Supplementary Information (SI) for Environmental Science: Atmospheres.

Comparison of oxidation products generated from the reaction of α-pinene with hydroxyl radicals, chlorine atoms, and bromine atoms measured using ammonium adduct chemical ionization mass spectrometry

Andrew T. Lambe,*[a] Jordan E. Krechmer[a‡], Anita M. Avery[a], Mitchell W. Alton[a], Neil M. Donahue[b], and Manjula R. Canagaratna[a]

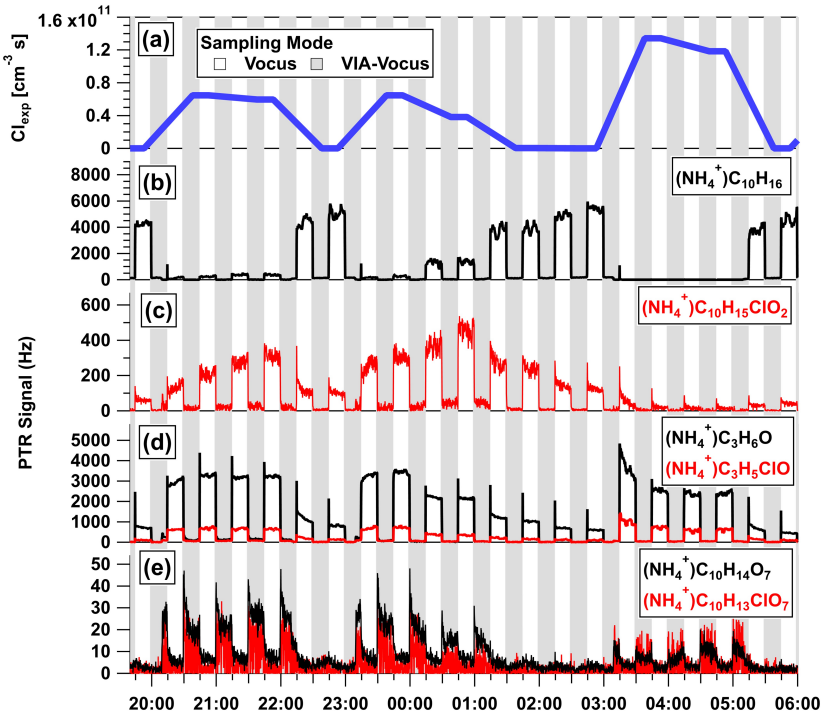

Fig. S1 (a) Time series of Cl exposure (Cl_{exp}) and (b)-(e) selected Vocus signals for representative ammonium adduct ions from an α-pinene/Cl oxidation experiment, showing alternating sampling between Vocus and VIA-Vocus modes (gray and white shaded regions, respectively). (b) $NH_4^+ \cdot C_{10}H_{16}$ (α-pinene) (c) $NH_4^+ \cdot C_{10}H_{15}ClO_2$ (d) $NH_4^+ \cdot C_3H_6O$ and $NH_4^+ \cdot C_3H_5ClO$ (e) $NH_4^+ \cdot C_{10}H_{14}O_7$ and $NH_4^+ \cdot C_{10}H_{13}O_7$. Signals enhanced during Vocus periods suggest higher volatility, while signals higher during VIA-Vocus periods indicate lower volatility.

[a] *Aerodyne Research, Billerica, Massachusetts, United States. E-mail: lambe@aerodyne.com*
[b] *Carnegie Mellon University Center for Atmospheric Particle Studies, Pittsburgh, Pennsylvania, United States.*

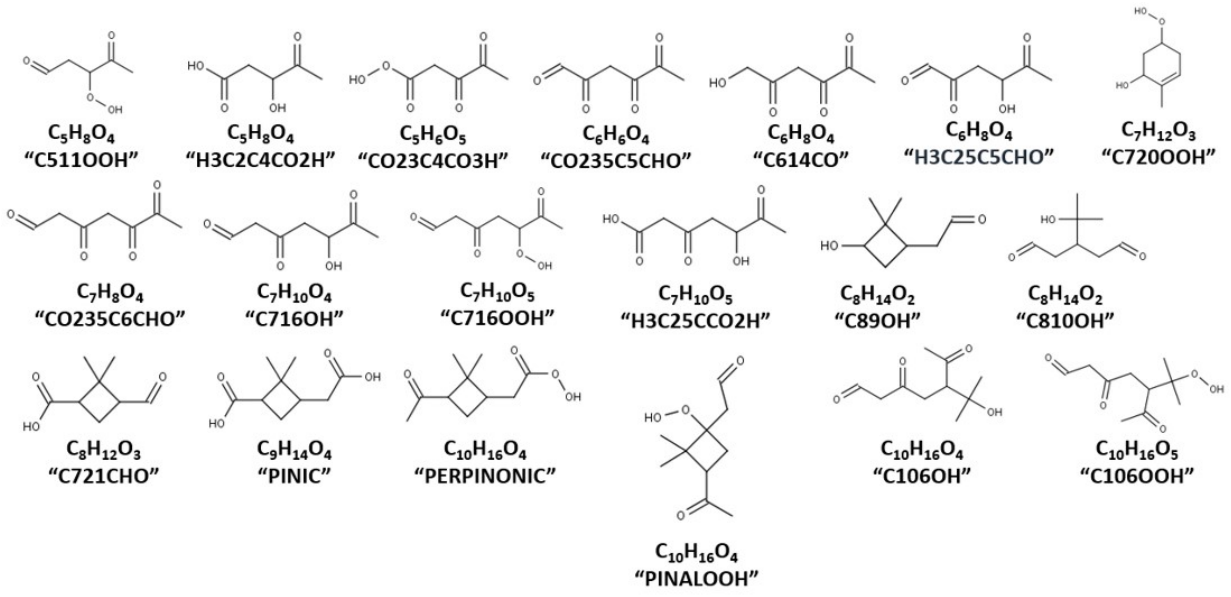

Fig. S2 Molecular formulas, names, and proposed structures of α-pinene oxidation products present in version 3.3.1 of the Master Chemical Mechanism (MCM) [1] and detected with the Vocus using ammonium adduct chemical ionization mass spectrometry in this work.

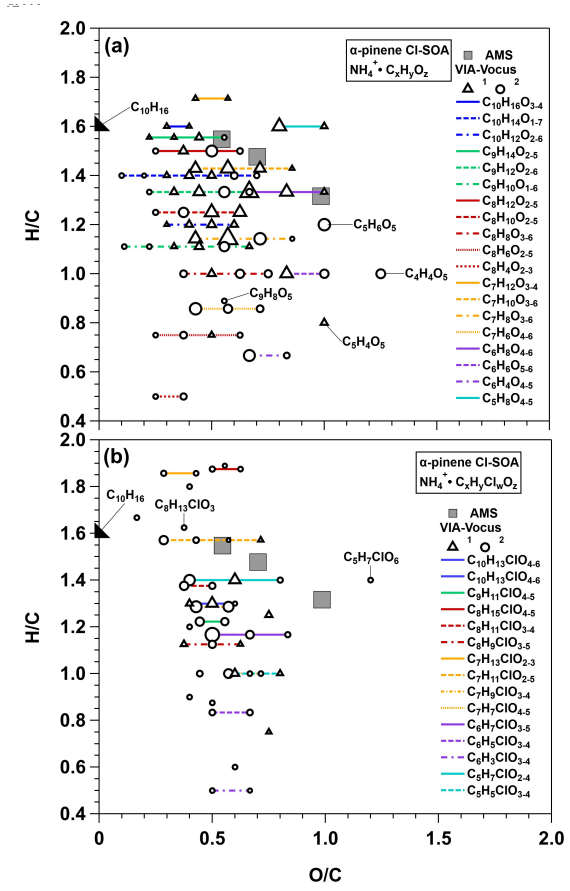

Fig. S3 Van Krevelen diagram showing hydrogen-to-carbon (H/C) and oxygen-to-carbon (O/C) ratios of SOA generated from the Cl oxidation of pinene. Data from an Aerosol Mass Spectrometer (AMS, gray squares) show bulk SOA elemental composition, while data from the VIA-Vocus identify individual (a) non-chlorinated and (b) chlorinated molecular formulas of Factor 4 components. Colored lines show homologous series of $C_xH_yO_z$ and $C_xH_yClO_z$ oxidation products. Additional figure notes: [1]Molecular formulas of oxidation products not included in the MCM[2], [3]Molecular formulas not previously reported in α-pinene/Cl studies.

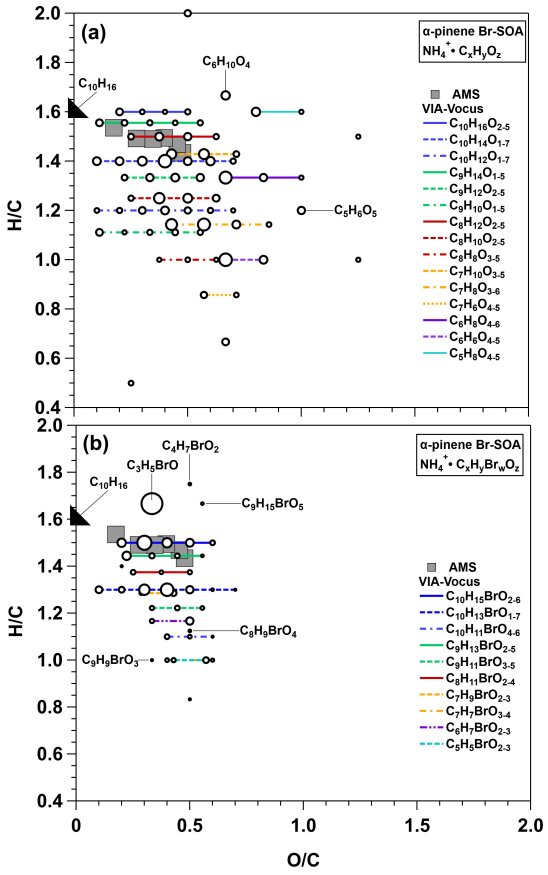

Fig. S4 Van Krevelen diagram showing hydrogen-to-carbon (H/C) and oxygen-to-carbon (O/C) ratios of SOA generated from the Br oxidation of pinene. Data from an Aerosol Mass Spectrometer (AMS, gray squares) show bulk SOA elemental composition, while data from the VIA-Vocus identify individual (a) non-brominated and (b) brominated molecular formulas of Factor 4 components. Colored lines show homologous series of $C_xH_yO_z$ and $C_xH_yBrO_z$ oxidation products.

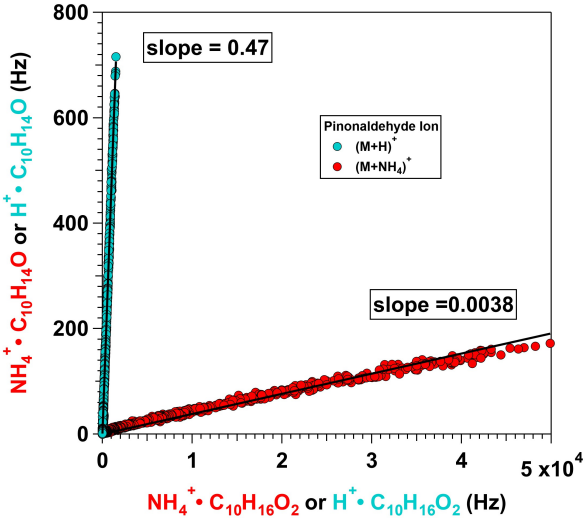

Fig. S5 Scatter plot of $NH_4^+ \cdot C_{10}H_{14}O$ versus $NH_4^+ \cdot C_{10}H_{16}O_2$ and $H^+ \cdot C_{10}H_{14}O$ versus $H^+ \cdot C_{10}H_{16}O_2$ signals detected in a 2-[(1R,3R)-3-acetyl-2,2-dimethylcyclobutyl]acetaldehyde (pinonaldehyde) standard (CAS #58558-22-8, 97.2% purity, Alfa Chemistry) with Vocus PTR following reaction with ammonium and hydronium reagent ions.

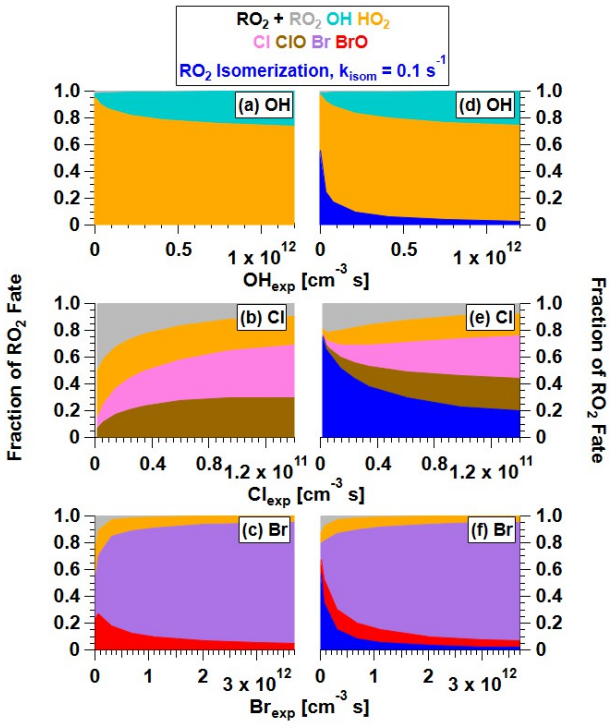

Fig. S6 Comparison of the modeled fates of the organic peroxy radical (RO_2) as a function of oxidant exposure during the OH, Cl, and Br oxidation of α-pinene in the (a-c) absence and (d-f) presence of isomerization/autooxidation reactions, with an assumed first-order isomerization rate coefficient (k_{isom} = 0.1 s^{-1}). Reactions and kinetic rate coefficients used in these calculations are provided in Table S2.

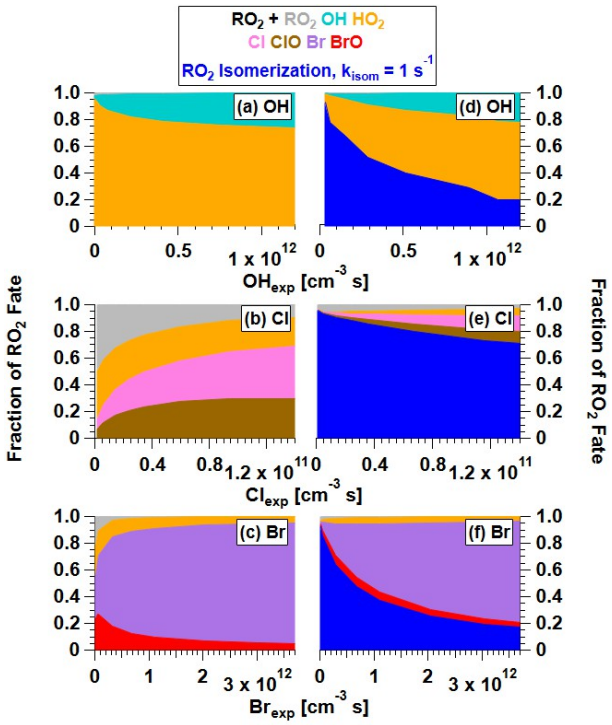

Fig. S7 Comparison of the modeled fates of the organic peroxy radical (RO_2) as a function of oxidant exposure during the OH, Cl, and Br oxidation of α-pinene in the (a-c) absence and (d-f) presence of isomerization/autooxidation reactions, with an assumed first-order isomerization rate coefficient (k_{isom} = 1 s^{-1}). Reactions and kinetic rate coefficients used in these calculations are provided in Table S2.

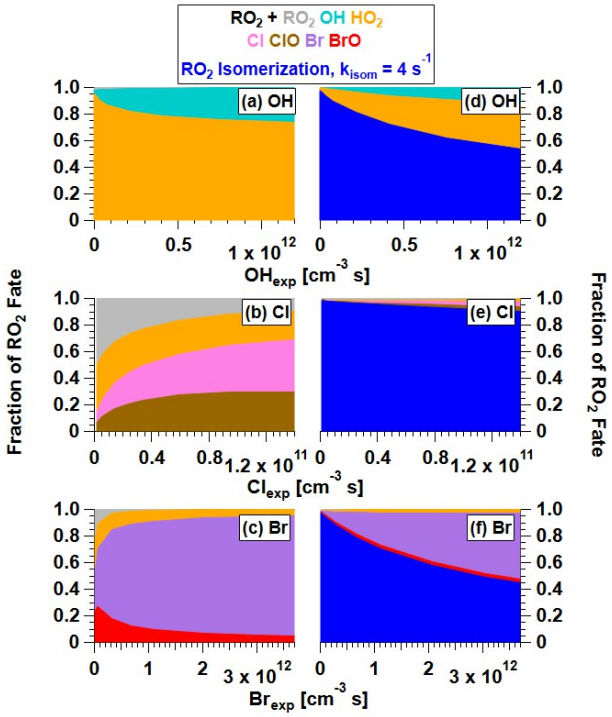

Fig. S8 Comparison of the modeled fates of the organic peroxy radical (RO_2) as a function of oxidant exposure during the OH, Cl, and Br oxidation of α-pinene in the (a-c) absence and (d-f) presence of isomerization/autooxidation reactions, with an assumed first-order isomerization rate coefficient (k_{isom} = 4 s^{-1}). Reactions and kinetic rate coefficients used in these calculations are provided in Table S2.

Table S1 KinSim mechanism used to model Cl and Br formation and destruction in the OFR.

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	A_∞	E_∞	n_∞	A_0	E_0	n_0	References
Cl_2	HV254	2 Cl			7.26×10^{-22}	0	0	0	0	0	3
Cl_2	HV313	2 Cl			2.032×10^{-19}	0	0	0	0	0	3
Cl_2	HV369	2 Cl			8.828×10^{-20}	0	0	0	0	0	3
Cl_2	$O(^1D)$	Cl_2	$O(^3P)$		2.19×10^{-10}	0	0	0	0	0	4
Cl_2	$O(^1D)$	ClO	Cl		1.99×10^{-10}	0	0	0	0	0	5
Cl_2	$O(^3P)$	ClO	Cl		4.17×10^{-12}	1370	0	0	0	0	6
Cl_2	OH	HOCl	Cl		3.6×10^{-12}	1200	0	0	0	0	6
Cl_2	Cl	Cl_3			1.51×10^{-16}	0	0	0	0	0	7
Cl_2	Br	BrCl	Cl		1.1×10^{-15}	0	0	0	0	0	8
Cl_2	ClCO	$COCl_2$	Cl		4.18×10^{-12}	1490.14	0	0	0	0	9
$C_2Cl_2O_2$	HV254	2 Cl	2 CO		2.76×10^{-19}	0	0	0	0	0	10
$C_2Cl_2O_2$	HV313	2 Cl	2 CO		8.19×10^{-20}	0	0	0	0	0	10
$C_2Cl_2O_2$	Cl	Cl_2	CO	COCl	4×10^{-14}	0	0	0	0	0	11
Br_2	HV369	2 Br			1.78×10^{-19}	0	0	0	0	0	12
Br_2	HV421	2 Br			6.45×10^{-19}	0	0	0	0	0	12
Br_2	$O(^3P)$	BrO	Br		5.11×10^{-13}	-989	0	0	0	0	13
Br_2	OH	Br	HOBr		2×10^{-11}	240.558	0	0	0	0	6
Br_2	Cl	Br	BrCl		2.3×10^{-10}	134.713	0	0	0	0	14
$C_2Br_2O_2$	HV254	2 Br	2 CO		1.68×10^{-18}	0	0	0	0	0	15
$C_2Br_2O_2$	Br	Br_2	CO	COBr	4×10^{-14}	0	0	0	0	0	16
O_3	HV254	O_2	$O(^1D)$		1.03×10^{-17}	0	0	0	0	0	17
O_3	HV313	O_2	$O(^1D)$		6.84×10^{-20}	0	0	0	0	0	17
O_3	HV369	O_2	$O(^1D)$		3.59×10^{-23}	0	0	0	0	0	17
O_3	HV421	O_2	$O(^1D)$		6.47×10^{-23}	0	0	0	0	0	17
O_3	Cl	ClO	O_2		2.3×10^{-11}	200	0	0	0	0	6
O_3	ClO	O_2	OClO		1×10^{-18}	0	0	0	0	0	6
O_3	ClO	O_2	ClOO		1.5×10^{-17}	0	0	0	0	0	6
O_3	OClO	O_2	ClO_3		2.1×10^{-12}	4700	0	0	0	0	6
O_3	Cl_2O_2	O_2	ClOO	ClO	1×10^{-19}	0	0	0	0	0	6
O_3	Br	O_2	BrO		1.7E-11	799.856	0	0	0	0	6
O_3	BrO	2 O_2	Br		2E-17	0	0	0	0	0	18
O_3	BrO_2				5E-16	0	0	0	0	0	19
Cl	OH	HCl	$O(^3P)$		9.8×10^{-12}	2860.24	0	0	0	0	20
Cl	HO_2	HCl	O_2		1.4×10^{-11}	-270	0	0	0	0	6
Cl	HO_2	OH	ClO		6.3×10^{-11}	570.123	0	0	0	0	6
Cl	Cl	Cl_2			6.15E-34	-905.701	0	0	0	0	20
Cl	O_2	ClOO			0	0	0	1.4×10^{-33}	0	3.9	6
Cl	H_2	HCl	H		3.9×10^{-11}	2310.56	0	0	0	0	6
Cl	H_2O_2	HCl	HO_2		1.1×10^{-11}	980	0	0	0	0	6
Cl	CO	ClCO			3.4×10^{-14}	0	0	0	0	0	21
ClCO		Cl	CO		4.1×10^{-10}	2960.07	0	0	0	0	6
Cl	ClCO	Cl_2	CO		2.16×10^{-9}	1670.68	0	0	0	0	20
ClO	HV254	Cl	$O(^3P)$		4.25×10^{-18}	0	0	0	0	0	22
ClO	HV313	Cl	$O(^3P)$		3.25×10^{-19}	0	0	0	0	0	22
ClO	$O(^3P)$	Cl	O_2		2.5×10^{-11}	-109.454	0	0	0	0	6
ClO	OH	HCl	O_2		1.2×10^{-12}	0	0	0	0	0	6
ClO	OH	HO_2	Cl		1.9×10^{-11}	0	0	0	0	0	6
ClO	HO_2	O_2	HOCl		4.8×10^{-13}	700.024	0	0	0	0	23
ClO	HO_2	HCl	O_3		2.01×10^{-14}	0	0	0	0	0	24
ClO	Cl	Cl_2	$O(^3P)$		1.74×10^{-12}	4589.85	0	0	0	0	20
ClO	ClO	OClO	Cl		3.5×10^{-13}	1370	0	0	0	0	6
ClO	ClO	Cl_2O_2			1×10^{-11}	0	0	2.05×10^{-32}	0	4	6

Table S1 KinSim mechanism used to model Cl and Br formation and destruction in the OFR (continued).

ClO	ClO	ClOO	Cl		8.06×10^{-15}	0	0	0	0	0	6
ClO	ClO	O_2	2 Cl		3×10^{-11}	2450	0	0	0	0	25
ClO	ClO	O_2	Cl_2		1×10^{-12}	1590	0	0	0	0	6
ClO	BrO	OClO	Br		1.6×10^{-12}	-430.599	0	0	0	0	6
ClO	BrO	ClOO	Br		2.9×10^{-12}	-220.111	0	0	0	0	6
ClO	BrO	BrCl	O_2		5.8×10^{-13}	-169.593	0	0	0	0	6
OClO	HV254	ClO	$O(^3P)$		3.49×10^{-19}	0	0	0	0	0	22
OClO	HV313	ClO	$O(^3P)$		1.74×10^{-18}	0	0	0	0	0	22
OClO	HV369	ClO	$O(^3P)$		9.03×10^{-18}	0	0	0	0	0	22
OClO	$O(^3P)$	ClO	O_2		2.4×10^{-12}	960	0	0	0	0	6
OClO	$O(^3P)$	ClO_3			3.11×10^{-11}	0	1	1.91E-31	0	0	6
OClO	OH	O_2	HOCl		1.4×10^{-12}	-600	0	0	0	0	6
OClO	Cl	2 ClO			3.2×10^{-11}	-169.593	0	0	0	0	6
OClO	ClO	Cl_2O_3			2.4×10^{-11}	0	0	6.2×10^{-32}	0	4.7	6
OClO	Br	ClO	BrO		2.7×10^{-11}	1300.22	0	0	0	0	6
ClOO	HV254	ClO	$O(^3P)$		1.24×10^{-17}	0	0	0	0	0	26
ClOO		Cl	O_2		0	0	0	2.8×10^{-10}	1820	0	6
ClOO	H	ClO	OH		5.65×10^{-11}	0	0	0	0	0	20
ClOO	$O(^3P)$	ClO	O_2		4.98×10^{-11}	0	0	0	0	0	27
ClOO	Cl	Cl_2	O_2		2.3×10^{-10}	0	0	0	0	0	23
ClOO	Cl	2 ClO			1.2×10^{-11}	0	0	0	0	0	23
ClOO	Br	O_2	BrCl		5.15×10^{-14}	0	0	0	0	0	28
Cl_2O	HV254	ClO	Cl		1.84×10^{-18}	0	0	0	0	0	29,30
Cl_2O	HV313	Cl_2	Cl		3.94×10^{-19}	0	0	0	0	0	29,30
Cl_2O	HV369	Cl_2	Cl		5.43×10^{-21}	0	0	0	0	0	29,30
Cl_2O	H	ClO	HCl		4.1×10^{-11}	0	0	0	0	0	31
Cl_2O	$O(^3P)$	2 ClO			2.7×10^{-11}	530	0	0	0	0	6
Cl_2O	OH	HOCl	ClO		5.1×10^{-12}	-100	0	0	0	0	32
Cl_2O	Cl	Cl_2	ClO		6.20×10^{-11}	129.901	0	0	0	0	6
Cl_2O	ClO	Cl_2	ClOO		4.32×10^{-16}	0	0	0	0	0	27
Cl_2O	ClO	Cl_2	Cl	O_2	1.08×10^{-15}	0	0	0	0	0	27
Cl_2O	Br	ClO	BrCl		2.1×10^{-11}	470.291	0	0	0	0	6
Cl_2O_2	HV254	ClOO	Cl		6.01×10^{-18}	0	0	0	0	0	30,33
Cl_2O_2	HV313	ClOO	Cl		3.81×10^{-19}	0	0	0	0	0	30,33
Cl_2O_2	HV369	ClOO	Cl		4.76×10^{-20}	0	0	0	0	0	30,33
Cl_2O_2		2 ClO			3.7×10^{-7}	7690.64	0	0	0	0	6
Cl_2O_2	OH	HOCl	ClOO		6×10^{-13}	-670	0	0	0	0	32
Cl_2O_2	Cl	Cl_2	ClOO		7.6×10^{-11}	-65	0	0	0	0	6
Cl_2O_2	Br	ClOO	BrCl		5.9×10^{-12}	169.593	0	0	0	0	6
Cl_2O_3	HV254				1.443×10^{-17}	0	0	0	0	0	22
Cl_2O_3	HV313				1.86×10^{-18}	0	0	0	0	0	22
Cl_2O_3		ClO	OClO		1.4×10^{-10}	3810.44	0	0	0	0	6
BrO	HV369	Br	$O(^3P)$		1.01×10^{-18}	0	0	0	0	0	34
BrO	$O(^3P)$	BrO_2			5×10^{-11}	0	0	0	0	0	34
BrO	$O(^3P)$	Br	O_2		1.9×10^{-11}	-230	0	0	0	0	6
BrO	OH	O_2	HBr		1×10^{-12}	0	0	0	0	0	35
BrO	OH				1.8×10^{-11}	-250.18	0	0	0	0	6
BrO	HO_2	O_2	HOBr		6.19×10^{-12}	500.361	0	0	0	0	36
BrO	BrO	Br	BrO_2		5.25×10^{-11}	449.844	0	0	0	0	37
BrO	BrO	O_2	2 Br		2.7×10^{-12}	0	0	0	0	0	6
BrO	BrO	Br_2	O_2		2.5×10^{-14}	0	0	0	0	0	6
BrO_2	HV421	BrO	$O(^3P)$		5.70×10^{-18}	0	0	0	0	0	22
BrO_2	$O(^3P)$	BrO	O_2		4.25×10^{-12}	0	0	0	0	0	34

Table S1 KinSim mechanism used to model Cl and Br formation and destruction in the OFR (continued).

BrO_2	Br			5×10^{-11}	0	0	0	0	0	34
BrO_2	ClO			1.5×10^{-13}	0	0	0	0	0	38
BrO_2	OClO			6×10^{-14}	0	0	0	0	0	38
HCl	H	H_2	Cl	1.32×10^{-11}	1710.37	0	0	0	0	20
HCl	$O(^1D)$	Cl	OH	1×10^{-10}	0	0	0	0	0	39
HCl	$O(^1D)$	ClO	H	3.6×10^{-11}	0	0	0	0	0	39
HCl	$O(^3P)$	Cl	OH	1×10^{-11}	3300	0	0	0	0	23
HCl	OH	Cl	H_2O	1.72×10^{-12}	229.733	0	0	0	0	6
HOCl	HV254	OH	Cl	1.46×10^{-19}	0	0	0	0	0	40
HOCl	HV313	OH	Cl	5.84×10^{-20}	0	0	0	0	0	40
HOCl	HV369	OH	Cl	9.19×10^{-21}	0	0	0	0	0	40
HOCl	H	HCl	OH	6.71×10^{-13}	0	0	0	0	0	41
HOCl	$O(^3P)$	ClO	OH	1.7×10^{-13}	0	0	0	0	0	6
HOCl	OH	ClO	H_2O	3.01×10^{-12}	500	0	0	0	0	23
HOCl	Cl	ClO	HCl	3.4×10^{-12}	130	0	0	0	0	23
HOCl	Cl	OH	Cl_2	3.4×10^{-13}	0	0	0	0	0	41
HBr	H	Br	H_2	8.32×10^{-12}	81.7898	1.05	0	0	0	42
HBr	$O(^1D)$			1.5×10^{-10}	0	0	0	0	0	23
HBr	$O(^3P)$	Br	OH	5.8×10^{-12}	1500	0	0	0	0	23
HBr	OH	Br	H_2O	6.7×10^{-12}	-155.16	0	0	0	0	6
HBr	Cl	Br	HCl	7.8×10^{-12}	0	0	0	0	0	20
HBr	ClO	Br	HOCl	5.60×10^{-15}	0	0	0	0	0	43
HBr	BrO	Br	HOBr	6.19×10^{-15}	0	0	0	0	0	43
HOBr	HV254	OH	Br	6.19×10^{-20}	0	0	0	0	0	22
HOBr	HV369	OH	Br	9.32×10^{-20}	0	0	0	0	0	22
HOBr	HV421	OH	Br	9.67×10^{-21}	0	0	0	0	0	22
HOBr	$O(^3P)$	BrO	OH	1.2×10^{-10}	430.6	0	0	0	0	6
HOBr	OH			5×10^{-13}	0	0	0	0	0	44
HOBr	Cl	BrCl	OH	8×10^{-11}	0	0	0	0	0	44
BrCl	HV254	Br	Cl	3.24×10^{-20}	0	0	0	0	0	12
BrCl	HV313	Br	Cl	2.51×10^{-20}	0	0	0	0	0	12
BrCl	HV369	Br	Cl	3.96×10^{-19}	0	0	0	0	0	12
BrCl	HV421	Br	Cl	1.78×10^{-19}	0	0	0	0	0	12
BrCl	$O(^3P)$	BrO	Cl	2.09×10^{-11}	0	0	0	0	0	45
BrCl	OH			1.5×10^{-12}	0	0	0	0	0	44
BrCl	Cl	Cl_2	Br	1.45×10^{-11}	0	0	0	0	0	46
BrCl	Br	Br_2	Cl	3.32×10^{-15}	0	0	0	0	0	20

Table S2 KinSim mechanism used to model peroxy radical RO_2 formation and destruction in the OFR.

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	A_∞	E_∞	n_∞	A_0	E_0	n_0	References
APINENE	OH	RO_2	H_2O		1.2×10^{-11}	-443.83	0	0	0	0	47
APINENE	Cl	RO_2	HCl		4.7×10^{-10}	0	0	0	0	0	48
APINENE	Br	RO_2	HBr		2.23×10^{-11}	0	0	0	0	0	49
RO_2		$RO_{2,Isom}$			0, 0.1, 1, or 4	0	0	0	0	0	50,51
RO_2	RO_2	2RO	O_2		2.55×10^{-13}	0	0	0	0	0	1
RO_2	RO_2	ROH	R(O)	O_2	1.09×10^{-13}	0	0	0	0	0	1
RO_2	$RO_{2,Isom}$	2RO	O_2		2.55×10^{-13}	0	0	0	0	0	1
RO_2	$RO_{2,Isom}$	ROH	R(O)	O_2	1.09×10^{-13}	0	0	0	0	0	1
RO_2	HO_2	ROOH			2.66×10^{-13}	-1300	0	0	0	0	1
$RO_{2,Isom}$	HO_2	ROOH			2.66×10^{-13}	-1300	0	0	0	0	1
RO_2	OH	ROH	O_2		1×10^{-10}	0	0	0	0	0	52
$RO_{2,Isom}$	OH	ROH	O_2		1×10^{-10}	0	0	0	0	0	52
RO	O_2	PINAL	HO_2		1×10^{6}	0	0	0	0	0	1
RO_2	Cl	RO	ClO		1.6×10^{-10}	0	0	0	0	0	23
$RO_{2,Isom}$	Cl	RO	ClO		1.6×10^{-10}	0	0	0	0	0	23
RO_2	ClO	RO	ClO_2		4.9×10^{-12}	329.565	0	0	0	0	18
$RO_{2,Isom}$	ClO	RO	ClO_2		4.9×10^{-12}	329.565	0	0	0	0	18
RO_2	ClO	ROCl	O_2		2.6×10^{-13}	-259.803	0	0	0	0	18
$RO_{2,Isom}$	ClO	ROCl	O_2		2.6×10^{-13}	-259.803	0	0	0	0	18
RO	O_2	CHLOROPINAL	HO_2		3.3×10^{5}	0	0	0	0	0	
RO	O_2	PINAL	Cl		6.7×10^{5}	0	0	0	0	0	
RO_2	Br	RO	BrO		1.6×10^{-10}	0	0	0	0	0	
$RO_{2,Isom}$	Br	RO	BrO		1.6×10^{-10}	0	0	0	0	0	
RO_2	BrO	RO2H	HOBr		4.6×10^{-13}	-797.45	0	0	0	0	53
$RO_{2,Isom}$	BrO	RO2H	HOBr		4.6×10^{-13}	-797.45	0	0	0	0	53
RO	O_2	BROMOPINAL	HO_2		6.6×10^{5}	0	0	0	0	0	
RO	O_2	PINAL	Br		3.4×10^{5}	0	0	0	0	0	
ROOH	OH	RO_2			1.83×10^{-11}		0	0	0	0	1
ROOH	Cl	RO_2			1.83×10^{-10}		0	0	0	0	
ROOH	Br	RO_2			2.23×10^{-13}		0	0	0	0	
ROH	OH	RO_2			1.49×10^{-11}		0	0	0	0	1
ROH	Cl	RO_2			1.49×10^{-10}		0	0	0	0	
ROH	Br	RO_2			2.23×10^{-13}		0	0	0	0	
R(O)	OH	RO_2			1.49×10^{-11}		0	0	0	0	1
R(O)	Cl	RO_2			1.49×10^{-10}		0	0	0	0	
R(O)	Br	RO_2			2.23×10^{-13}		0	0	0	0	
PINAL	OH	RO_2			4.5×10^{-12}	-600.192	0	0	0	0	54
PINAL	Cl	RO_2			3.86×10^{-10}	0	0	0	0	0	55
CHLOROPINAL	Cl	RO_2			3.86×10^{-10}	0	0	0	0	0	
PINAL	Br	RO_2			3.9×10^{-12}	0	0	0	0	0	56
BROMOPINAL	Br	RO_2			3.9×10^{-12}	0	0	0	0	0	

References

1 M. Jenkin, S. Saunders and M. Pilling, *Atmospheric Environment*, 1997, **31**, 81–104.

2 C. G. Masoud and L. Hildebrandt Ruiz, *ACS Earth Space Chem.*, 2021, **5**, 2307–2319.

3 D. Maric, J. Burrows, R. Meller and G. Moortgat, *Journal of Photochemistry and Photobiology A: Chemistry*, 1993, **70**, 205 – 214.

4 I. S. Fletcher and D. Husain, *Berichte der Bunsengesellschaft für physikalische Chemie*, 1976, **80**, 982–985.

5 K. Freudenstein and D. Biedenkapp, *Colloid and Polymer Science*, 1977, **255**, 928–928.

6 R. Atkinson, D. L. Baulch, R. A. Cox, J. N. Crowley, R. F. Hampson, R. G. Hynes, M. E. Jenkin, M. J. Rossi and J. Troe, *Atmospheric Chemistry and Physics*, 2007, **7**, 981–1191.

7 E. Hutton and M. Wright, *Trans. Faraday Soc.*, 1965, **61**, 78–89.

8 D. A. Dolson and S. R. Leone, *The Journal of Physical Chemistry*, 1987, **91**, 3543–3550.

9 W. G. Burns and F. S. Dainton, *Trans. Faraday Soc.*, 1952, **48**, 39–52.

10 B. Ghosh, D. K. Papanastasiou and J. B. Burkholder, *The Journal of Chemical Physics*, 2012, **137**, 164315.

11 A. V. Baklanov and L. N. Krasnoperov, *J. Phys. Chem. A*, 2001, **105**, 97–103.

12 D. Maric, J. Burrows and G. Moortgat, *Journal of Photochemistry and Photobiology A: Chemistry*, 1994, **83**, 179 – 192.

13 M. H. Harwood, D. M. Rowley, R. A. Cox and R. L. Jones, *J. Phys. Chem. A*, 1998, **102**, 1790–1802.

14 Y. Bedjanian, G. Laverdet and G. Le Bras, *J. Phys. Chem. A*, 1998, **102**, 953–959.

15 H. Shimada, R. Shimada and Y. Kanda, *Bulletin of the Chemical Society of Japan*, 1968, **41**, 1289–1295.

16 C.-C. Wu, H.-C. Lin, Y.-B. Chang, P.-Y. Tsai, Y.-Y. Yeh, H. Fan, K.-C. Lin and J. S. Francisco, *The Journal of Chemical Physics*, 2011, **135**, 234308.

17 J. Burrows, A. Richter, A. Dehn, B. Deters, S. Himmelmann, S. Voigt and J. Orphal, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 1999, **61**, 509–517.

18 R. Atkinson, D. Baulch, R. Cox, J. Crowley, J. Hampson, R.F, J. Kerr, M. Rossi and J. Troe, *IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry - Web Version*, 2001.

19 Z. Li, *J. Phys. Chem. A*, 1999, **103**, 1206–1213.

20 D. L. Baulch, J. Duxbury, S. J. Grant and D. C. Montague, *J. Phys. Chem. Ref. Data*, 1981, **10**, year.

21 A. D. Hewitt, K. M. Brahan, G. D. Boone and S. A. Hewitt, *International Journal of Chemical Kinetics*, 1996, **28**, 763–771.

22 S. Sander, R. Friedl, D. Golden, M. Kurylo, G. Moortgat, H. Keller-Rudek, P. Wine, A. R. Ravishankara, C. Kolb, M. Molina, B. Finlayson-Pitts, R. Huie and V. Orkin, *JPL Publication*, 2006, 1–523.

23 W. B. DeMore, S. P. Sander, D. M. Golden, R. F. Hampson, M. J. Kurylo, C. J. Howard, A. R. Ravishankara, C. E. Kolb and M. J. Molina, *JPL Publication 97-4*, 1997.

24 R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, J. A. Kerr (Chairman) and J. Troe, *Journal of Physical and Chemical Reference Data*, 1989, **18**, 881–1097.

25 A. Horowitz, D. Bauer, J. N. Crowley and G. K. Moortgat, *Geophysical Research Letters*, 1993, **20**, 1423–1426.

26 H. S. Johnston, E. D. Morris and J. Van den Bogaerde, *J. Am. Chem. Soc.*, 1969, **91**, 7712–7727.

27 N. Basco, S. K. Dogra and R. G. W. Norrish, *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 1971, **323**, 401–415.

28 M. A. A. Clyne, J. A. Coxon and J. W. Linnett, *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 1967, **298**, 424–452.

29 C. M. Nelson, T. A. Moore, M. Okumura and T. K. Minton, *The Journal of Chemical Physics*, 1994, **100**, 8055–8064.

30 D. K. Papanastasiou, K. J. Feierabend and J. B. Burkholder, *The Journal of Chemical Physics*, 2011, **134**, 204310.

31 S. J. Wategaonkar and D. W. Setser, *The Journal of Chemical Physics*, 1989, **90**, 251–264.

32 J. C. Hansen, R. R. Friedl and S. P. Sander, *J. Phys. Chem. A*, 2008, **112**, 9229–9237.

33 T. A. Moore, M. Okumura, J. W. Seale and T. K. Minton, *J. Phys. Chem. A*, 1999, **103**, 1691–1695.

34 N. Butkovskaya, I. Morozov, V. Tal'rose and E. Vasiliev, *Chemical Physics*, 1983, **79**, 21–30.

35 Y. Bedjanian, V. Riffault, G. Le Bras and G. Poulet, *J. Phys. Chem. A*, 2001, **105**, 6154–6166.

36 W. DeMore, S. Sander, D. Golden, R. Hampson, M. Kurylo, C. Howard, A. Ravishankara, C. Kolb and M. Molina, *JPL Publication 94-26*, 1994.

37 M. A. A. Clyne and H. W. Cruse, *Trans. Faraday Soc.*, 1970, **66**, 2214–2226.

38 Z. Li, G. R. Jeong and E. C. Person, *International Journal of Chemical Kinetics*, 2002, **34**, 430–437.

39 A. Chichinin, *Chemical Physics Letters - CHEM PHYS LETT*, 2000, **316**, 425–432.

40 R. J. Barnes, A. Sinha and H. A. Michelsen, *J. Phys. Chem. A*, 1998, **102**, 8855–8859.

41 R. Vogt and R. N. Schindler, *Berichte der Bunsengesellschaft für physikalische Chemie*, 1993, **97**, 819–829.

42 M. Seakins, P.W.; Pilling, *J. Phys. Chem.*, 1991, 9878–9881.
43 A. A. Turnipseed, J. W. Birks and J. G. Calvert, *J. Phys. Chem.*, 1991, **95**, 4356–4364.
44 A. Kukui, U. Kirchner, T. Benter and R. N. Schindler, *ChemInform*, 1996, **27**, year.
45 M. A. A. Clyne, P. B. Monkhouse and L. W. Townsend, *International Journal of Chemical Kinetics*, 1976, **8**, 425–449.
46 M. A. A. Clyne and H. W. Cruse, *J. Chem. Soc., Faraday Trans. 2*, 1972, **68**, 1377–1387.
47 R. Atkinson, *Chemical Reviews*, 1986, **86**, 69–201.
48 B. J. Finlayson-Pitts, C. J. Keoshian, B. Buehler and A. A. Ezell, *International Journal of Chemical Kinetics*, 1999, **31**, 491–499.
49 A. Bierbach, I. Barnes and K. H. Becker, *Int. J. Chem. Kinet.*, 1996, **28**, 565–577.
50 F. Bianchi, T. Kurtén, M. Riva, C. Mohr, M. P. Rissanen, P. Roldin, T. Berndt, J. D. Crounse, P. O. Wennberg, T. F. Mentel, J. Wildt, H. Junninen, T. Jokinen, M. Kulmala, D. R. Worsnop, J. A. Thornton, N. Donahue, H. G. Kjaergaard and M. Ehn, *Chemical Reviews*, 2019, **119**, 3472–3509.
51 L. Xu, K. H. Møller, J. D. Crounse, R. V. Otkjær, H. G. Kjaergaard and P. O. Wennberg, *J. Phys. Chem. A*, 2019, **123**, 1661–1674.
52 C. Fittschen, *Chemical Physics Letters*, 2019, **725**, 102–108.
53 S. Enami, T. Yamanaka, T. Nakayama, S. Hashimoto, M. Kawasaki, D. E. Shallcross, Y. Nakano and T. Ishiwata, *J. Phys. Chem. A*, 2007, **111**, 3342–3348.
54 M. E. Davis, R. K. Talukdar, G. Notte, G. B. Ellison and J. B. Burkholder, *Environ. Sci. Technol.*, 2007, **41**, 3959–3965.
55 B. Srinivasulu, G.; Rajakumar, *Journal of Chemical Sciences*, 2016, **128**, 977–989.
56 B. Nozière and I. Barnes, *Journal of Geophysical Research: Atmospheres*, 1998, **103**, 25587–25597.