SUPPORTING INFORMATION

Production of Gas Phase NO_2 and Halogens from the Photolysis of Thin Water Films Containing Nitrate, Chloride and Bromide Ions at Room Temperature

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Molecular Dynamics (MD) Force Field Parameters

The force field parameters are provided in Table S1 for MD simulations for NaCl/NaBr/$NaNO_3$.

Atom	Parameter Set	q (e)[a]	α (Å^3)[b]	Rmin/2 (Å)[c]	ε (kcal/mol)[d]
Na^+	PB[e]	1	0.240	1.3190	0.1300
Br^-	S[f]	-1	4.530	2.6380	0.1000
Cl^-	PB[e]	-1	3.250	2.4192	0.100
Nitrate (N)	Thomas[h]	0.950	0.000	1.88	0.1700
Nitrate (O)	Thomas[h]	-0.650	1.490	1.80	0.1600
Water (O)	POL3[i]	-0.730	0.528	1.798	0.156
Water (H)	POL3[i]	0.365	0.170	0.0	0.0

[a]Charge or partial charge of atom or ion, [b]Atomic polarizability, [c]R_{min} is the position of the minimum in the Lennard-Jones potential, [d]Lennard-Jones well depth, [e]Perera and Berkowitz[1], [f]Sremaniak et al.[2], [h]Thomas et al.[3] and [i]Caldwell and Kollman[4].

Table S2: Gas Phase Chemistry

no	reaction	k	ref
G1	$NO_2 + O(^3P) = NO + O_2$	1.04×10^{-11}	5
G2	$NO_2 + O(^3P) = NO_3$	3.3×10^{-11}	5
G3	$NO_2 + O_3 = NO_3 + O_2$	3.2×10^{-17}	5
G4	$NO_2 + NO_3 = N_2O_5$	1.84×10^{-12}	6
G5	$NO_2 + NO_3 = NO + NO_2 + O_2$	6.6×10^{-16}	7
G6	$NO_2 + OH = HNO_3$	1.0×10^{-11}	8
G7	$NO_2 + HO_2 = HNO_2 + O_2$	5×10^{-16}	9
G8	$NO + O(^3P) = NO_2$	3×10^{-11}	5
G9	$NO + O_3 = NO_2 + O_2$	1.9×10^{-14}	5
G10	$NO + NO_3 = NO_2 + NO_2$	2.6×10^{-11}	5
G11	$NO + HO_2 = OH + NO_2$	8.1×10^{-12}	5
G12	$NO + HO_2 = HNO_3$	1.4×10^{-13}	10
G13	$NO_3 + O(^3P) = NO_2 + O_2$	1.7×10^{-11}	5
G14	$NO_3 + NO_3 = NO_2 + NO_2 + O_2$	2.3×10^{-16}	7
G15	$NO_3 + HO_2 = OH + NO_2$	3.5×10^{-12}	11
G16	$NO_3 + OH = HO_2 + NO_2$	2.2×10^{-11}	5
G17	$N_2O_5 = NO_3 + NO_2$	4.0×10^{-20}	5
G18	$N_2O_5 + H_2O = HNO_3 + HNO_3$	2×10^{-21}	5
G19	$HNO_2 + O_3 = O_2 + HNO_3$	5×10^{-19}	7
G20	$HNO_2 + OH = NO_2 + H_2O$	6×10^{-12}	5
G21	$HNO_3 + O(^3P) = NO_3 + OH$	3×10^{-17}	7
G22	$HNO_3 + OH = H_2O + NO_3$	1.5×10^{-13}	5
G23	$OH + O_3 = HO_2 + O_2$	7.3×10^{-14}	7
G24	$OH + H_2O_2 = HO_2 + H_2O$	1.8×10^{-12}	5
G25	$OH + OH = H_2O + O(^3P)$	1.48×10^{-12}	7
G26	$OH + OH = H_2O_2$	6.3×10^{-12}	7
G27	$OH + HO_2 = H_2O + O_2$	1.1×10^{-10}	7
G28	$O(^3P) + O_2 = O_3$	1.5×10^{-14}	7
G29	$O(^3P) + O_3 = O_2 + O_2$	8×10^{-15}	7
G30	$O(^3P) + HO_2 = OH + O_2$	5.9×10^{-11}	7
G31	$O(^3P) + H_2O_2 = OH + HO_2$	1.7×10^{-15}	7
G32	$HO_2 + O_3 = OH + O_2 + O_2$	1.9×10^{-15}	7

G33	$HO_2 + HO_2 = H_2O_2 + O_2$	2.7×10^{-12}	7
G34	$BrO + O(^3P) = O_2 + Br$	4.11×10^{-11}	12
G35	$BrO + OH = Br + HO_2$	7.5×10^{-11}	12
G36	$BrO + O_3 = Br + O_2 + Br + O_2$	2×10^{-17}	13
G37	$BrO + BrO = Br + O_2 + Br$	2.7×10^{-12}	12
G38	$BrO + BrO = Br_2 + O_2$	4.86×10^{-13}	12
G39	$BrO + O(^3P) = BrO_2$	5×10^{-11}	14
G40	$BrO + HO_2 = HBr + O_3$	2.3×10^{-3}	15
G41	$BrO + HO_2 = O_2 + HOBr$	5×10^{-12}	16
G42	$BrO + OH = O_2 + HBr$	1×10^{-12}	12
G43	$BrO + NO = NO_2 + Br$	2.1×10^{-11}	12
G44	$BrO + NO_2 = BrONO_2$	1.4×10^{-11}	17
G45	$BrO + NO_3 = BrO_2 + NO_2$	1×10^{-12}	12
G46	$HBr + HOBr = OH + Br_2$	2.41×10^{-17}	18
G47	$HBr + O(^3P) = OH + Br$	5×10^{-12}	16
G48	$HBr + OH = H_2O + Br$	1.1×10^{-11}	12
G49	$HBr + NO_3 = HNO_3 + Br$	1×10^{-16}	12
G50	$Br + BrONO_2 = Br_2 + NO_3$	6.71×10^{-11}	19
G51	$Br + HOBr = OH + Br_2$	2.41×10^{-17}	20
G52	$Br + NO = BrNO$	3.32×10^{-11}	21
G53	$Br + HO_2 = HBr + O_2$	1.93×10^{-12}	13
G54	$Br + O_3 = BrO + O_2$	1.16×10^{-12}	12
G55	$Br + H_2O_2 = HBr + HO_2$	5×10^{-16}	16
G56	$Br + NO_2 = BrNO_2$	2.7×10^{-11}	12
G57	$Br + NO_3 = BrO + NO_2$	1.6×10^{-11}	12
G58	$HOBr + O(^3P) = BrO + OH$	2.83×10^{-11}	12
G59	$Br_2 + OH = HOBr + Br$	4.25×10^{-11}	13
G60	$BrONO_2 + O(^3P) = NO_3 + BrO$	3.9×10^{-13}	13
G61	$BrONO_2 + BrNO = Br_2 + NO_2 + NO_2$	1×10^{-16}	22
G62	$BrONO_2 + NO = NO_3 + BrNO$	3.01×10^{-19}	22
G63	$BrONO_2 + Br = Br_2 + NO_3$	4.9×10^{-11}	22
G64	$O_2 + O(^1D) = O(^3P) + O_2$	3.95×10^{-11}	7
G65	$O(^1D) + O_3 = O_2 + O_2$	1.2×10^{-10}	7
G66	$O(^1D) + N_2 = O(^3P) + N_2$	3.1×10^{-10}	7

G67	$O(^1D) + H_2O = OH + OH$	2×10^{-10}	7
G68	$O(^1D) + CO_2 = O(^3P) + CO_2$	1.1×10^{-10}	7
G69	$O(^1D) + O_3 = 2\ O\ (^3P) + O_2$	1.2×10^{-10}	7
G70	$NO + OH = HNO_2$	3.3×10^{-12}	5
G71	$HNO_3 + NO_2 = OH + NO + NO$	1×10^{-18}	7
G72	$BrNO + Br = Br_2 + NO$	3.72×10^{-10}	21
G73	$BrNO_2 + Br = Br_2 + NO_2$	1×10^{-10}	23
G74	$HOBr + NO = BrNO + OH$	5×10^{-14}	24
G75	$Cl + HO_2 = OH + ClO$	9.1×10^{-12}	7
G76	$Cl + O_3 = ClO + O_2$	1.2×10^{-11}	7
G77	$Cl + H_2O_2 = HO_2 + HCl$	4.1×10^{-13}	7
G78	$Cl + ClO_2 = ClO + ClO$	5.8×10^{-11}	7
G79	$Cl + ClO_2 = Cl_2 + O_2$	2.3×10^{-10}	7
G80	$Cl + HOCl = OH + Cl_2$	1.6×10^{-12}	7
G81	$Cl + HOCl = HCl + ClO$	1.22×10^{-14}	25
G82	$Cl + O_2 = ClO_2$	5.2×10^{-14}	7
G83	$Cl + Cl_2O = Cl_2 + ClO$	9.6×10^{-11}	7
G84	$Cl + Cl_2O_2 = Cl_2 + O_2$	1×10^{-10}	5
G85	$Cl + NO = ClNO$	1.9×10^{-12}	7
G86	$Cl + NO_2 = ClNO_2$	1×10^{-10}	7
G87	$Cl + NO_3 = ClO + NO_2$	2.4×10^{-11}	5
G88	$Cl + HNO_3 = HCl + NO_3$	2×10^{-16}	5
G89	$Cl + ClNO = NO + Cl_2$	7.61×10^{-11}	7
G90	$Cl + ClONO_2 = Cl_2 + NO_3$	1×10^{-11}	5
G91	$ClO + O_3 = ClO_2 + O_2$	1.4×10^{-17}	5
G92	$ClO + O_3 = OClO + O_2$	1.0×10^{-18}	5
G93	$ClO + ClO = Cl_2 + O_2$	4.8×10^{-15}	7
G94	$ClO + ClO = ClO_2 + Cl$	8×10^{-15}	7
G95	$ClO + ClO = Cl + Cl + O_2$	3.5×10^{-15}	7
G96	$ClO + ClO = Cl_2O_2$	2.4×10^{-13}	7
G97	$ClO + OH = Cl + HO_2$	1.8×10^{-11}	7
G98	$ClO + OH = HCl + O_2$	2.2×10^{-12}	7
G99	$ClO + O\ (^3P) = Cl + O_2$	3.7×10^{-11}	7
G100	$ClO + HO_2 = HOCl + O_2$	5.6×10^{-12}	7

G101	$ClO + NO = NO_2 + Cl$	1.7×10^{-17}	5
G102	$ClO + NO_2 = ClONO_2$	2.3×10^{-12}	5
G103	$ClO + NO_3 = ClO_2 + NO_2$	4.7×10^{-13}	5
G104	$OClO + O(^3P) = ClO + O_2$	9.6×10^{-14}	7
G105	$OClO + O(^3P) = ClO_3$	3.1×10^{-11}	5
G106	$OClO + O_3 = ClO + 2O_2$	3×10^{-19}	12
G107	$OClO + OH = HOCl + O_2$	6.8×10^{-12}	7
G108	$OClO + NO = NO_2 + ClO$	3.4×10^{-13}	12
G109	$ClO_2 = Cl + O_2$	6.2×10^{-13}	12
G110	$Cl_2O + O(^3P) = ClO + ClO$	4.5×10^{-12}	7
G111	$Cl_2O + ClO = Cl_2 + ClO_2$	4.3×10^{-16}	26
G112	$Cl_2O + ClO = Cl_2 + Cl + O_2$	2.7×10^{-15}	26
G113	$HOCl + O(^3P) = OH + ClO$	1.7×10^{-13}	7
G114	$HOCl + OHg = H_2O + ClO$	5.6×10^{-13}	7
G115	$HCl + OH = H_2O + Cl$	8×10^{-13}	7
G116	$HCl + O(^3P) = OH + Cl$	1.5×10^{-16}	7
G117	$Cl_2 + OH = HOCl + Cl$	6.7×10^{-14}	7
G118	$ClONO_2 + O(^3P) = ClO + NO_3$	2×10^{-13}	12
G119	$ClONO_2 + OH = ClO + HNO_3$	3.9×10^{-13}	12
G120	$ClONO_2 + NO = Cl + N_2O_5$	4×10^{-17}	27
G121	$ClONO_2 + H_2O = HNO_3 + HOCl$	5×10^{-21}	16
G122	$ClNO_2 + OH = HOCl + NO_2$	3.6×10^{-14}	12
G123	$BrCl + Cl = Cl_2 + Br$	1.45×10^{-11}	28
G124	$BrCl + Br = Br_2 + Cl$	3.32×10^{-15}	29
G125	$BrCl + O(^3P) = BrO + Cl$	2.09×10^{-11}	30
G126	$Cl_2 + Br = BrCl + Cl$	1.1×10^{-15}	31
G127	$HOBr + Cl = OH + BrCl$	3.7×10^{-14}	20
G128	$ClNO + Br = NO + BrCl$	1.26×10^{-11}	32

Table S3: Aqueous Phase Chemistry

no	Reaction	k	Ref/comment
A1	$NO_3^- = NO_2 + O^-$	1.8×10^{-4}	a
A2	$NO_3^- = NO_2^- + O\ (^3P)$	1.8×10^{-5}	b
A3	$NO_2^- = NO + O^-$	1.5×10^{-3}	c
A4	$H_2O_2 = OH + OH$	1.26×10^{-3}	c
A5	$NO_2^- + OH = NO_2 + OH^-$	1.2×10^{10}	33
A6	$NO_2^- + O_3 = O_2 + NO_3^-$	5×10^{5}	34
A7	$NO + OH = HNO_2$	1.7×10^{10}	33
A8	$NO + NO_2 = H^+ + NO_2^- + H^+ + NO_2^-$	2×10^{8}	35
A9	$NO + NO + O_2 = NO_2 + NO_2$	2.1×10^{6}	36
A10	$2\ NO_2 + H_2O = H^+ + NO_3^- + H^+ + NO_2^-$	1×10^{8}	35
A11	$NO_2 + OH = H^+ + NO_3^-$	4.5×10^{9}	37
A12	$NO_2 + O_2^- = NO_2^- + O_2$	1×10^{8}	38
A13	$2H^+ + NO_2^- + NO_2^- = NO + NO_2 + H_2O$	5.8	38
A14	$H^+ + NO_2^- + OH = NO_2 + H_2O$	1×10^{10}	33
A15	$NO_2^- + O(^3P) = NO_3^-$	3×10^{10}	38
A16	$NO_3^- + O(^3P) = NO_2^- + O_2$	2×10^{8}	39
A17	$O\ (^3P) + O_2 = O_3$	4×10^{9}	40
A18	$O(^3P) + OH^- = HO_2^-$	4.2×10^{8}	41
A19	$O(^3P) + H_2O_2 = OH + HO_2$	1.6×10^{9}	41
A20	$O\ (^3P) + HO_2^- = OH + O_2^-$	5.3×10^{9}	41
A21	$O_3 = O\ (^3P) + O_2$	3×10^{-6}	42
A22	$O_3 + OH = HO_2 + O_2$	1.1×10^{8}	43
A23	$O_3 + O_2^- = O_3^- + O_2$	1.5×10^{9}	44
A24	$O_3 + OH^- = HO_2^- + O_2$	70	45
A25	$O_3 + OH^- = O_2^- + HO_2$	57	45
A26	$O_3 + H_2O_2 = OH + HO_2 + O_2$	6.5×10^{-2}	42
A27	$O_3 + HO_2^- = HO_3 + O_2^-$	5.5×10^{6}	45
A28	$2\ OH = H_2O_2$	5.5×10^{9}	46
A29	$OH + HO_2 = H_2O + O_2$	1×10^{10}	47
A30	$OH + O^- = HO_2^-$	2×10^{10}	48

A31	$OH + HO_2^- = OH^- + HO_2$	7.5×10^9	49
A32	$OH + H_2O_2 = HO_2 + H_2O$	2.72×10^7	46
A33	$OH + O_2^- = OH^- + O_2$	9.4×10^9	50
A34	$OH + O_3^- = O_2^- + HO_2$	8.5×10^9	51
A35	$OH + O_3^- = O_3 + OH^-$	2.5×10^9	51
A36	$O^- + H_2O = OH + OH^-$	9.4×10^7	52
A37	$O^- + HO_2^- = O_2^- + OH^-$	4×10^8	46
A38	$O^- + O_2^- + H_2O = OH^- + OH^- + O_2$	6×10^8	53
A39	$O^- + O_3 = O_2^- + O_2$	1×10^8	54
A40	$O^- + O_3^- = O_2^- + O_2^-$	7×10^8	53
A41	$O^- + H_2O_2 = O_2^- + H_2O$	2.5×10^8	46
A42	$2\ O_2^- + 2\ H_2O = H_2O_2 + 2\ OH^- + O_2$	1.75×10^{-1}	51
A43	$O_2^- + H_2O_2 = OH + OH^- + O_2$	1.3×10^{-1}	55
A44	$O_2^- + O_3^- + H_2O = OH^- + OH^- + O_2 + O_2$	5×10^4	54
A45	$O^- + O_2 = O_3^-$	3.54×10^9	46
A46	$O^{-2} + H_2O = OH^- + OH^-$	1×10^8	Estimated
A47	$H_2O_2 + HO_2 = OH + O_2 + H_2O$	5×10^{-1}	55
A48	$HO_2 + O_3 = OH + O_2 + O_2$	5×10^3	43
A49	$HO_2 + HO_2 = H_2O_2 + O_2$	8.3×10^5	56
A50	$CO_2 + OH = CO_3^- + H+;$	1×10^6	57
A51	$CO_3^- + H_2O_2 = HCO_3^- + HO_2$	5.7×10^5	58
A52	$CO_3^- + HO_2^- = HCO_3^- + HO_2^-$	3.5×10^7	58
A53	$CO_3^- + HO_2 = HCO_3^- + O_2$	3.5×10^8	59
A54	$CO_3^- + O_2^- = HCO_3^- + OH^-$	3.53×10^8	59
A55	$CO_3^- + O_3^- = CO_3^{2-} + O_3$	6×10^7	60
A56	$HCO_3^- + O_2^- = CO_3^- + HO_2^-$	1.5×10^6	61
A57	$HCO_3^- + OH = CO_3^- + H_2Oa$	8.25×10^6	46
A58	$CO_3^{2-} + OH = CO_3^- + OH^-$	3.79×10^8	59
A59	$CO_3^{2-} + O^- + H_2O = CO_3^- + OH^- + OH^-$	2.5×10^5	59
A60	$Br^- + O_3 + H_2O = HOBr + O_2 + OH^-$	258	62
A61	$Br^- + O_3 = BrO^- + O_2$	239	62
A62	$BrO^- + O_3 = Br^- + O_2 + O_2$	330	62

A63	$BrO^- + O_3 + O_3 = BrO_3^- + O_2 + O_2$	100	62
A64	$BrO^- + O_3 = BrO_2^- + O_2$	100	62
A65	$BrO^- + BrO^- = BrO_2^- + Br^-$	6×10^{-7}	63
A66	$BrO^- + Br = Br^- + BrO$	4.1×10^{9}	63
A67	$BrO^- + O_2^- = Br_2^- + O_2 + OH^-$	2×10^{8}	64
A68	$BrO^- + OH = BrO + OH^-$	4.2×10^{9}	65
A69	$BrO^- + O^- + H_2O = BrO + OH^- + OH^-$	3.55×10^{9}	65
A70	$BrO^- + Br_2^- = BrO + Br^- + Br^-$	8×10^{7}	65
A71	$BrO^- + H_2O = HOBr + OH^-$	1×10^{8}	65
A72	$HOBr + O_3 = BrO_2^- + O_2 + H+$	1.3×10^{-2}	62
A73	$HOBr + Br^- + H^+ = Br_2 + H_2O$	1.6×10^{10}	66
A74	$HOBr + Br^- = Br_2 + OH^-$	3.4×10^{4}	66
A75	$HOBr + Br^- + H_2O_2 = Br_2 + HO_2^- + H_2O$	3.9×10^{4}	67
A76	$HOBr + H_2O_2 = H^+ + Br^- + O_2 + H_2O$	1.5×10^{4}	67
A77	$HOBr + HO_2^- = H^+ + Br^- + O_2 + H_2O$	7.6×10^{8}	68
A78	$2\ HOBr = HBrO_2 + Br^- + H^+$	2.3×10^{-3}	69
A79	$2\ HOBr + OH^- = HBrO_2 + Br^- + H_2O$	1.5×10^{-1}	69
A80	$HOBr + O_2^- = Br + O_2 + OH^-$	3.5×10^{9}	64
A81	$HOBr + OH = BrO + H_2O$	2×10^{9}	63
A82	$HOBr + OH^- = BrO^- + H_2O$	1.5×10^{-1}	69
A83	$HOBr^- = Br^- + OH$	3.3×10^{7}	70
A84	$HOBr^- = OH^- + Br;$	4.2×10^{6}	70
A85	$HOBr^- + H^+ = Br + H_2O$	4.4×10^{10}	70
A86	$HOBr^- + Br^- = Br_2^- + OH^-$	1.9×10^{8}	70
A87	$BrO_2^- + O_3 = BrO_3^- + O_2$	1×10^{6}	71
A88	$BrO_2^- + HBrO_2 = HOBr + BrO_3^-$	3.91×10^{1}	72
A89	$BrO_2^- + O(^3P) = BrO^- + O_2$	1.24×10^{9}	72
A90	$BrO_2^- + Br_2^- = BrO + BrO^- + Br^-$	8×10^{7}	65
A91	$BrO_2^- + OH = BrO_2 + OH^-$	2.05×10^{9}	65
A92	$BrO_2^- + O^- + H_2O = BrO_2 + OH^- + OH^-$	1.8×10^{9}	65
A93	$BrO + BrO + H_2O = HOBr + HBrO_2$	2.6×10^{9}	63
A94	$BrO + BrO_2^- = BrO^- + BrO_2$	3.4×10^{8}	72

A95	$HBrO_2 + HBrO_2 = HOBr + H^+ + BrO_3^-$	8×10^2	73
A96	$BrO_2 + OH = BrO_3^- + H^+$	2×10^9	74
A97	$BrO_2 + BrO_2 = Br_2O_4$	3×10^9	74
A98	$Br_2O_4 = BrO_2 + BrO_2$	3.1×10^5	74
A99	$Br_2O_4 + OH^- = BrO_3^- + H^+ + BrO_2^-$	7.45×10^8	65
A100	$BrO_3^- + O(^3P) = BrO_2^- + O_2$	1.5×10^7	40
A101	$Br^- + OH = HOBr^-$	1.06×10^{10}	70
A102	$Br^- + H_2O_2 + H^+ = HOBr + H_2O$	1.4×10^{-2}	75
A103	$Br^- + H_2O_2 = HOBr + OH^-$	2.14×10^{-5}	75
A104	$Br^- + Br = Br_2^-$	1.17×10^{10}	76
A105	$Br + Br = Br_2$	1.5×10^{10}	76
A106	$Br + Br_2^- = Br_2 + Br^-$	5×10^9	76
A107	$Br + H_2O_2 = Br^- + HO_2 + H^+$	2.5×10^9	77
A108	$Br + OH^- = HOBr^-$	1.3×10^{10}	63
A109	$Br + H_2O = HOBr^- + H^+$	1.36	63
A110	$Br_2^- = Br + Br^-$	4.71×10^4	76
A111	$Br_2^- + Br_2^- = Br_3^- + Br^-$	2.04×10^8	78
A112	$Br_2^- + OH^- = HOBr^- + Br^-$	5.14×10^7	79
A113	$Br_2^- + H_2O_2 = Br^- + H^+ + Br^- + HO_2$	1×10^3	80
A114	$Br_2 + HO_2 = Br_2^- + O_2 + H^+$	1.3×10^8	64
A115	$Br_2^- + HO_2 + H^+ = Br_2 + H_2O_2$	3.8×10^9	77
A116	$Br_3^- + HO_2 = Br_2^- + Br^- + O_2 + H^+$	1×10^8	81
A117	$Br_3^- + O_2^- = Br_2^- + Br^- + O_2$	1.5×10^9	64
A118	$Br_3^- = Br_2 + Br^-$	5×10^7	82
A119	$Br_2 + H_2O = HOBr + Br^- + H^+$	9.7×10^1	11
A120	$Br_2 + OH^- + H_2O = HOBr + Br^- + H_2O$	7×10^9	66
A121	$Br_2 + Br^- = Br_3^-$	1.5×10^9	82
A122	$Br_2 + O_2^- = Br_2^- + O_2$	5.3×10^9	64
A123	$Br_2 + HO_2^- + H_2O = HOBr + Br^- + H_2O_2$	8.8×10^7	66
A124	$Br_2 + HCO_3^- + H_2O = HOBr + Br^- + CO_2$	1.6×10^5	66
A125	$Br_2 + CO_3^{2-} = HOBr + Br^- + HCO_3^-$	1.5×10^7	66
A126	$HOBr + Br^- + CO_2 = Br_2 + HCO_3^-$	1.2×10^7	66

A127	$HOBr + Br^- + HCO_3^- = Br_2 + CO_3^{2-}$	1.1×10^5	66
A128	$HOBr + CO_3^{2-} = BrO^- + HCO_3^-$	3×10^8	83
A129	$2\ HOBr + CO_3^{2-} = HBrO_2 + Br^- + HCO_3^-$	3.2×10^{-1}	69
A130	$BrO^- + HCO_3^- = HOBr + CO_3^{2-}$	3.9×10^7	83
A131	$BrO^- + CO_3^- = BrO + CO_3^{2-}$	4.3×10^7	65
A132	$BrO_2^- + CO_3^- = BrO_2 + CO_3^{2-}$	8×10^7	65
A133	$Br_2^- + NO_2^- = Br^- + Br^- + NO_2$	2×10^7	84
A134	$Br^- + O^- = Br + O^{-2}$	1.8×10^8	70
A135	$Cl + Cl^- = Cl_2^-$	8.6×10^9	85
A136	$Cl + H_2O = HOCl^- + H^+$	2.5×10^5	86
A137	$Cl + Cl = Cl_2$	8.8×10^7	87
A138	$Cl + OH^- = HOCl^-$	1.8×10^{10}	63
A139	$Cl + HO_2 = Cl^- + H^+ + O_2$	3.1×10^{10}	88
A140	$Cl + H_2O_2 = Cl^- + HO_2 + H^+$	4.1×10^7	89
A141	$Cl^- + OH = HOCl^-$	4.3×10^9	90
A142	$Cl^- + HOCl^- = Cl_2^- + OH^-$	1×10^4	91
A143	$Cl^- + O_3 = ClO^- + O_2$	3×10^{-3}	71
A144	$Cl^- + HOCl + H^+ = Cl_2 + H_2O$	2.1×10^4	88
A145	$Cl^- + HOCl + CO_2 = Cl_2 + HCO_3^-$	2.7	92
A146	$Cl^- + HOCl + HCO_3^- = Cl_2 + CO_3^{2-}$	1.2×10^{-2}	92
A147	$ClO^- + H_2O = HOCl + OH^-$	1×10^2	92
A148	$ClO^- + O_3 = Cl^- + O_2 + O_2$	1.1×10^2	62
A149	$Cl_2 + HO_2 = Cl_2^- + H^+ + O_2$	1×10^9	93
A150	$Cl_2 + H_2O = HOCl + Cl^- + H^+$	22	88
A151	$Cl_2 + OH^- = HOCl + Cl^-$	1×10^8	88
A152	$Cl_2 + HO_2^- = 2\ Cl^- + H^+ + O_2$	1.1×10^8	94
A153	$Cl_2 + HCO_3^- = HOCl + Cl^- + CO_2$	3.2×10^3	92
A154	$Cl_2 + CO_3^{2-} = HOCl + Cl^- + HCO_3^-$	1.4×10^5	92
A155	$Cl_2^- + H_2O = HOCl^- + H+ + Cl^-$	1.3×10^3	86
A156	$Cl_2^- + Cl_2^- = Cl_2 + Cl^- + Cl^-$	1.8×10^9	95
A157	$Cl_2^- + OH^- = HOCl^- + Cl^-$	4.5×10^7	96
A158	$Cl_2^- + HO_2 = Cl^- + Cl^- + H^+ + O_2$	1×10^9	97

A159	$Cl_2^- + O_2^- = Cl^- + Cl^- + O_2$	1×10^9	98
A160	$Cl_2^- + H_2O_2 = Cl^- + Cl^- + HO_2 + H^+$	4.1×10^4	99
A161	$Cl_2^- + OH = HOCl + Cl^-$	1×10^9	96
A162	$Cl_2^- + O_3 = ClO^- + Cl + O_2$	9×10^7	100
A163	$Cl_2^- = Cl + Cl^-$	6×10^4	101
A164	$Cl_2^- + CO_3^{2-} = CO_3^- + Cl^- + Cl^-$	2.7×10^6	102
A165	$HOCl + Cl = Cl^- + ClO + H^+$	3×10^9	63
A166	$HOCl + O_2^- = Cl + OH + O_2$	7.5×10^6	103
A167	$HOCl + HO_2^- = Cl^- + O_2 + H_2O$	4.4×10^7	104
A168	$HOCl + HOCl = Cl_2O + H_2O$	0.08×10^{-2}	105
A169	$HOCl + HOCl = Cl_2O + H_2O$	3.1	105
A170	$HOCl^- + H^+ = Cl + H_2O$	3.2×10^{10}	90
A171	$HOCl + H^+ + Cl^- = Cl_2 + H_2O$	2.2×10^4	106
A172	$HOCl + OH^- = ClO^- + H_2O$	2.8×10^{10}	106
A173	$Cl_2O + H_2O = HOCl + HOCl$	7	105
A174	$Cl_2O + H_2O = HCl + HCl + O_2$	0	105
A175	$Cl + HCO_3^- = CO_3^- + Cl^- + H^+$	2.2×10^8	102
A176	$Cl + CO_3^{2-} = CO_3^- + Cl^-$	5×10^8	102
A177	$HOCl + Br^- + H^+ = BrCl + H_2O$	2.3×10^6	106
A178	$Cl_2^- + Br^- = BrCl^- + Cl^-$	4.9×10^9	88
A179	$BrCl^- + Cl^- = Cl_2^- + Br^-$	1.1×10^2	88
A180	$BrCl^- + Br^- = Br_2^- + Cl^-$	8×10^9	88
A181	$Br_2^- + Cl^- = BrCl^- + Br^-$	4.3×10^6	88
A182	$HOCl^- + Br^- = BrCl^- + OH^-$	1×10^8	Estimated

[a]Obtained by matching NO_2 production from pure $NaNO_3$. This value was varied as the halide to ni nitrate ratio changed.
[b]Based on published quantum yields the rate is 10 times slower than A1.
[c] Based on published quantum yields the rate is 10 times faster than A1.

Table S4: Henry's Law Constants

no	Species	H_{298} (M^{-1}/atm)	ref	no	Species	H_{298} (M^{-1}/atm)	ref
H1	O_3	1.09 E-2	107	H14	$BrNO_2$	0.3	108
H2	O_2	0.00125	109	H15	Br	1.2	110
H3	OH	30	111	H16	HCl	2500	109
H4	CO_2	0.035	112	H17	HOCl	480	111
H5	HO_2	3900	111	H18	ClNO	0.05	113
H6	H_2O_2	110000	114	H19	$ClNO_2$	0.046	108
H7	HNO_3	210000	115	H20	$ClONO_2$	1.0 E10[a]	116
H8	NO_3	12	117	H21	Cl_2	0.093	118
H9	Br_2	0.7	119	H22	Cl_2O	17	118
H10	HBr	0.913	120	H23	ClO_2	1	118
H11	HOBr	93	121	H24	Cl	0.2	110
H12	NO	0.0019	115	H25	BrCl	0.94	122
H13	NO_2	49	115				

[a]Used in lieu of estimated value of ∞ in ref. 116

Table S5: Photolysis Rate Constants

no	reaction	kp	no	reaction	kp
P1	$NO_2 = NO + O(^3P)$	6.92×10^{-4}	P11	$BrNO = Br + NO$	1.75×10^{-3}
P2	$HNO_3 = OH + NO$	5.35×10^{-6}	P12	$BrO_2 = BrO + O(^3P)$	1.05×10^{-2}
P3	$HONO = OH + NO$	1.45×10^{-4}	P13	$BrONO_2 = Br + NO_3$	4.13×10^{-4}
P4	$O_3 = O_2 + O(^1D)$	8.00×10^{-4}	P14	$Cl_2 = Cl + Cl$	2.94×10^{-4}
P5	$O_3 = O_2 + O(^3P)$	8.90×10^{-5}	P15	$ClNO = Cl + NO$	3.41×10^{-4}
P6	$H_2O_2 = OH + OH$	1.0×10^{-6}	P16	$ClNO_2 = Cl + NO_2$	3.51×10^{-4}
P7	$Br_2 = Br + Br$	7.62×10^{-5}	P17	$HOCl = OH + Cl$	1.07×10^{-4}
P8	$BrO + O_2 = Br + O_3$	6.30×10^{-3}	P18	$ClO_2 = ClO + O1$	9.66×10^{-4}
P9	$HOBr = Br + OH$	2.87×10^{-4}	P19	$ClONO_2 = Cl + NO_3$	5.48×10^{-5}
P10	$BrNO_2 = Br + NO_2$	6.10×10^{-3}	P20	$ClONO_2 = ClO + NO_2$	3.56×10^{-5}

Calculated based on the measured kp for NO_2 over the range 240 – 600 nm from cross sections and quantum yields available in JPL publication[7] as well as our own narrow band UVB lamp intensity data. For example, the kp for HONO was calculated as follows:

$$\frac{k_p^{HONO}}{k_p^{NO_2}} = \frac{\int_{240\,nm}^{600\,nm} \Phi_{HONO}(\lambda)\,\sigma_{HONO}(\lambda) F(\lambda)\,d(\lambda)}{\int_{240\,nm}^{600\,nm} \Phi_{NO2}(\lambda)\,\sigma_{NO2}(\lambda)\,F(\lambda) d(\lambda)}$$

EDX Images of NaCl/NaBr/$NaNO_3$

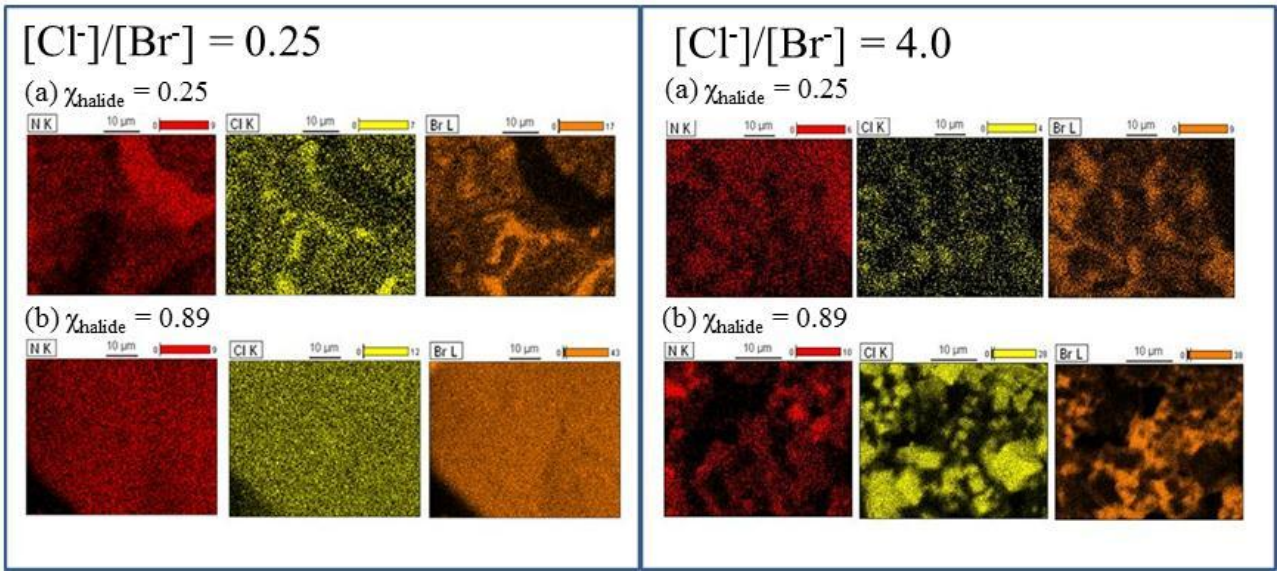

Figure S1: Elemental maps for mixtures of $[Cl^-]/[Br^-]$ = 0.25 and 4.0 as function of χ_{halide} [from left to right nitrogen (red) , chlorine (yellow) and bromine (orange)].

MD Simulations for NaCl/NaBr/$NaNO_3$ mixtures

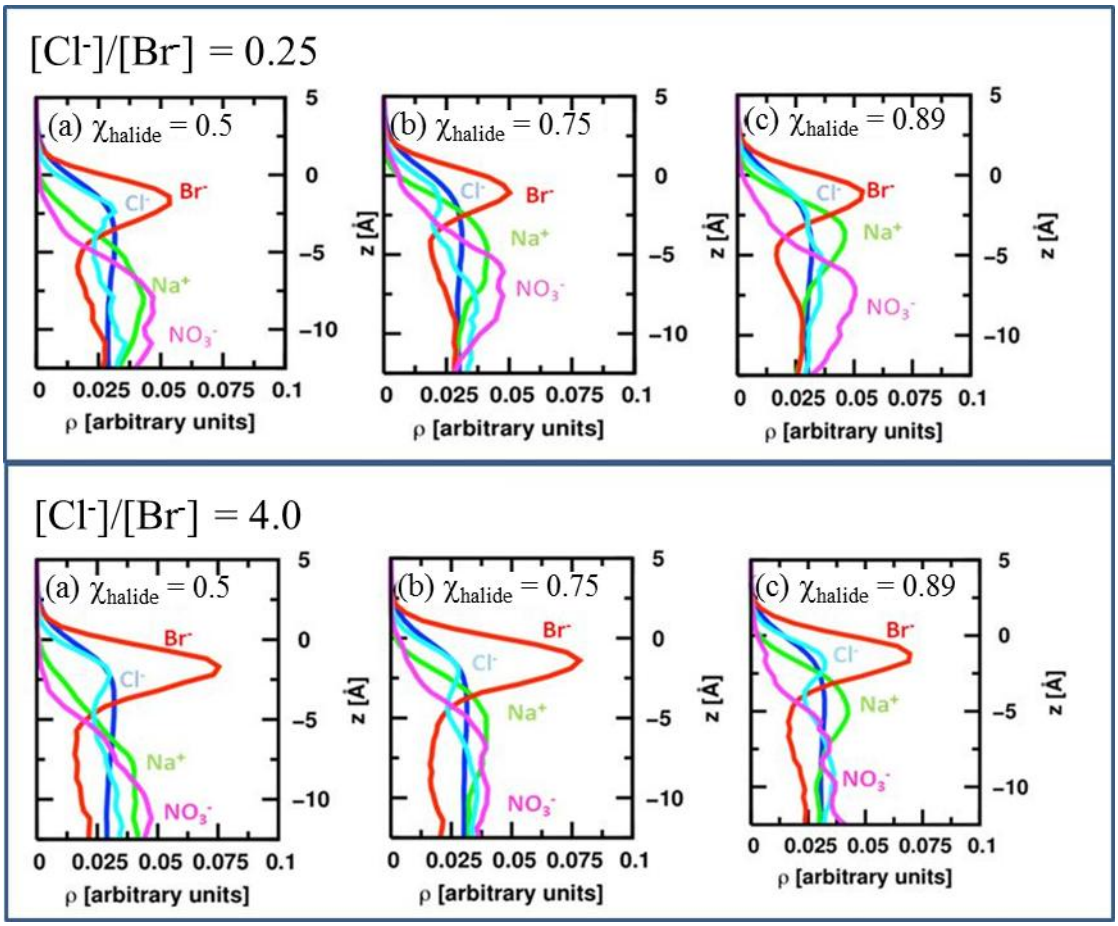

Figure S2: Density profiles for MD simulations of the air-water interface of $[Cl^-]/[Br^-]$ = 0.25 and 4.0 of (a) χ_{halide}= 0.5, (b) χ_{halide} = 0.75, and (c) χ_{halide} = 0.89.

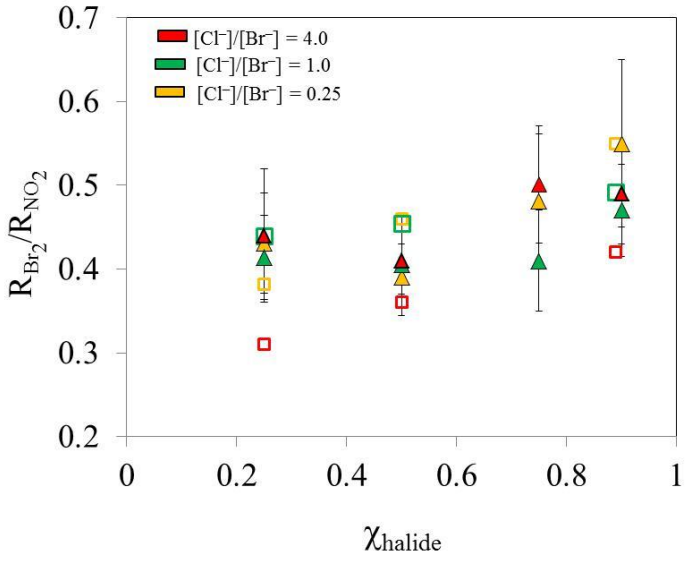

Figure S3: The rate of Br_2/the rate of NO_2 for NaCl/NaBr/$NaNO_3$ photolysis experiments. The open symbols are the model predicted values and the closed are the experimental values.

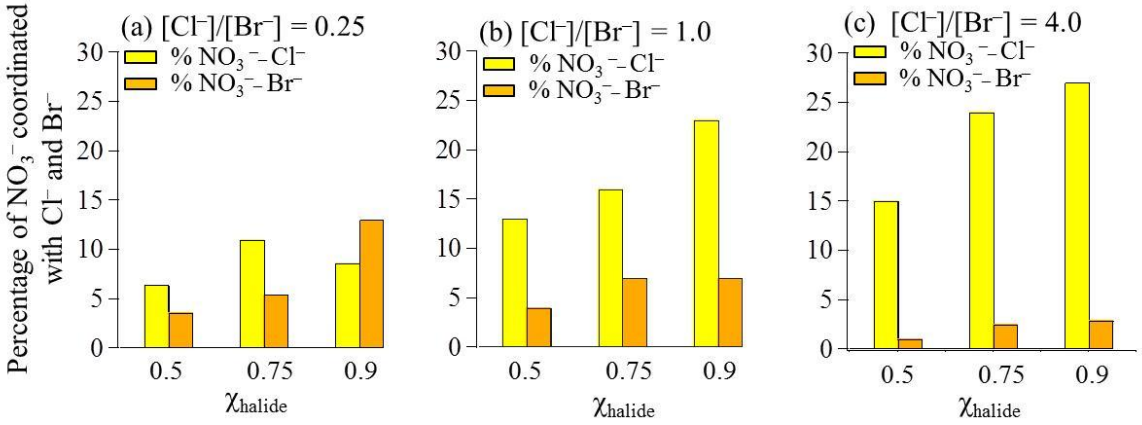

Figure S4. Percentage of NO_3^- coordinated within 3.8 Å with Cl^- or Br^- for NaCl/NaBr/$NaNO_3$ mixtures.

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