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Supplementary Material

Kinetic Measurements of Cl Atom Reactions with C_5–C_8 Unsaturated Alcohols

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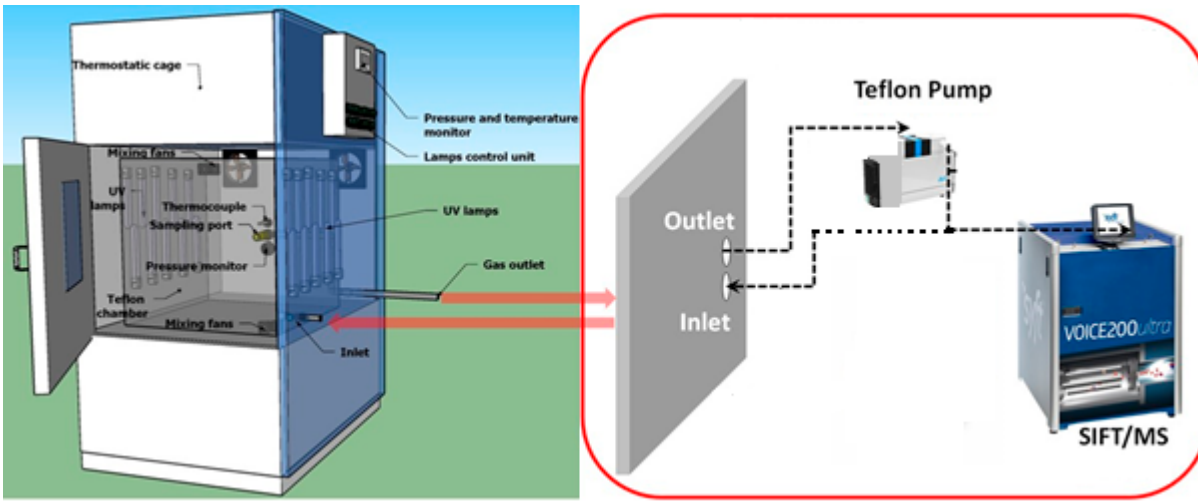


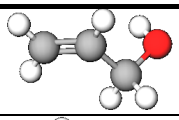
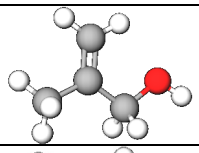
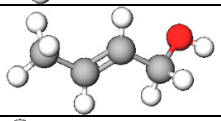
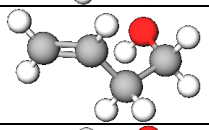
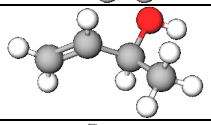
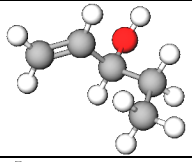
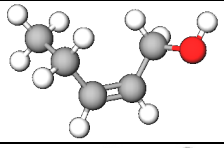
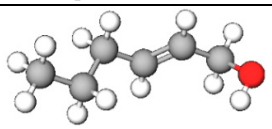
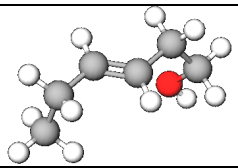
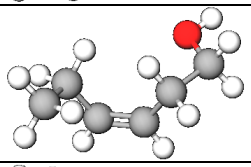
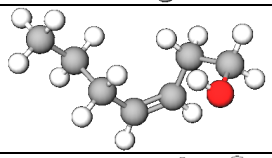
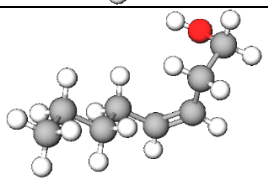
Figure S1. General description of THALAMOS facility.

Table S1. Product ion distributions of the H_3O^+, NO^+ and O_2^+ reactions with the studied unsaturated alcohols and reference compounds (BR—branching ratios of product ions). (Data come from the SIFT-MS library; BR could vary depending on the experimental conditions and working status of the instrument).

Compound	M (g mol^{-1})	H_3O^+			NO^+			O_2^+		
		m/z	Ion	BR (%)	m/z	Ion	BR (%)	m/z	Ion	BR (%)
(Z)-2-penten-1-ol ($C_5H_{10}O$)	86	69	$C_5H_9^+$	100	68	$C_5H_8^+$	4	44	$C_2H_4O^+$	7
					69	$C_5H_9^+$	24	56	$C_3H_4O^+$	3
					85	$C_5H_9O^+$	68	57	$C_3H_5O^+$	56
					86	$C_5H_{10}O^+$	4	68	$C_5H_8^+$	15
								71	$C_4H_7O^+$	4
								86	$C_5H_{10}O^+$	9
									others	6
(E)-2-hexen-1-ol ($C_6H_{12}O$)	100	83	$C_6H_{11}^+$	100	83	$C_6H_{11}^+$	31	44	$C_2H_4O^+$	6
					99	$C_6H_{11}O^+$	55	56	$C_3H_4O^+$	5
					100	$C_6H_{12}O^+$	10	57	$C_3H_5O^+$	44
						others	4	67	$C_5H_7^+$	5
								71	$C_4H_7O^+$	7
								72	$C_4H_8O^+$	4
								82	$C_6H_{10}^+$	15
								100	$C_6H_{12}O^+$	5
									others	9
(E)-3-hexen-1-ol ($C_6H_{12}O$)	100	83	$C_6H_{11}^+$	65	71	$C_5H_{11}^+$	5	67	$C_5H_7^+$	20
		101	$C_6H_{12}OH^+$	35	72	$C_4H_8O^+$	5	69	$C_5H_9^+$	10
					82	$C_6H_{10}^+$	25	70	$C_4H_6O^+$	10
					99	$C_6H_{11}O^+$	50	82	$C_6H_{10}^+$	50
					100	$C_6H_{12}O^+$	15	83	$C_6H_{11}^+$	5
								101	$C_6H_{12}O.H^+$	5
(Z)-3-hexen-1-ol ($C_6H_{12}O$)	100	83	$C_6H_{11}^+$	90	71	$C_4H_7O^+$	10	67	$C_5H_7^+$	30
		101	$C_6H_{12}OH^+$	10	72	$C_4H_8O^+$	30	69	$C_5H_9^+$	5
					82	$C_6H_{10}^+$	30	70	$C_4H_6O^+$	10
					99	$C_6H_{11}O^+$	20	82	$C_6H_{10}^+$	45
					100	$C_6H_{12}O^+$	10	83	$C_6H_{11}^+$	8
								101	$C_6H_{12}O.H^+$	2
1-Octen-3-ol ($C_8H_{16}O$)	128	69	$C_5H_9^+$	8	69	$C_4H_5O^+$	2	57	$C_3H_5O^+$	28
		111	$C_8H_{15}^+$	83	99	$C_6H_{11}O^+$	7	68	$C_5H_8^+$	4
		129	$C_8H_{16}OH^+$	9	111	$C_8H_{15}^+$	29	71	$C_4H_7O^+$	3
					127	$C_8H_{15}O^+$	57	72	$C_4H_8O^+$	24
						others	5	81	$C_6H_9^+$	3
								82	$C_6H_{10}^+$	4
								85	$C_5H_9O^+$	7
								99	$C_6H_{11}O^+$	6
								110	$C_8H_{14}^+$	4
									others	17
THF (C_4H_8O)	72	73	$C_4H_8OH^+$	100	71	$C_4H_7O^+$	100	42	CH_2CO^+ or $C_3H_6^+$	40
								43	CH_3CO^+	5

									or $C_3H_7^+$	
								71	$C_4H_7O^+$	55
Propan-1-ol (C_3H_8O)	60	43	$C_3H_7^+$	90	59	$C_3H_7O^+$	100	31	CH_3O^+	90
		61	$C_3H_9O^+$	10				42	$C_3H_6^+$	10
Octane (C_8H_{18})	114	113	$C_8H_{17}^+$	100	113	$C_8H_{17}^+$	80	114	$C_8H_{18}^+$	30
						others	20		others	70

Table S2. Rate constants for the reactions of Cl atoms with unsaturated alcohols at 298 K and atmospheric pressure (all rate constants are expressed in 10^{-10} cm^3 $molecule^{-1}$ s^{-1}).

Compound	Structure	k_{Alc+Cl}	Reference
2-propen-1-ol		1.72 ± 0.19	[49]
2-methyl-2-propen-1-ol		2.17 ± 0.39	[50]
2-buten-1-ol		3.12 ± 0.64	[50]
		3.90 ± 0.35	[62]
3-buten-1-ol		2.63 ± 0.25	[62]
3-buten-2-ol		1.44 ± 0.17	[49]
1-penten-3-ol		2.35 ± 0.31	[38]
(*Z*)-2-penten-1-ol		3.00 ± 0.49	[38]
		3.00 ± 0.51	This work
(*E*)-2-hexen-1-ol		3.49 ± 0.82	[39]
		3.41 ± 0.63	This work
(*E*)-3-hexen-1-ol		3.42 ± 0.79	[39]
		3.05 ± 0.54	This work
(*Z*)-3-hexen-1-ol		2.94 ± 0.72	[39]
		3.14 ± 0.58	This work
(*Z*)-3-hepten-1-ol		3.80 ± 0.86	[39]
(*Z*)-3-octen-1-ol		4.13 ± 0.68	[39]

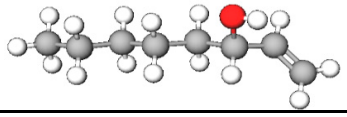
1-octen-3-ol		4.03 ± 0.77	This work

Table S3. Rate constants for the reactions of Cl atoms with alkenes at 298 K and atmospheric pressure (all rate constants are expressed in 10^{-10} cm^3 $molecule^{-1}$ s^{-1}).

Compound	k_{Alc+Cl}	Reference
propene	2.70 ± 0.40	[67]
1-butene	3.52 ± 0.07	[65]
1-pentene	3.97 ± 0.36	[22]
(Z)-3-hexene	4.13 ± 0.51	[61]
1-octene	5.5 ± 0.9	[66]