

Supplement of:

Introducing the Extended Volatility Range Proton-Transfer-Reaction Mass Spectrometer (EVR PTR-MS)

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Table S1: Table of investigated analytes, their molecular formula, phases investigated, drift tube temperatures used, and supplier

Compound	Molecular formula	gas	particle	Temperatures [°C]	Manufacturer
4-Nitrocatechol	C ₆ H ₅ NO ₄	X		120	ALDRICH
1,6-Anhydro-beta-D-glucose (Levoglucozan)	C ₆ H ₁₀ O ₅	X	X	80, 100, 120	ALDRICH
2,6-Dimethoxyphenol	C ₈ H ₁₀ O ₃	X		120	SIGMA-ALDRICH
2,7-Dihydroxynaphthalene	C ₁₀ H ₈ O ₂	X	X	120	ALDRICH
2-Tridecanone	C ₁₃ H ₂₆ O	X		40, 60, 80, 100, 120	SIGMA-ALDRICH
4-Nitroguaiacol	C ₇ H ₇ NO ₄	X		120	SIGMA-ALDRICH
Adipic acid	C ₆ H ₁₀ O ₄		X	120	SIGMA
Ammonium nitrate	NH ₄ NO ₃	X	X	60, 80, 100, 120	SIGMA-ALDRICH
Ammonium sulphate	(NH ₄) ₂ SO ₄		X	120	SIGMA
Arabitol	C ₅ H ₁₂ O ₅	X		120	SIGMA
Azelaic acid	C ₉ H ₁₆ O ₄	X	X	120	ALDRICH
Benzocaine	C ₉ H ₁₁ NO ₂	X		120	SIGMA
<i>Cis</i> -pinic acid	C ₉ H ₁₄ O ₄		X	120	
<i>Cis</i> -Pionic acid	C ₁₀ H ₁₆ O ₃	X		80, 100, 120	ALDRICH
D-(+)-Glucose	C ₆ H ₁₂ O ₆	X		120	SIGMA
Diglycolic acid	C ₄ H ₆ O ₅	X	X	120	ALDRICH
Erythritol	C ₄ H ₁₀ O ₄	X		120	SIGMA
Fructose	C ₆ H ₁₂ O ₆	X		120	SIGMA
Glycolic acid	C ₂ H ₄ O ₃	X		120	SIGMA-ALDRICH
MBTCA (3-methyl-1,2,3-butanetricarboxylic acid)	C ₈ H ₁₂ O ₆		X	120	self-synthesized
Methyl-β-d-xylopyranoside	C ₆ H ₁₂ O ₅		X	120	SIGMA
Norpinonic acid	C ₉ H ₁₄ O ₃		X	120	synthesized at TROPOS
Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	X		120	SIGMA
Phenoxyacetic acid	C ₈ H ₈ O ₃	X		120	FLUKA
Stearic acid	C ₁₈ H ₃₆ O ₂	X	X	120	SIGMA
Tartaric acid	C ₄ H ₆ O ₆		X	120	
Vanillic acid	C ₈ H ₈ O ₄	X	X	120	SIGMA-ALDRICH
Vanillin	C ₈ H ₈ O ₃	X		80, 100, 120	SIGMA-ALDRICH
Xylitol	C ₅ H ₁₂ O ₅	X		120	SIGMA

Table S2: Parameters of the double-exponential decay fit functions shown in Fig. 1

compound	A1	b1	A2	b2
2-tridecanone _(g)	1.08	-3.75	0.00	-1.27
<i>cis</i> -pinonic acid _(g)	0.78	-0.65	0.22	-0.04
4-nitrocatechol _(g)	0.72	-0.05	0.22	-0.01
nitrate _(p)	0.73	-0.38	0.28	-0.04
levoglucosan _(p)	0.70	-0.21	0.28	-0.02
2,7-dihydroxynaphthalene _(p)	0.73	-0.10	0.24	-0.01

Table S3: Parameters of the double-exponential decay fit functions shown in Fig. 3

compound	A1	b1	A2	b2
2-tridecanone _(g) RT	0.50	-0.07	0.48	-0.03
2-tridecanone _(g) 60°C	0.89	-0.55	0.09	-0.03
2-tridecanone _(g) 80°C	1.07	-1.93	0.05	-0.03
2-tridecanone _(g) 100°C	1.08	-3.75	0.00	-1.27
<i>cis</i> -pinonic acid _(g) 80°C	0.75	-0.22	0.25	-0.04
<i>cis</i> -pinonic acid _(g) 100°C	0.71	-0.39	0.27	-0.03
<i>cis</i> -pinonic acid _(g) 120°C	0.78	-0.65	0.22	-0.04

Table S4: List of m/z signals generated from limonene/O₃ SOA, the assigned ionic formulas, and tentatively assigned neutral precursors

m/z	ion formula	neutral precursor
176.09	C ₇ H ₁₀ O ₄ ·NH ₄ ⁺	3,6-oxoheptanoic acid
188.13	C ₉ H ₁₄ O ₃ ·NH ₄ ⁺	limonic acid, ketolimononaldehyde, norlimonic acid
190.11	C ₈ H ₁₂ O ₄ ·NH ₄ ⁺	norlimonic acid
202.14	C ₁₀ H ₁₆ O ₃ ·NH ₄ ⁺	limonic acid, 7-hydroxylimononaldehyde
204.12	C ₉ H ₁₄ O ₄ ·NH ₄ ⁺	limonic acid, ketolimononic acid
206.10	C ₈ H ₁₂ O ₅ ·NH ₄ ⁺	ketolimononic acid
218.14	C ₁₀ H ₁₆ O ₄ ·NH ₄	5-hydroxylimononic acid, 7-hydroxylimononic acid

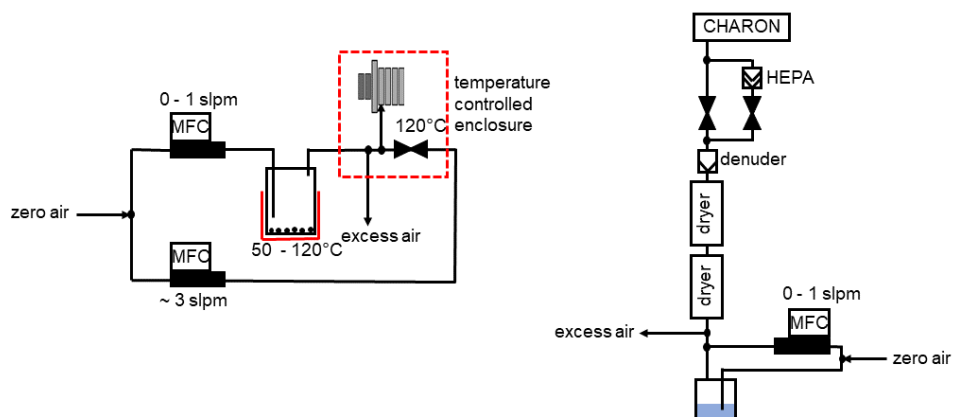


Figure S1: Schemes of the experimental set-ups used for measuring $\tau_{1/e}$ of gas phase (left panel) and particle phase (right panel) analytes

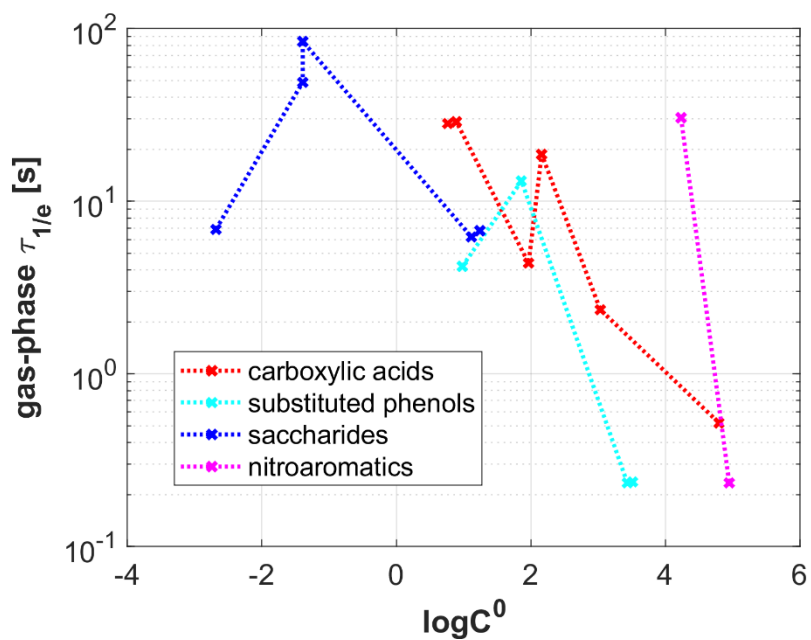
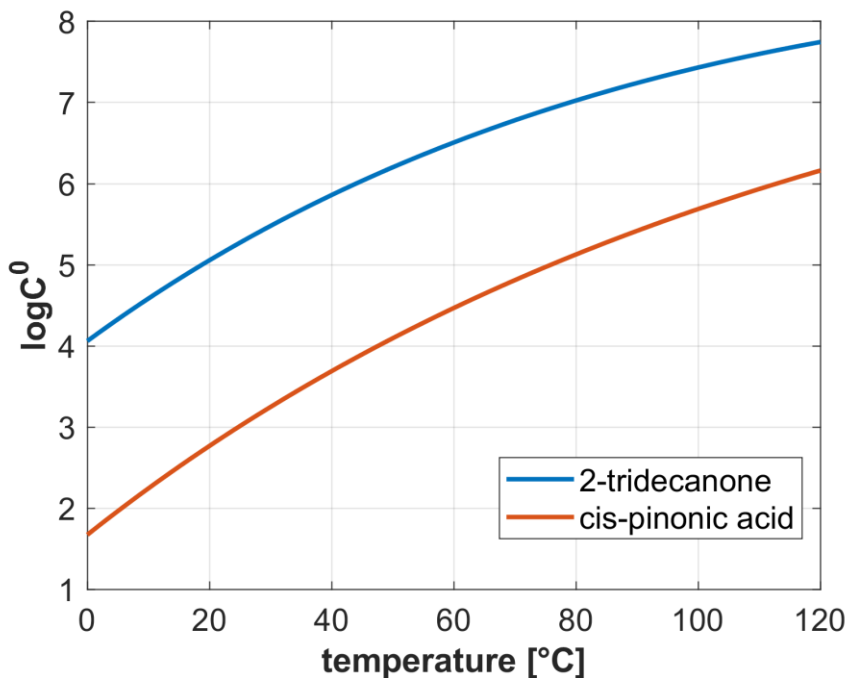
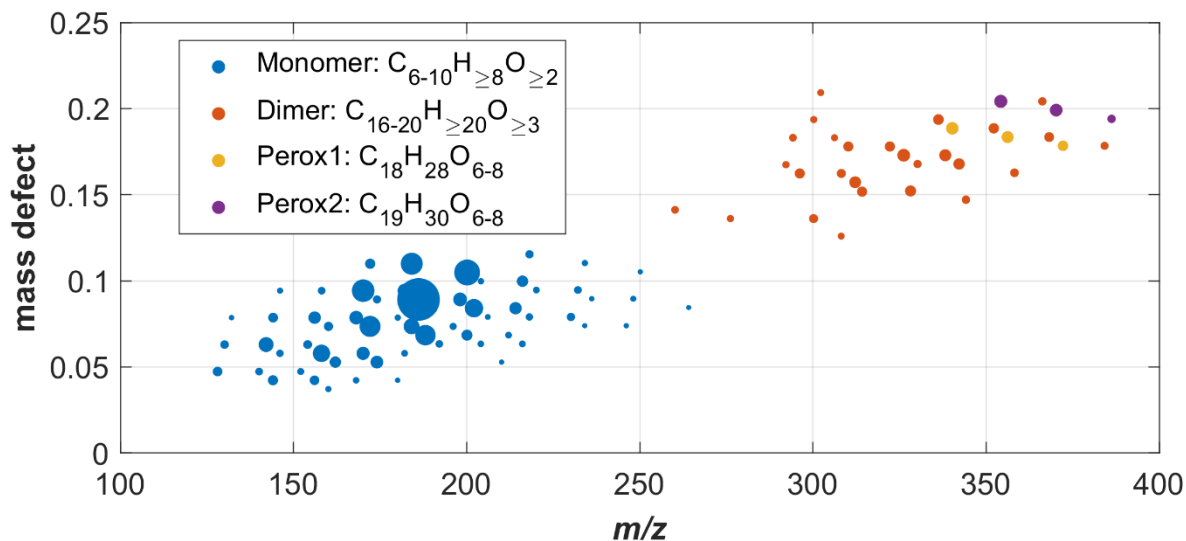


Figure S2: Graph showing the decrease of $\tau_{1/e}$ with increasing $\log C^0$ for selected carboxylic acids (red), substituted phenols (cyan), saccharides (blue) and nitroaromatics (magenta)



35

Figure S3: Graph showing the increase in $\log C^0$ of 2-tridecanone and *cis*-pinonic acid with increasing temperature, as calculated using the SIMPOL.1 method



40

Figure S4: Mass defect plot obtained from the ion signals measured by a CHARON EVR PTR-MS analyzer when limonene/ O_3 SOA was sampled. The points highlighted in orange and purple have been associated with analytes containing a hydroperoxy functional group.