Supporting Information

REACTIVE TANDEM ION MOBILITY SPECTROMETRY WITH ELECTRIC FIELD FRAGMENTATION OF ALCOHOLS AT AMBIENT PRESSURE

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Table S1. Supporting information for Figure 5 (data supplement Table 1).

Compound	t_d	K_o	t_d	K_o	t_d	K_o	Δt_d	ΔK_o	Ion Mass(g/mol)
	$MH^+(H_2O)_n$		M_2H^+		Fragment ion		$MH^+(H_2O)_n$ - Fragment ion		$MH^+(H_2O)_n$
isopropyl acetate	4.85	1.80	6.35	1.38	4.14	2.11	0.71	0.31	139.13
butyl acetate	5.11	1.72	6.90	1.28	4.15	2.12	0.96	0.40	153.16
isopentyl acetate	5.46	1.61	7.54	1.17	4.10	2.15	1.36	0.54	167.19
pentyl acetate	5.52	1.60	7.60	1.16	4.14	2.13	1.38	0.53	167.19
hexanal	5.18	1.68	6.62	1.31	4.78	1.82	0.40	0.14	137.16
heptanal	5.50	1.58	7.22	1.21	4.88	1.79	0.62	0.21	151.18
octanal	5.80	1.50	7.78	1.12	5.25	1.66	0.55	0.16	165.21
nonanal	6.14	1.42	8.30	1.05	5.39	1.62	0.75	0.20	179.24
octane	4.91	1.77	-	-	3.89	2.24	1.02	0.47	151.23
nonane	5.16	1.69	-	-	4.02	2.17	1.14	0.48	165.20
decane	5.43	1.60	-	-	4.20	2.07	1.23	0.47	179.29

Drift Time, t_d, in ms.

Reduced mobility coefficient, K_o, in cm^2/Vs

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Table S2. Influence of Electric Field Strength on Percent Fragmentation of Protonated Monomer

	Percent Fragmentation at 67˚C and Field Strength (E/N)						Terms for Linear Regression of Percent Fragmentation vs E/N	
	69 Td	77 Td	90 Td	99 Td	112 Td	120 Td		
	Normal alcohols						Slope	Intercept
1-propanol	0.0	0.6	2.0	1.9	5.1	16.5	0.181	-13.28
1-butanol	0.0	2.5	12.2	15.6	25.8	42.5	0.772	-56.52
1-pentanol	8.4	11.4	34.4	46.5	58.8	65.6	1.199	-75.76
1-hexanol	7.6	7.4	26.0	35.0	51.4	54.6	1.029	-66.95
1-heptanol	10.8	16.9	29.5	37.0	49.2	54.4	0.876	-49.81
1-octanol	9.7	17.3	20.4	39.4	44.2	50.5	0.818	-47.03
1-nonanol	0.2	1.3	8.2	30.0	27.9	33.7	0.663	-45.17
	Other alcohols							
cyclohexanol	23.6	38.8	51.3	70.4	80.4	93.8	1.332	-66.18
2-butanol	7.6	13.8	26.0	35.0	42.1	51.1	0.818	-47.03
isobutanol	3.1	14.5	25.6	28.3	45.2	56.1	0.973	-63.15

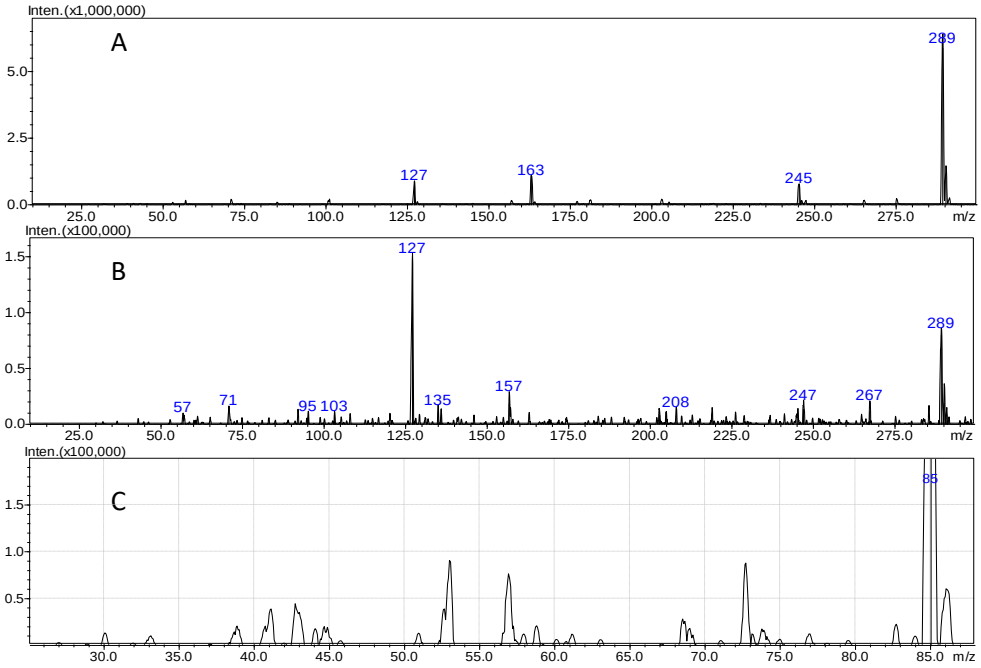

Figure S1. Mass spectra for 1-nonanol with a drift tube-mass spectrometer at 60˚C. Spectra are shown without (A) and with (B) electric field fragmentation at 168 Td. In Frame C, an expanded mass axis is shown for ions of low abundance ions from 25 to 90 Da.

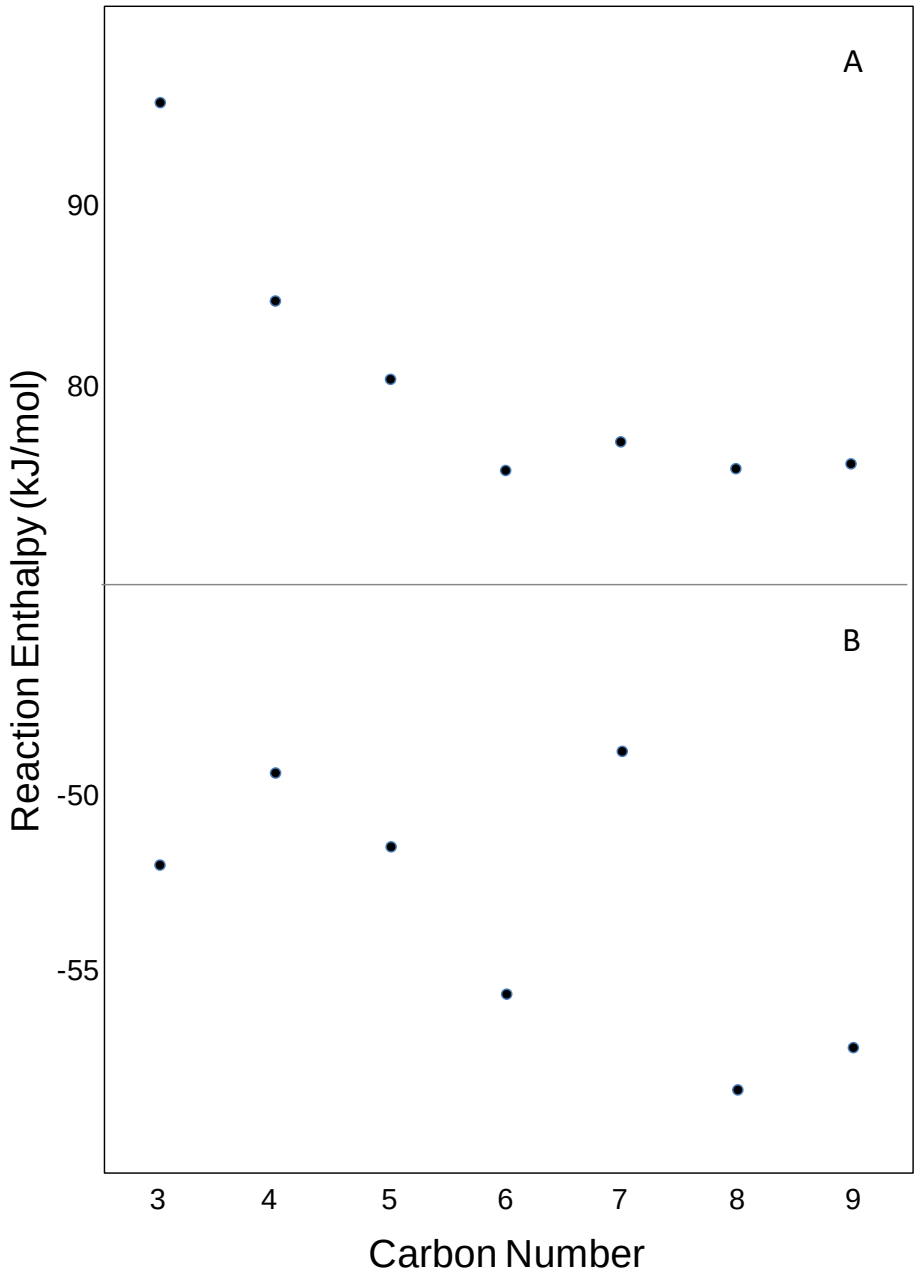

Figure S2. Enthalpy of fragmentation of normal alcohols in: A- a first step of water elimination from protonated monomer to a primary carbocation and B- a second step of charge migration to a secondary carbocation.