0.01
Methomyl	1.695 ± 0.01
Carbaryl	1.528 ± 0.01
Isoprocarb	1.483 ± 0.01
Nitenpyram	1.372 ± 0.01
Acetamiprid	1.450 ± 0.01
Thiacloprid	1.403 ± 0.01
Dimethomorph	1.445 ± 0.01
Triadimenol	1.284 ± 0.01
Triadimefon	1.282 ± 0.01
Propiconazol	1.244 ± 0.01
Tebuconazole	1.318 ± 0.01
Myclobutanil	1.278 ± 0.01
Paclobutrazol	1.303 ± 0.01
Tricyclazole	1.619 ± 0.01
Atrazine	1.479 ± 0.01
Simazine	1.542 ± 0.01
Ametryn	1.436 ± 0.01
Diazinon	1.653 ± 0.01
	1.310 ± 0.01
Alachlor	1.382 ± 0.01
Metolachlor	1.380 ± 0.01
Acephate	1.683 ± 0.01
RH-5849	1.307 ± 0.01
Uniconazole	1.303 ± 0.01
Propyzamide	1.392 ± 0.01
Chlorbenzuron	1.322 ± 0.01

Experimental conditions used in this study: Drift tube temperature 60°C, and 3-methylpyridine was used as calibrant.

Table S2. Mobility constant values for explosives analysed in Reference. [2]

Analyte	K_0 ($cm^2 V^{-1} s^{-1}$)	Reactant
TNT	1.48	NaCl and ammonium acetate
2 ADNT	1.57	
2,4 DNT	1.62	
4-NT	1.79	
TNB	1.42	
RDX	1.40	
HMX	1.25	
EGDN	1.57	

Table S3. Mobility constant values for explosives analysed in Reference.[3]

Analyte		K_0 ($cm^2\ V^{-1}\ s^{-1}$)
DMNB	$[NO_2]^-$ – major ion	2.50
DNT	$[DNT–H]^-$ – major ion	1.68
TNT	$[TNT–H]^-$ – major ion	1.54
RDX	$[RDX–HNO_2+Cl]^-$ – minor ion	1.57
	$[RDX+Cl]^-$ – major ion	1.47
	$[RDX+NO_2]^-$ – major ion	1.42
	$[RDX+Cl_2]^-$ – minor ion	1.36
	$[2RDX+Cl]^-$ – minor ion	1.00
HMX	$[HMX–HNO_2+Cl]^-$ – minor ion	1.42
	$[HMX+Cl]^-$ – major ion	1.34
	–	1.28
	$[2HMX+Cl]^-$ – minor ion	0.89
EGDN, NG, PETN, NH_4NO_3	$[NO_3]^-$ – major ion	2.40
NG	$[NG–NO_2+H+Cl]^-$ – minor ion	1.54
	$[NG–NO_2+H+NO_3]^-$ – minor ion	1.44
	$[NG+Cl]^-$ – major ion	1.42
	$[NG+NO_3]^-$ – major ion	1.35
	$[NG+Cl_2]^-$ – minor ion	1.32
PETN	$[PETN–NO_2+H+Cl]^-$ – minor ion	1.29
	$[PETN–H]^-$ – minor ion	1.27
	$[PETN–NO_2+H+NO_3]^-$ – minor ion	1.24
	$[PETN+Cl]^-$ – major ion	1.22
	$[PETN+NO_3]^-$ – major ion	1.18
	$[PETN+Cl_2]^-$ – minor ion	1.12
NH_4NO_3	$[HNO_3+NO_3]^-$ – major ion	2.05
HMTD	$[NC_2H_2O_2]^-$ – minor ion	2.33
	$[NC_2H_2O_2+H+Cl]^-$ – minor ion	2.05
	$[HMTD–NC_3H_6O_3–H+Cl]^-$ – minor ion	1.82
	$[HMTD–NC_3H_6O_3+H+Cl]^-$ – major ion	1.83
	$[NC_3H_8O_2]^+$ – minor ion	2.12
	$[HMTD+H–CH_2O–H_2O_2]^+$ – major ion	1.74
TATP	$[C_3H_8O_4+Cl]^-$ – major ion	1.77
	$[C_4H_9NH_2]^+$ – minor ion	2.30
	$[C_4H_9O_2]^+$ – major ion	2.17

Experimental conditions used in this study: 4-nitrobenzylnitrile standard in negative mode; isobutyramide standard in positive mode.

References

1 N. Zou, K. Gu, S. Liu, Y. Hou, J. Zhang, X. Xu, X. Li and C. Pan, J. Sep. Sci., 2016, **39**, 1202-1212.

2 G.R. Asbury, J. Klasmeier, H.H. Hill Jr, Talanta, 2000, **50**, 1291-1298.

3 J. Kozole, A. Levine, J. Tomlinson-Phillips and J.R. Stairs, Talanta, 2015, **140**, 10-19.