Supplement to Technical note: Gas-phase nitrate radical generation via irradiation of aerated ceric ammonium nitrate mixtures

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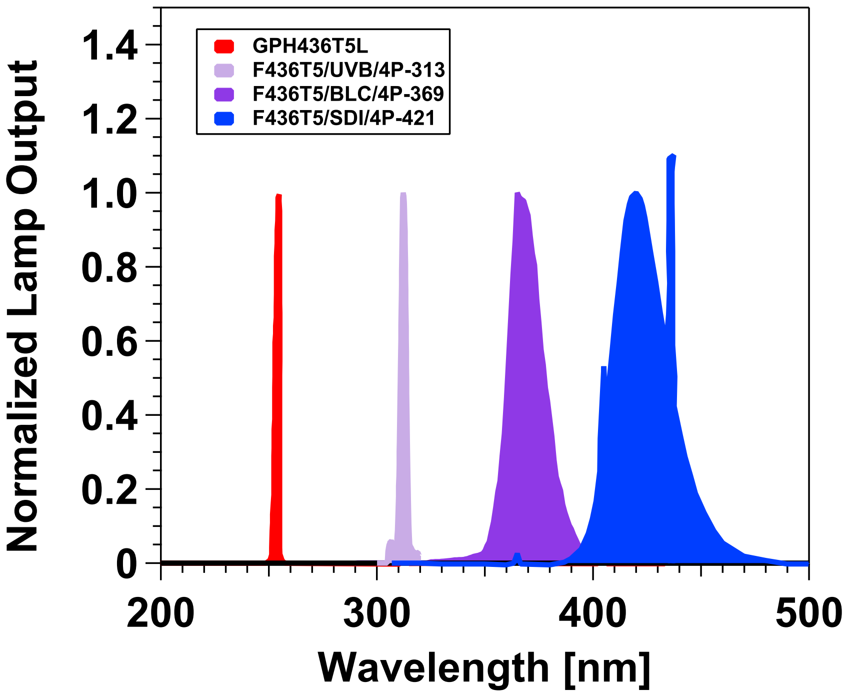


Figure S1. Normalized emission spectra for low-pressure GPH436T5L/4P, F436T5/UVB/4P-313, F436T5/BLC/4P-369, and F436T5/SDI/4P-421 mercury lamps used in this study. Spectra are provided by the manufacturer (GPH436T5L/4P: Light Sources Inc.; all others: LCD Lighting, Inc.)

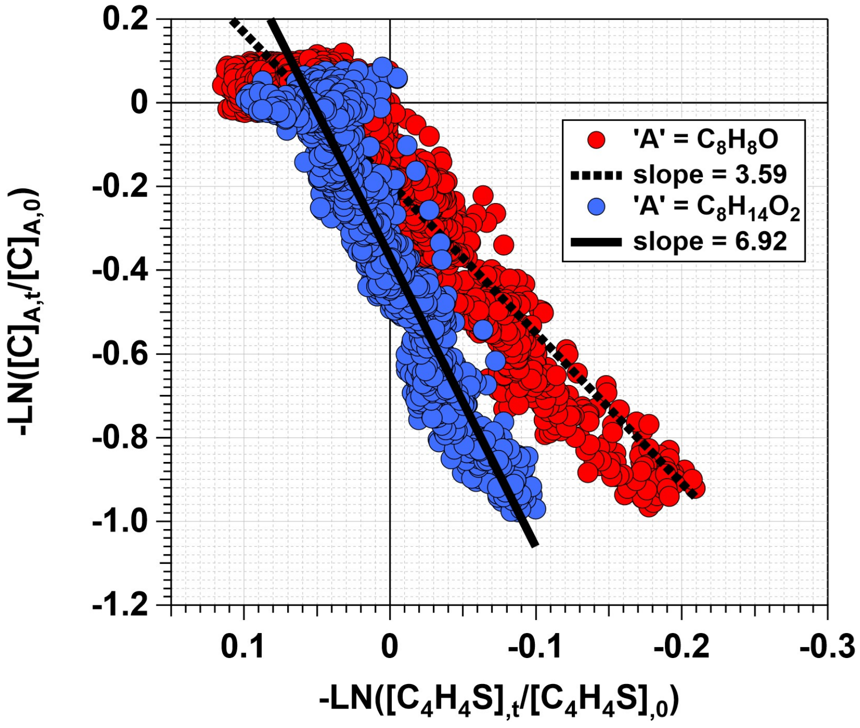


Figure S2. Relative rate coefficients obtained from Vocus measurements of acetonitrile, thiophene (C_4H_4S), 2,3-dibenzofuran (C_8H_8O), and cis-3-hexynyl-acetate ($C_8H_{14}O_2$) tracers used in characterization studies described in Sect. 3.2. Literature relative rate coefficients obtained from kinetic data published by Atkinson (1991) and Atkinson et al. (1995).

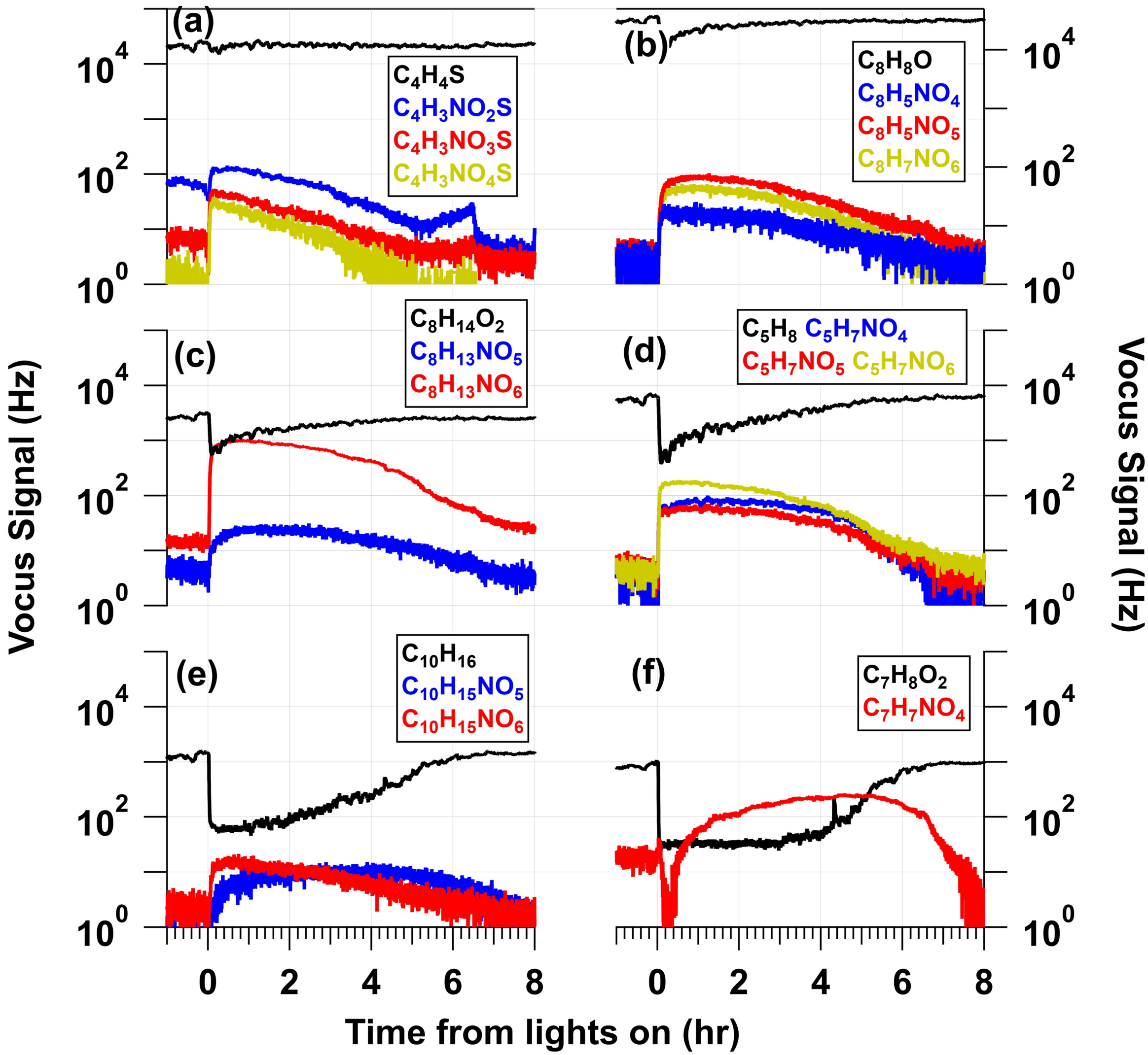


Figure S3. Time series of Vocus PTR ions measured following irradiation of a mixture containing 0.5 M CAN and 6.0 M HNO_3 mixture: **(a)** thiophene (C_4H_4S) and nitrothiophenes ($C_4H_3NO_{2-4}S$), **(b)** 2,3-dibenzofuran (C_8H_8O) and $C_8H_{5,7}NO_{4-6}$, **(c)** cis-3-hexynyl-acetate ($C_8H_{14}O_2$) and $C_8H_{13}NO_{5-6}$, **(d)** isoprene C_5H_8 and $C_5H_7NO_{4-6}$, **(e)** α-pinene ($C_{10}H_{16}$) and $C_{10}H_{15}NO_{5,6}$, and **(f)** guaiacol $C_7H_8O_2$ and nitroguiacol ($C_7H_7NO_4$).

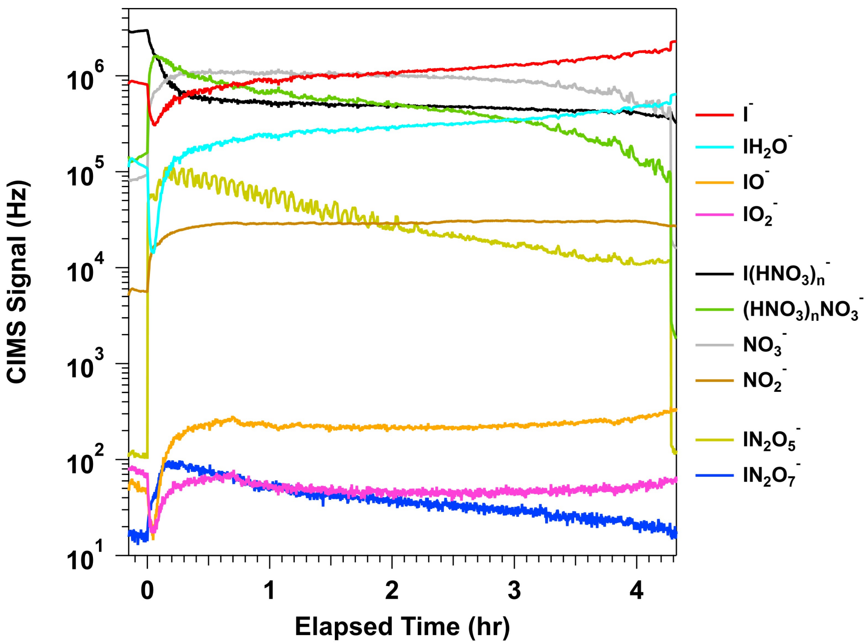


Figure S4. HR-ToF-CIMS time series of I^-, IH_2O^-, IO^-, IO_2^-, NO_2^-, NO_3^-, $IHNO_3^-$, and $HNO_3NO_3^-$, $IN_2O_5^-$, and $IN_2O_7^-$ signals detected following irradiation of a mixture containing 0.5 M CAN and 1.0 M $NaNO_3$ (see Fig. 7).

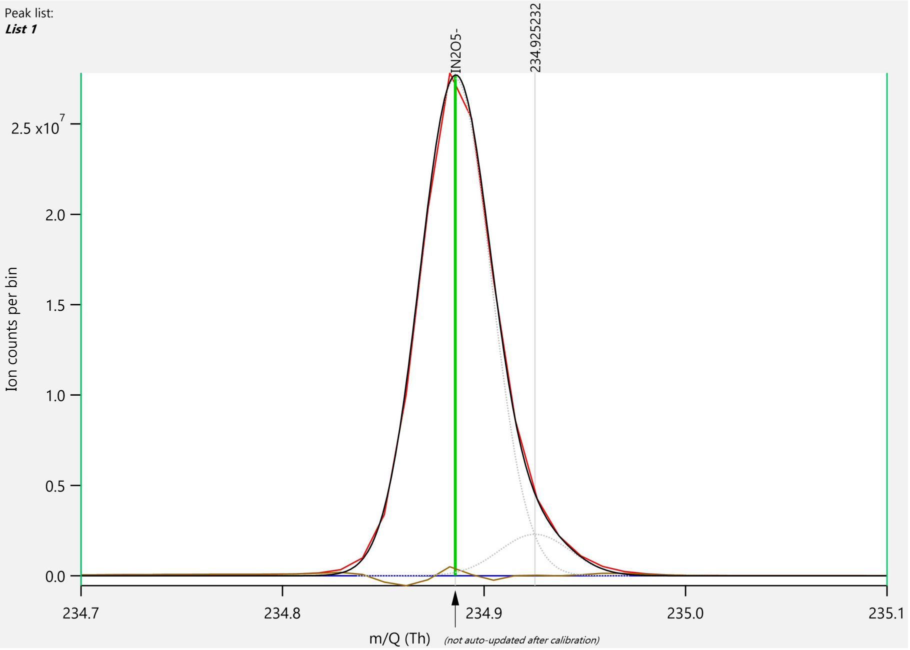


Figure S5. HR-ToF-CIMS spectrum of m/Q=235 obtained following irradiation of CAN/HNO_3 mixtures.

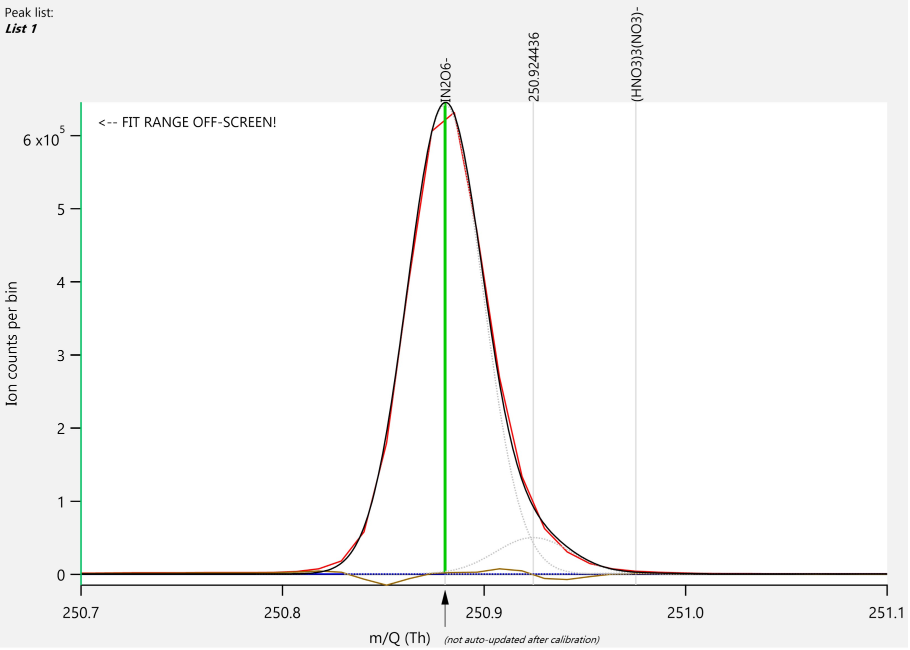


Figure S6. HR-ToF-CIMS spectrum of m/Q=251 obtained following irradiation of CAN/HNO_3 mixtures.

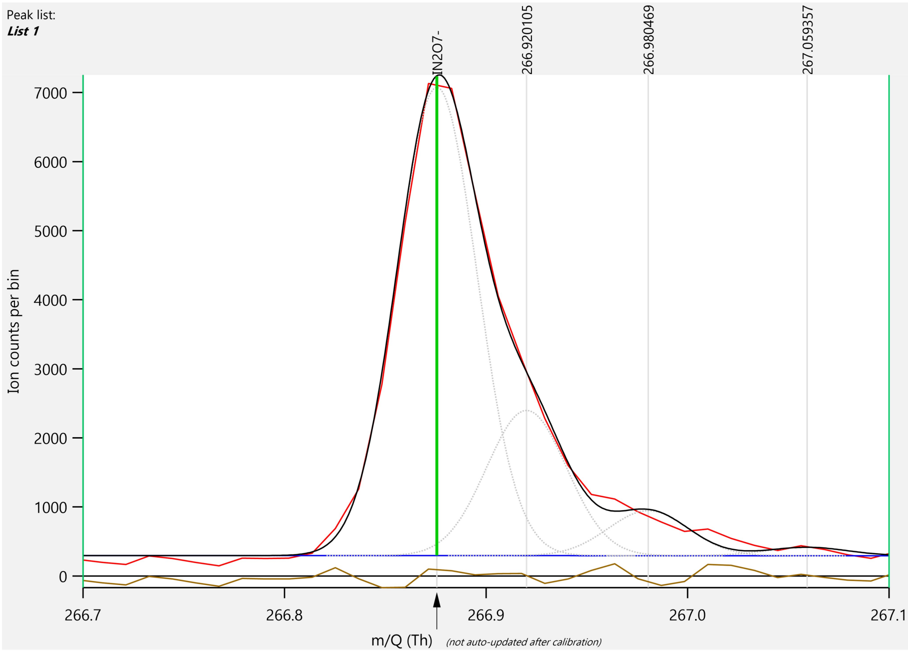


Figure S7. HR-ToF-CIMS spectrum of m/Q=267 obtained following irradiation of CAN/HNO_3 mixtures.

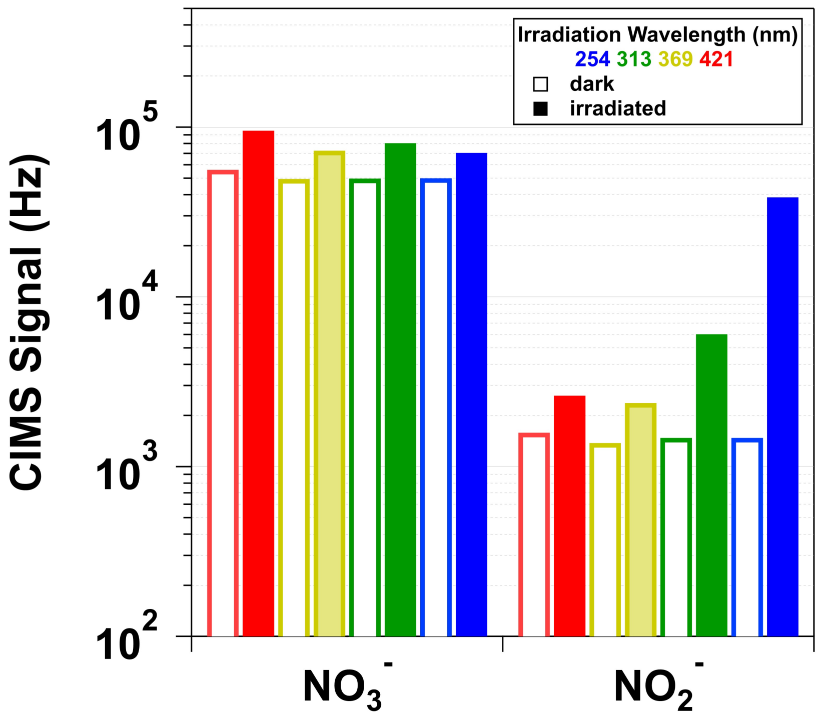


Figure S8. HR-ToF-CIMS NO_2^- and NO_3^- signals obtained during sampling of dark and irradiated neat CAN samples.

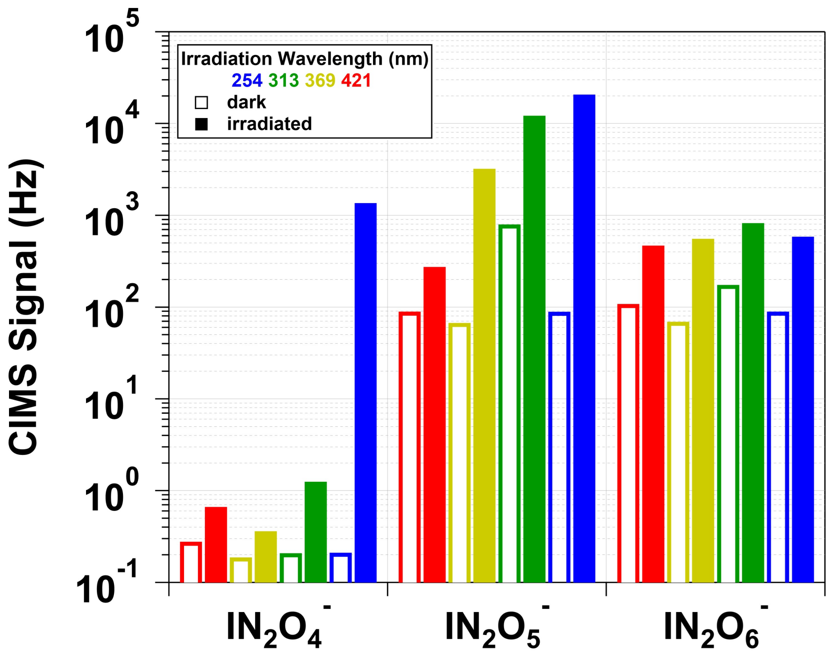


Figure S9. HR-ToF-CIMS $IN_2O_4^-$, $IN_2O_5^-$, and $IN_2O_6^-$ signals obtained during sampling of dark and irradiated neat CAN samples.

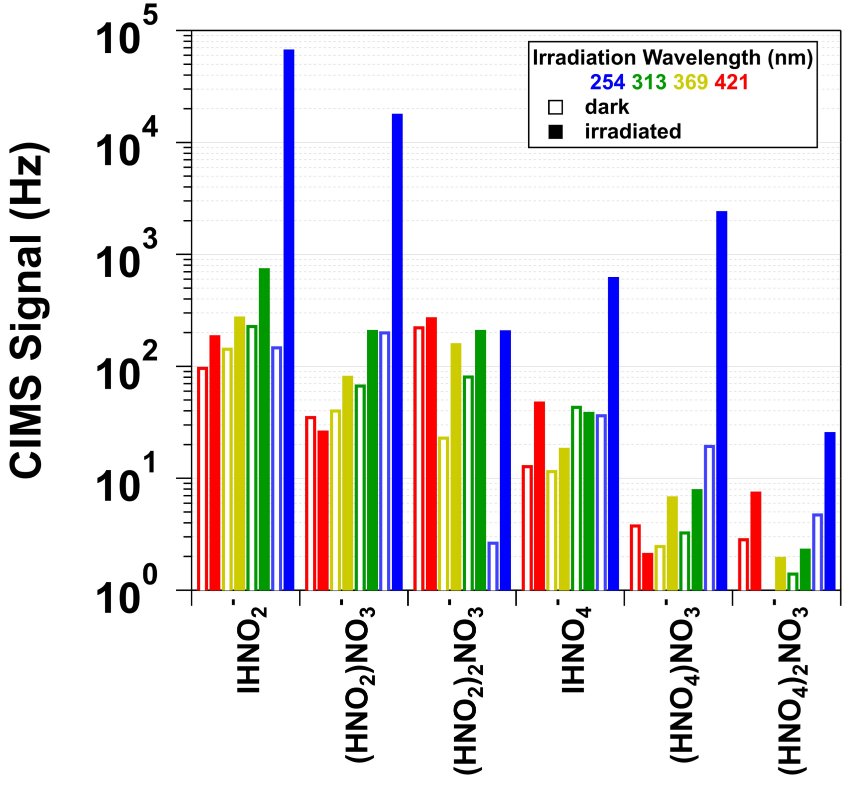


Figure S10. HR-ToF-CIMS $I(HNO_2)_n^-$, $(HNO_2)_nNO_3^-$, $I(HNO_4)_n^-$, and $(HNO_4)_nNO_3^-$ signals obtained during sampling of dark and irradiated neat CAN samples.

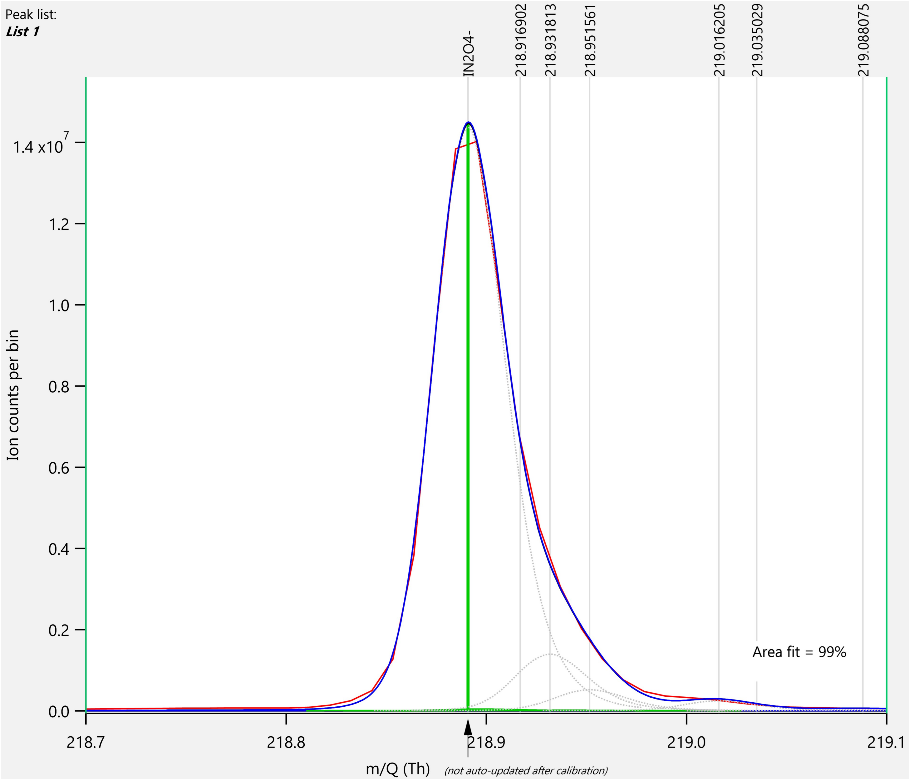


Figure S11. HR-ToF-CIMS spectrum of m/Q=219 obtained following irradiation of neat CAN samples.

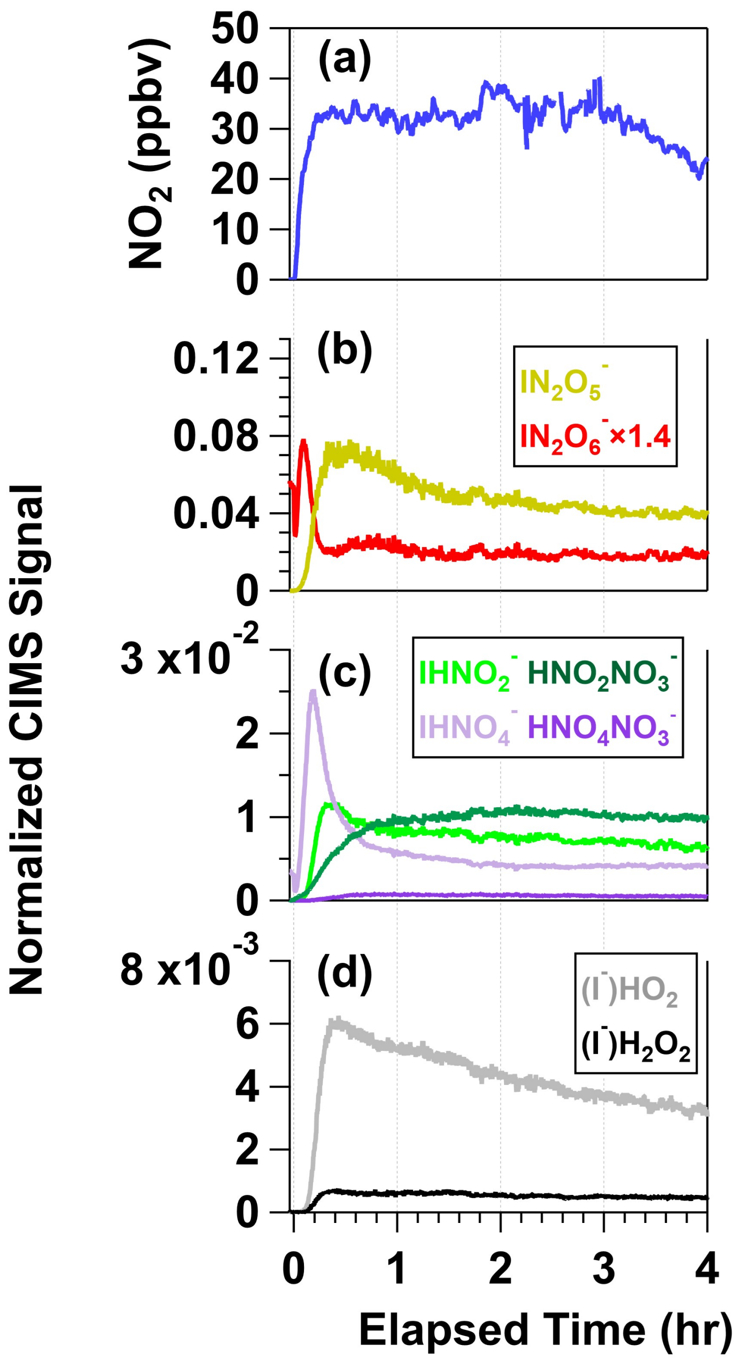


Figure S12. Time series of **(a)** NO_2, **(b)** N_2O_5 and N_2O_6, **(c)** HNO_2 and HNO_4, and **(d)** HO_2 and H_2O_2 measured with NO_x analyzer and HR-ToF-CIMS during irradiation of a mixture containing 0.5 M CAN and 3.0 M HNO_3. N_2O_5, N_2O_6, HO_2 and H_2O_2 were detected as I^- adducts, and HNO_2 and HNO_4 were detected as both I^- and NO_3^- adducts.

Table S1: KinSim mechanism used to calculate concentrations of species associated with irradiation of CAN/HNO_3 mixtures. Rate coefficients or absorption cross sections are given in units of cm^3 $molecules^{-1}$ s^{-1} (blue text), M^{-1} s^{-1} (red text), cm^{-2} (teal text), or s^{-1} (**black text**). Condensed-phase reaction rate coefficients were used where possible, and otherwise were obtained from gas-phase reaction rate coefficients. Reaction rate coefficients in parentheses were obtained by applying a 6.022E+020 conversion factor to the other reaction coefficient listed in the same row. Additional table notes: [1]$[HNO_3]$=1.0 M, [2]$[HNO_3]$=3.0 M, [3]$[HNO_3]$=6.0 M.

Reactant 1	**Reactant 2**	**Product 1**	**Product 2**	**Product 3**	**RateCoeff**	**Citation**
$Ce^{IV}NO_3^-$	$h\nu_{254}$	$[Ce^{III}...NO_3]^*$	NO_3		2.7E-17	this work[1]
					3.1E-17	this work[2]
					3.1E-17	this work[3]
$Ce^{IV}NO_3^-$	$h\nu_{313}$	$[Ce^{III}...NO_3]^*$	NO_3		3.1E-17	this work[1]
					3.5E-17	this work[2]
					4.5E-17	this work[3]
$Ce^{IV}NO_3^-$	$h\nu_{369}$	$[Ce^{III}...NO_3]^*$	NO_3		8.7E-18	this work[1]
					1.2E-17	this work[2]
					2.5E-17	this work[3]
$Ce^{IV}NO_3^-$	$h\nu_{421}$	$[Ce^{III}...NO_3]^*$	NO_3		1.0E-18	this work[1]
					1.5E-18	this work[2]
					4.4E-18	this work[3]
$[Ce^{III}...NO_3]^*$		$Ce^{IV}NO_3^-$			5.12E+04	Martin and Stevens (1978)[1]
					6.30E+03	Martin and Stevens (1978)[2]
					0	Martin and Stevens (1978)[3]
$[Ce^{III}...NO_3]^*$		Ce^{III}	NO_3		4.36E+04	Martin and Stevens (1978)[1]
					6.76E+04	Martin and Stevens (1978)[2]
					7.74E+04	Martin and Stevens (1978)[3]
Ce^{III}	NO_3	$Ce^{IV}NO_3^-$			6.00E+07 (9.96E-14)	Martin and Stevens (1978)[1]
					1.08E+06 (1.79E-15)	Martin and Stevens (1978)[2]
					1.78E+06 (2.96E-15)	Martin and Stevens (1978)[3]
NO_3	$h\nu_{254}$	NO_2	O		1.20E-19	Sander (1986)
NO_3	$h\nu_{313}$	NO_2	O		N/A	N/A
NO_3	$h\nu_{369}$	NO_2	O		9.56E-19	Schott and Davidson (1958)
NO_3	$h\nu_{421}$	NO_2	O		8.00E-20	Wayne et al. (1991)
NO_3	H_2O	H^+	NO_3^-	OH	5.30E+05 (8.80E-16)	Jiang et al. (1992)
NO_3	NO	2 NO_2			(1.57E+10) 2.6E-11	Atkinson et al. (2004)

Table S1 – continued from previous page

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	RateCoeff	Citation
NO_3	NO_2	N_2O_5			1.70E+09 (2.82E-12)	Katsumura et al. (1991)
NO_3	NO_2^-	NO_3^-	NO_2		1.2E+09 (2.0E-12)	Daniels (1969)
NO_3	NO_3	N_2O_6			9.2E+05 (1.53E-15)	Martin and Stevens (1978)
NO_3	H	NO_2	OH		(5.66E+10) 9.4E-11	Becker et al. (1992)
NO_3	O	NO_2	O_2		(6.02E+09) 1.0E-11	DeMore et al. (1994)
NO_3	OH	NO_2	HO_2		(1.20E+10) 2.0E-11	Atkinson et al. (1994)
NO_3	HO_2	H^+	NO_3^-	O_2	3E+09 (4.98E-12)	Jiang et al. (1992)
NO_3	H_2O_2	H^+	NO_3^-	HO_2	7.1E+06 (1.7E-14)	Herrmann et al. (1994)
NO_3	HNO_2	H^+	NO_3^-	NO_2	8.0E+06 (1.3E-14)	Katsumura et al. (1991)
NO_2	$h\nu_{254}$	NO	O		1.1E-20	Sander et al. (2011)
NO_2	$h\nu_{313}$	NO	O		2.2E-19	Sander et al. (2011)
NO_2	$h\nu_{369}$	NO	O		5.6E-19	Sander et al. (2011)
NO_2	NO	N_2O_3			1.1E+09 (1.8E-12)	Grätzel et al. (1970)
NO_2	NO_2	N_2O_4			4.7E+08 (7.8E-13)	Poskrebyshev et al. (2001)
NO_2	O	NO	O_2		(6.02E+09) 1.0E-11	Atkinson et al. (2004)
NO_2	O	NO_3			(1.39E+10) 2.3E-11	Atkinson et al. (2004)
NO_2	H	HNO_2			1E+10 (1.7E-11)	Loegager and Sehested (1993)
NO_2	OH	H^+	NO_3^-		4.5E+09 (2.0E-11)	Loegager and Sehested (1993)
NO_2	HO_2	HNO_4			1.8E+09 (3.0E-12)	Loegager and Sehested (1993)
NO	O	NO_2			(1.81E+10) 3.0E-11	Atkinson et al. (2004)
NO	OH	HNO_2			2E+10 (3.3E-11)	Strehlow and Wagner (1982)
NO	HO_2	H^+	NO_3^-		3.2E+09 (5.3E-12)	Goldstein and Czapski (1995)
N_2O_3	$h\nu_{313}$	NO	NO_2		9.4E-19	Stockwell and Calvert (1978)
N_2O_3	$h\nu_{369}$	NO	NO_2		2.7E-19	Stockwell and Calvert (1978)
N_2O_3		NO	NO_2		3.6E+08	Atkinson et al. (2004)
N_2O_3	H_2O	2 HNO_2			2.0E+08 (3.3E-13)	Park and Lee (1988)
N_2O_4	$h\nu_{254}$	2 NO_2			6.5E-19	Sander et al. (2011)
N_2O_4	$h\nu_{313}$	2 NO_2			2.5E-19	Sander et al. (2011)
N_2O_4	$h\nu_{369}$	2 NO_2			1.3E-19	Sander et al. (2011)
N_2O_4		2 NO_2			6800	Poskrebyshev et al. (2001)
N_2O_4	H_2O	H^+	NO_3^-	HNO_2	1.5E+08 (2.49E-13)	Park and Lee (1988)
N_2O_5	$h\nu_{254}$	NO_2	NO_3		3.2E-19	Sander et al. (2011)
N_2O_5	$h\nu_{313}$	NO_2	NO_3		1.6E-20	Sander et al. (2011)

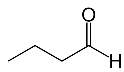
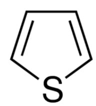
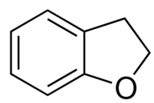
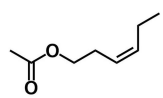
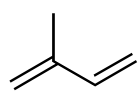
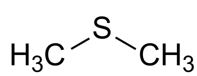
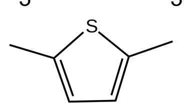
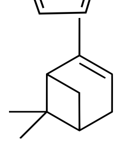
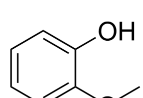
Table S1 – continued from previous page

Reactant 1	Reactant 2	Product 1	Product 2	Product 3	RateCoeff	Citation
N_2O_5	$h\nu_{369}$	NO_2	NO_3		7.2E-22	Sander et al. (2011)
N_2O_5	$h\nu_{421}$	NO_2	NO_3		8.0E-23	Sander et al. (2011)
N_2O_5		NO_2	NO_3		0.06	Atkinson et al. (2004)
N_2O_5	H_2O	2 H^+	2 NO_3^-		(7.8) 1.3E-20	Morris and Niki (1973)
HNO_2	$h\nu_{254}$	NO	OH		1.4E-19	Sander et al. (2011)
HNO_2	$h\nu_{313}$	NO	OH		2.2E-20	Sander et al. (2011)
HNO_2	$h\nu_{369}$	NO	OH		3.1E-19	Sander et al. (2011)
HNO_2	$h\nu_{421}$	NO	OH		2.4E-21	Sander et al. (2011)
HNO_2	H	NO	H_2O		4.5E+08 (7.5E-13)	Halpern and Rabani (1966)
HNO_2	OH	NO_2	H_2O		(3.61E+09) 6.0E-12	Atkinson et al. (2004)
HNO_3	$h\nu_{254}$	NO_2	OH		2.0E-20	Sander et al. (2011)
HNO_3	$h\nu_{313}$	NO_2	OH		6.3E-22	Sander et al. (2011)
HNO_3	$h\nu_{369}$	NO_2	OH		4.2E-24	Sander et al. (2011)
HNO_3	OH	NO_3	H_2O		5.3E+07 (8.8E-14)	Jiang et al. (1992)
HNO_4	$h\nu_{254}$	NO_2	HO_2		3.5E-19	Sander et al. (2011)
HNO_4	$h\nu_{313}$	NO_2	HO_2		4.7E-21	Sander et al. (2011)
HNO_4	$h\nu_{369}$	NO_2	HO_2		1.7E-22	Sander et al. (2011)
HNO_4		NO_2	HO_2		4.6E-03	Lammel et al. (1990)
HNO_4		HNO_2	O_2		7E-04	Loegager and Sehested (1993)
HNO_4	OH				(2.83E+09) 4.70E-12	Atkinson et al. (2004)
H	O_2	HO_2			1.0E+10 (1.7E-11)	Elliot et al. (1990)
H	O_2	H_2O_2			2.0E+10 (3.3E-11)	Feng et al. (1970)
OH	O	O_2	H		(2.0E+10) 3.3E-11	DeMore et al. (1997)
OH	OH	H_2O_2			4.2E+09 (7.0E-12)	Elliot et al. (1990)
OH	HO_2	O_2	H_2O		1.0E+10 (1.7E-11)	Elliot and Buxton (1992)
OH	HO_2	H_2O_3			(2.14E+09) 3.55E-12	Badenes et al. (2017)
OH	H_2O_2	HO_2	H_2O		(1.0E+09) 1.7E-12	Atkinson et al. (2004)
H_2O_2	$h\nu_{254}$	2OH			6.7E-20	Sander et al. (2011)
H_2O_2	$h\nu_{313}$	2OH			3.4E-21	Sander et al. (2011)
H_2O_2	$h\nu_{369}$	2OH			7.2E-23	Kahan et al. (2012)
H_2O_2	$h\nu_{421}$	2OH			9.2E-24	Kahan et al. (2012)
H_2O_2	H	H_2O	OH		3.6E+07 (6.0E-14)	Mezyk and Bartels (1995)

Table S1 – continued from previous page

Reactant 1	**Reactant 2**	**Product 1**	**Product 2**	**Product 3**	**RateCoeff**	**Citation**
H_2O_2	O	HO_2	OH		1.6E+09 (2.7E-12)	Sauer et al. (1984)
NO_3^-	H	H_2O	NO_2		1.0E+07 (1.7E-14)	Jiang et al. (1992)
NO_3^-	H^+	HNO_3			6.0E+08 (1.0E-12)	Poskrebyshev et al. (2001)

Table S2. VOC tracers used in CAN/HNO_3 and CAN/$NaNO_3$ irradiation studies. Bimolecular rate coefficients for reaction with NO_3 are given in units of cm^3 $molecule^{-1}$ s^{-1}.

Compound	Formula	Structure	Mixing Ratio (ppb)	k_{NO_3}	References
Acetonitrile	C_2H_3N		517	$<3.01\times10^{-19}$	Cantrell et al. (1987)
Butanal	C_4H_8O		42	1.22×10^{-14}	D'Anna et al. (2001)
Thiophene	C_4H_4S		48	3.94×10^{-14}	Atkinson (1991)
2,3-Dihydrobenzofuran	C_8H_8O		34	1.15×10^{-13}	Atkinson (1991)
cis-3-Hexenyl-1-Acetate	$C_8H_{14}O_2$		24	2.46×10^{-13}	Atkinson et al. (1995)
Isoprene	C_5H_8		38	3.77×10^{-16}	Atkinson (1991)
Dimethyl Sulfide	C_2H_6S		6.5	1.09×10^{-12}	Atkinson et al. (2004)
2,5-Dimethylthiophene	C_6H_8S		4.2	2.52×10^{-12}	Cabañas et al. (2006)
α-Pinene	$C_{10}H_{16}$		3.0	6.16×10^{-12}	Atkinson (1991)
Guaiacol	$C_7H_8O_2$		2.1	2.69×10^{-11}	Lauraguais et al. (2016)

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