Halogen activation in the plume of Masaya volcano: field observations and box model investigations

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Table S 1: Gas species used in the HSC model and the mixing ratio of the atmospheric background composition taken from (Roberts et al., 2014).

Species	Mixing ratio	Species	Mixing ratio
H_2O(g)	-	Cl(g)	-
Ar(g)	0.0095	I(g)	-
N_2(g)	0.78	F(g)	-
O_2(g)	0.21	BrO(g)	-
CO_2(g)	0.0004	ClO(g)	-
CH_4(g)	1.70E-06	IO(g)	-
CO(g)	1.5E-07	O(g)	-
O_3(g)	6.40E-08	Cl_2(g)	-
OH(g)	6.90E-13	Br_2(g)	-
H_2O_2(g)	-	I_2(g)	-
HO_2(g)	3.00E-11	BrCl(g)	-
NO(g)	5.00E-11	HOCl(g)	-
NO_2(g)	1.10E-10	H_2(g)	-
HNO_2(g)	-	H(g)	-
NO_3(g)	5.00E-14	H_2SO_4(g)	-
HNO_3(g)	-	N_2O(g)	-
N_2O_5(g)	-	HNO(g)	-
CH_3OH(g)	-	OClO(g)	-
SO_2(g)	-	HF(g)	-
HCl(g)	-	HI(g)	-
HBr(g)	-	Br(g)	-

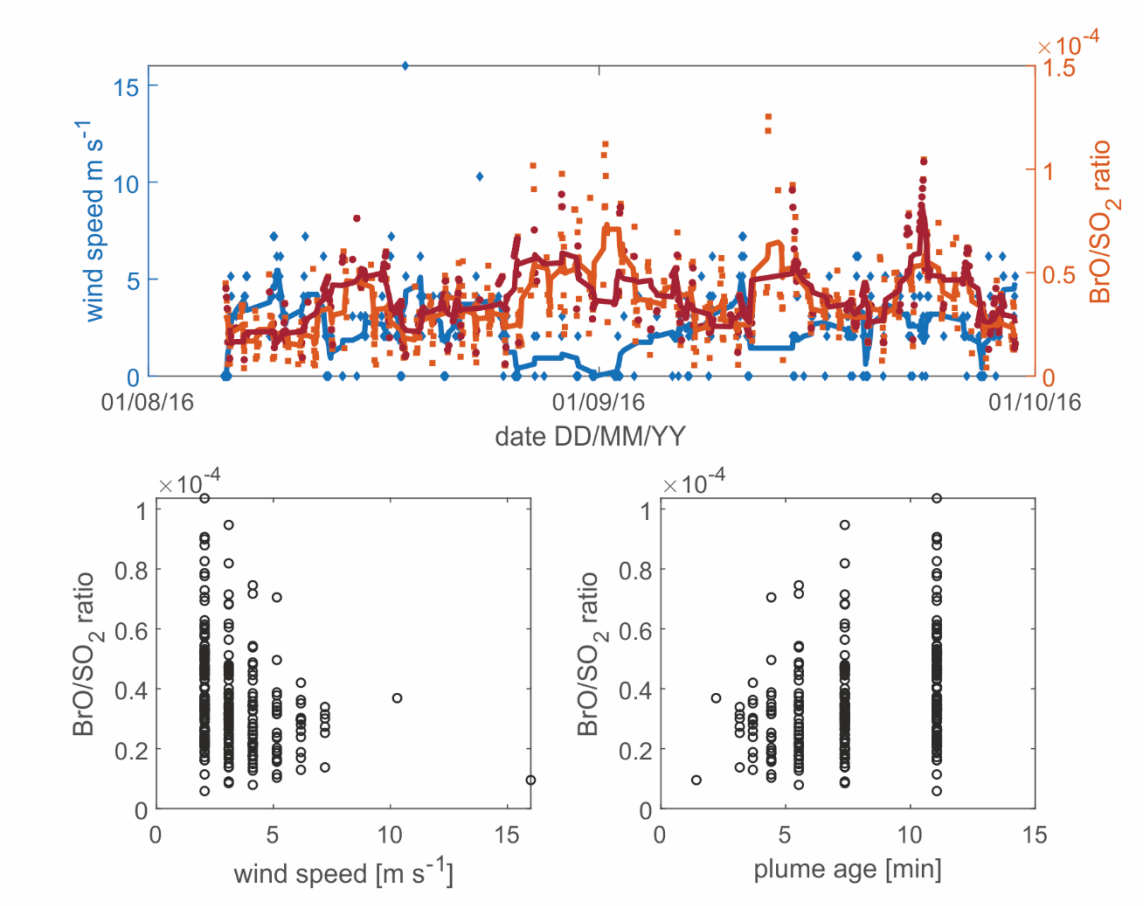
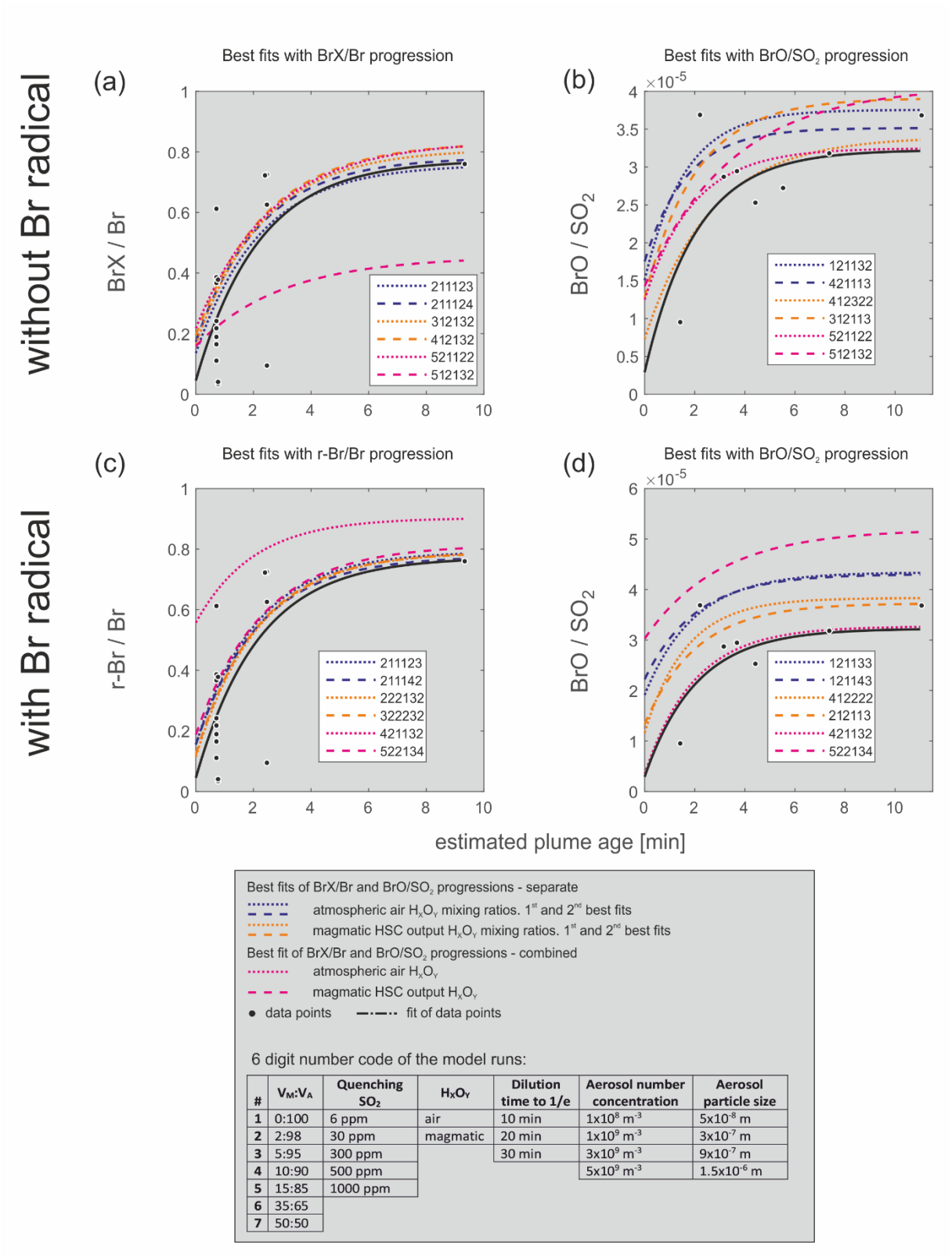


Figure S 1: (a) Wind speed at the meteorological measurement station at Managua airport (blue) and BrO/SO_2 mixing ratios at Masaya volcano (orange) and interpolated BrO/SO_2 mixing ratios (red) at the time of wind speed measurements; (b) BrO/SO_2 mixing ratio vs. wind speed and (c) BrO/SO_2 mixing ratio vs. estimated plume age



#	V_M:V_A	Quenching SO_2	H_XO_Y	Dilution time to 1/e	Aerosol number concentration	Aerosol particle size
1	0:100	6 ppm	air	10 min	$1x10^{8}$ m^{-3}	$5x10^{-8}$ m
2	2:98	30 ppm	magmatic	20 min	$1x10^{9}$ m^{-3}	$3x10^{-7}$ m
3	5:95	300 ppm		30 min	$3x10^{9}$ m^{-3}	$9x10^{-7}$ m
4	10:90	500 ppm			$5x10^{9}$ m^{-3}	$1.5x10^{-6}$ m
5	15:85	1000 ppm				
6	35:65					
7	50:50					

Figure S 21: (a) BrX/Br samples (black circles), fit through the sample data points using *f(x) = a*exp(-b*x) + c* (Eq. 1, see text) as a fit function (black line), fits of the closest model runs see description in legend (modelled BrX includes: Br_2, BrCl, $BrNO_2$, $BrNO_3$, HOBr and BrO), (b) BrO/SO_2 median values for different plume ages and fits through measurement and model data using Eq. 1 similar to (a), (c) and (d) similar procedure as in (a) and (b), but modelled reactive Br species (r-Br) also include Br radicals.

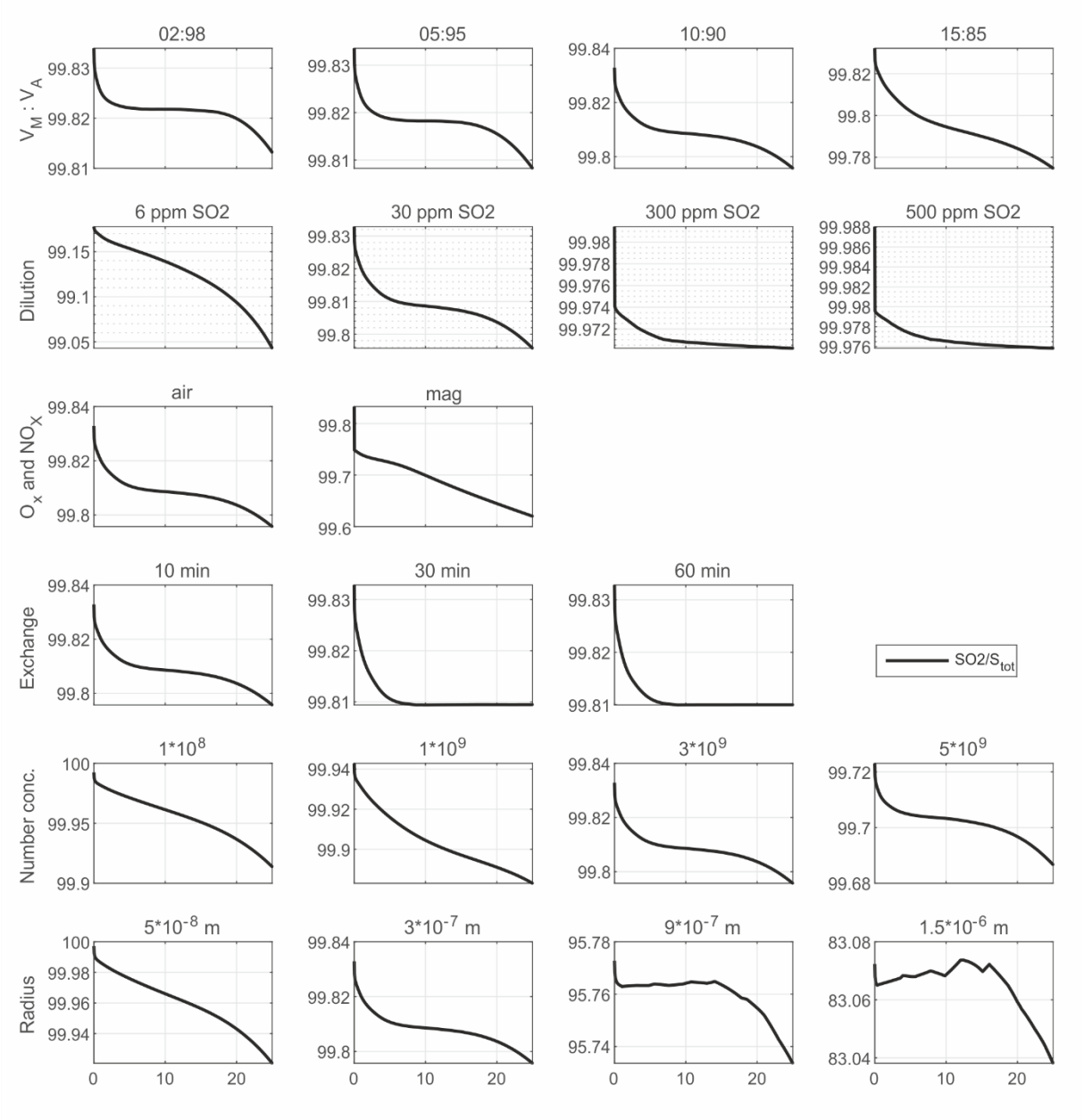


Figure S 2: SO_2 over total sulfur for selected CAABA/MECCA model runs corresponding to Figure 9. Variations of the base run by changes of one parameter (horizontal rows).

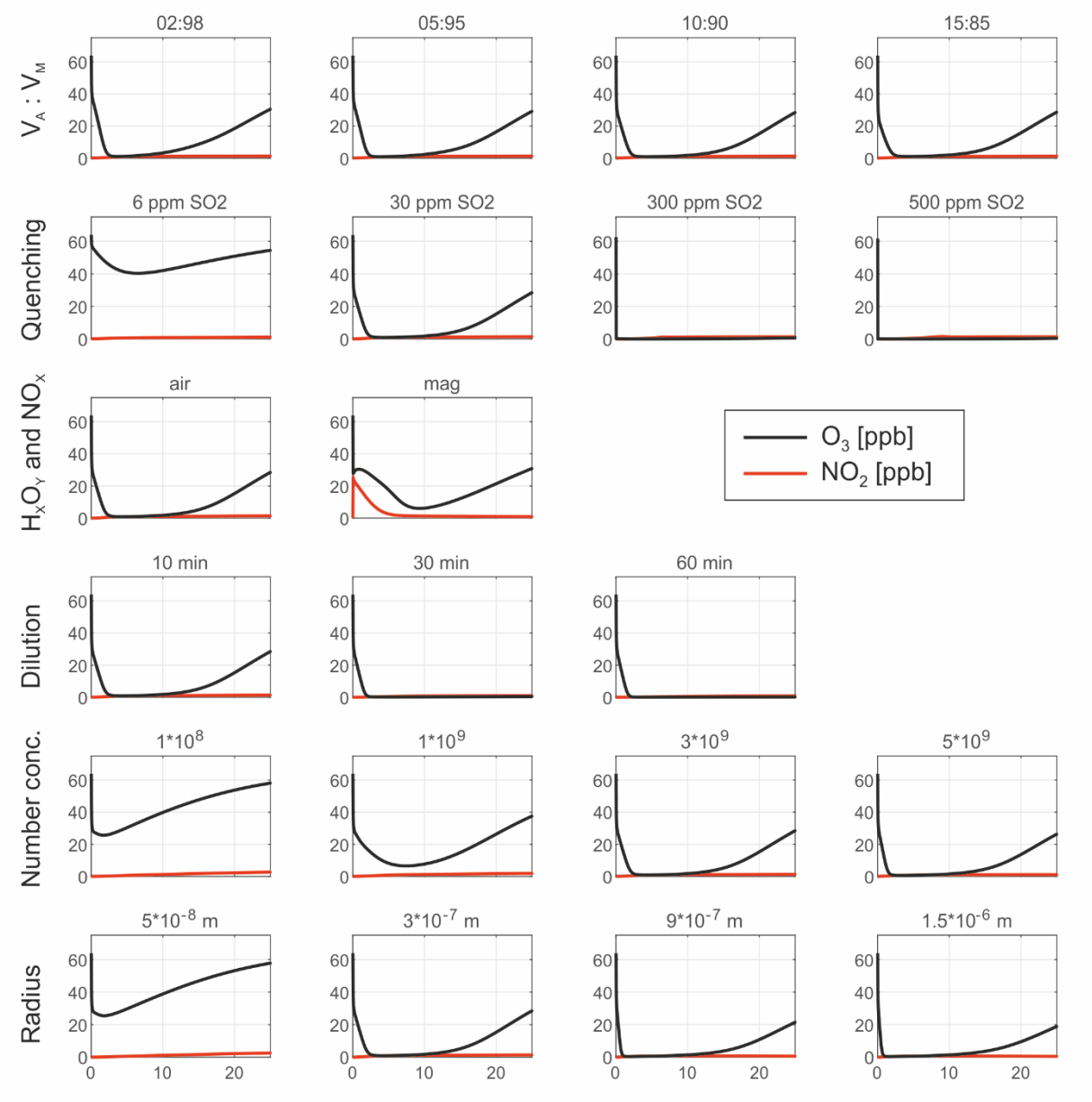


Figure S 3: O_3 and NO_2 mixing ratios during the model runs in Figure 9. Variations of the base run by changes of one parameter (horizontal rows)

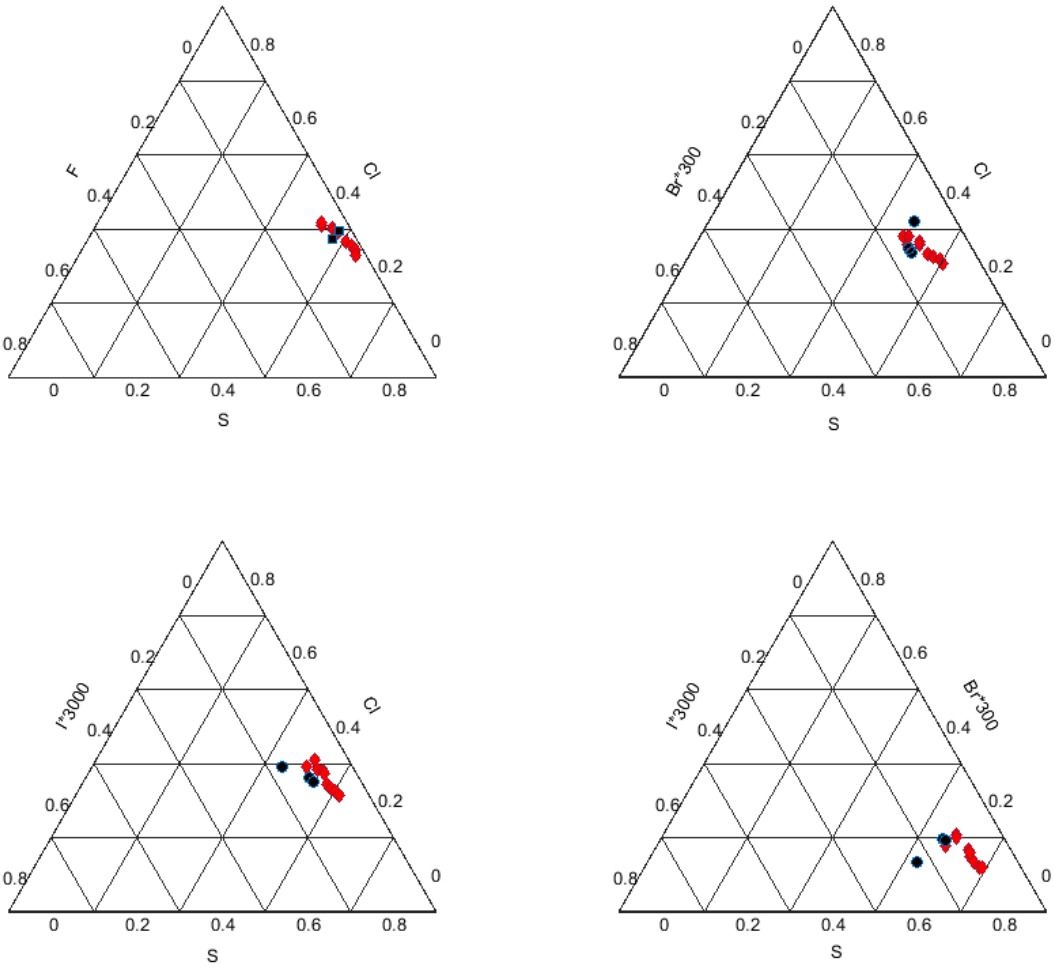


Figure S 4: Ternary plots of Halogen to Sulfur ratios; red diamonds: July samples, black circles: September samples

Table S 2: Results of denuder, alkaline and electrochemical sensor measurements (G = ground, R = Raschig tube, D = Drechsel bottle, UAV = unmanned aerial vehicle, Type 1 = 1 M NaOH, 4 = 4 M NaOH). HalX (e.g., Br_2, Cl_2 or BrCl) mixing ratios were derived from denuder samples with known volume of sampled plume gas; for certain alkaline trap samples the sampled volume is unknown and only a ratio of the respective halogen to sulfur was calculated from sample concentrations.

No.	Date	Type	Location	Distance [m]	S (SO_2) [ppm]	F [ppm]	F/S	Cl [ppm]	Cl/S	ClX [ppb]	ClX/S	ClX/Cl	Br_Y [ppb]	Br/S	BrX [ppb]	BrX/S	BrX/Br	I [ppb]	I/S	IX [ppb]	IX/S	IX/I
1	14.07.2016	GR 1	Lookout (s)	231 ± 20	4.18 ± 0.22	0.12 ± 0.01	1.6E-01 ± 1.2E-02	3.24 ± 0.17	0.77 ± 0.06				3.72 ± 0.07	8.89E-04 ± 4.95E-05				0.30 ± 0.07	7.2E-05 ± 1.8E-05			
2	14.07.2016	GD 1	Pole	214 ± 20	0.71 ± 0.04		1.1E-01 ± 8.1E-03	0.53 ± 0.03	0.75 ± 0.06	0.17 ± 0.24	2.4E-04 ± 3.4E-04	3.2E-04 ± 4.6E-04	1.11 ± 0.06	1.57E-03 ± 1.14E-04	0.68 ± 0.15	9.6E-04 ± 2.2E-04	0.61 ± 0.14	0.06 ± 0.06	8.5E-05 ± 7.9E-05	0.11 ± 0.01	1.6E-04 ± 2.0E-05	
3	14.07.2016	GR 1	Pole	214 ± 20		0.15 ± 0.01	1.8E-01 ± 1.3E-02	2.83 ± 0.15	0.80 ± 0.06				3.54 ± 0.06	1.00E-03 ± 5.48E-05				0.18 ± 0.06	5.2E-05 ± 1.7E-05			
4	14.07.2016	GD 1	Pole	214 ± 20	0.83 ± 0.04		5.6E-02 ± 4.0E-03	0.63 ± 0.03	0.76 ± 0.06	0.17 ± 0.24	2.1E-04 ± 3.0E-04	2.7E-04 ± 3.9E-04	1.85 ± 0.08	2.24E-03 ± 1.50E-04	0.68 ± 0.15	8.2E-04 ± 1.9E-04	0.37 ± 0.08	0.05 ± 0.08	5.6E-05 ± 9.5E-05	0.11 ± 0.01	1.4E-04 ± 1.7E-05	
5	14.07.2016	GD 4	Pole	214 ± 20		0.52 ± 0.03	1.2E-01 ± 8.8E-03		0.90 ± 0.06					5.46E-04 ± 3.02E-05					6.2E-05 ± 7.4E-06			
6	15.07.2016	GR 1	Nindirí Rim	740 ± 50	1.13 ± 0.06	0.34 ± 0.02	3.8E-02 ± 2.7E-03	0.54 ± 0.03	0.48 ± 0.04	0.73 ± 0.18	6.5E-04 ± 1.6E-04	1.3E-03 ± 3.3E-04	0.77 ± 0.03	6.86E-04 ± 4.71E-05	0.56 ± 0.10	5.0E-04 ± 8.9E-05	0.72 ± 0.13	0.05 ± 0.03	4.7E-05 ± 3.1E-05	0.07 ± 0.01	5.9E-05 ± 7.0E-06	
7	15.07.2016	GR 1	Pole	214 ± 20	8.81 ± 0.46		1.0E-01 ± 7.1E-03	4.45 ± 0.23	0.51 ± 0.04	0.26 ± 0.26	3.0E-05 ± 3.0E-05	5.9E-05 ± 5.9E-05	4.44 ± 0.08	5.04E-04 ± 2.76E-05	1.71 ± 0.19	1.9E-04 ± 2.4E-05	0.39 ± 0.04	0.33 ± 0.08	3.8E-05 ± 8.8E-06	0.17 ± 0.02	1.9E-05 ± 2.1E-06	0.51 ± 0.13
8	15.07.2016	GD 4	Pole	214 ± 20			7.9E-02 ± 5.6E-03		0.72 ± 0.05					8.79E-04 ± 8.08E-05					7.2E-05 ± 2.5E-05			
9	15.07.2016	GD 4	Pole	214 ± 20					0.84 ± 0.06					7.74E-04 ± 4.32E-05					4.0E-05 ± 2.7E-06			
10	16.07.2016	GR 1	Nindirí Rim	740 ± 50	0.98 ± 0.05	0.37 ± 0.02	4.9E-02 ± 3.5E-03	1.32 ± 0.07	1.35 ± 0.10				1.62 ± 0.04	1.66E-03 ± 9.65E-05	0.15 ± 0.07	1.6E-04 ± 6.8E-05	0.09 ± 0.04	0.09 ± 0.04	9.6E-05 ± 4.3E-05	0.03 ± 0.00	2.6E-05 ± 4.3E-06	0.27 ± 0.13
11	16.07.2016	GR 1	Pole	214 ± 20	7.56 ± 0.39			4.54 ± 0.24	0.60 ± 0.04				4.97 ± 0.10	6.57E-04 ± 3.66E-05				0.36 ± 0.10	4.7E-05 ± 1.3E-05			
12	17.07.2016	UAV	Caldera Valley	1989 ± 100	1.92 ± 0.09										1.26 ± 0.69	6.6E-04 ± 3.6E-04				0.18 ± 0.04	9.5E-05 ± 2.2E-05	
13	18.07.2016	GR 1	Nindirí Rim	740 ± 50	0.74 ± 0.04	0.10 ± 0.01	2.7E-02 ± 1.9E-03	1.70 ± 0.09	2.30 ± 0.17				1.31 ± 0.03	1.78E-03 ± 9.89E-05				0.05 ± 0.03	6.9E-05 ± 3.5E-05	0.03 ± 0.00	3.9E-05 ± 5.2E-06	0.57 ± 0.30
14	18.07.2016	GR 1	Pole	214 ± 20	3.61 ± 0.19			1.95 ± 0.10	0.54 ± 0.04				1.85 ± 0.04	5.11E-04 ± 2.86E-05	0.45 ± 0.06	1.2E-04 ± 1.7E-05	0.24 ± 0.03	0.15 ± 0.04	4.2E-05 ± 1.1E-05	0.09 ± 0.00	2.6E-05 ± 1.5E-06	0.62 ± 0.15
15	20.07.2016	GR 1	Pole	214 ± 20	2.65 ± 0.14	0.09 ± 0.01	3.3E-02 ± 2.3E-03	1.51 ± 0.08	0.57 ± 0.04				1.55 ± 0.03	5.84E-04 ± 3.28E-05	0.34 ± 0.05	1.3E-04 ± 2.1E-05	0.22 ± 0.03	0.12 ± 0.03	4.5E-05 ± 1.3E-05	0.08 ± 0.01	3.1E-05 ± 2.6E-06	0.70 ± 0.20
16	20.07.2016	GR 1	Nindirí Rim	740 ± 50	0.96 ± 0.05			0.89 ± 0.05	0.93 ± 0.07				1.22 ± 0.03	1.28E-03 ± 7.30E-05				0.06 ± 0.03	6.6E-05 ± 3.0E-05	0.02 ± 0.00	2.0E-05 ± 3.0E-06	0.31 ± 0.15
17	20.07.2016	UAV	Caldera Valley	1896 ± 100	0.51 ± 0.05										2.91 ± 0.75	5.7E-03 ± 1.6E-03				0.08 ± 0.03	1.5E-04 ± 6.4E-05	
18	20.07.2016	UAV	Caldera Valley	2122 ± 100	0.59 ± 0.05										1.19 ± 0.62	2.0E-03 ± 1.1E-03				0.06 ± 0.03	1.1E-04 ± 5.1E-05	
19	21.07.2016	GR 1	Nindirí Rim	740 ± 50	2.74 ± 0.14	0.29 ± 0.01	7.0E-02 ± 5.0E-03	2.00 ± 0.10	0.73 ± 0.05				2.56 ± 0.06	9.33E-04 ± 5.27E-05				0.17 ± 0.06	6.3E-05 ± 2.1E-05			
20	21.07.2016	GR 1	Nindirí Rim	740 ± 50	1.61 ± 0.08	0.56 ± 0.03	7.3E-02 ± 5.1E-03	1.46 ± 0.08	0.91 ± 0.07				1.81 ± 0.04	1.12E-03 ± 6.34E-05				0.09 ± 0.04	5.7E-05 ± 2.5E-05			
21	21.07.2016	GR 1	Pole	214 ± 20	4.06 ± 0.21		1.1E-01 ± 8.1E-03	2.76 ± 0.14	0.68 ± 0.05				3.05 ± 0.05	7.52E-04 ± 4.10E-05				0.19 ± 0.05	4.6E-05 ± 1.2E-05			
22	21.07.2016	GR 1	Pole	214 ± 20	7.67 ± 0.40		1.1E-01 ± 7.5E-03	5.36 ± 0.28	0.70 ± 0.05				5.57 ± 0.55	7.26E-04 ± 8.07E-05	0.92 ± 0.08	1.2E-04 ± 1.2E-05	0.17 ± 0.02	0.34 ± 0.55	4.4E-05 ± 7.1E-05	0.11 ± 0.01	1.4E-05 ± 1.2E-06	0.32 ± 0.52
23	21.07.2016	GD 1	Pole	214 ± 20		0.20 ± 0.01	7.4E-02 ± 5.2E-03		0.63 ± 0.04					6.16E-04 ± 3.09E-05					4.9E-05 ± 2.5E-06			
24	21.07.2016	GD 1	Pole	214 ± 20		0.14 ± 0.01	8.4E-02 ± 6.0E-03		0.84 ± 0.06					1.24E-03 ± 6.86E-05					9.2E-05 ± 4.8E-06			
25	22.07.2016	GR 1	Lookout (s)	231 ± 20	6.01 ± 0.31	0.46 ± 0.02	7.6E-02 ± 5.4E-03	4.34 ± 0.23	0.72 ± 0.05				5.86 ± 0.11	9.75E-04 ± 5.38E-05	0.20 ± 0.07	3.3E-05 ± 1.1E-05	0.03 ± 0.01	0.32 ± 0.11	5.3E-05 ± 1.8E-05	0.05 ± 0.01	8.7E-06 ± 1.0E-06	0.16 ± 0.06
26	22.07.2016	GR 1	Lookout (s)	231 ± 20	6.01 ± 0.31			4.34 ± 0.23	0.72 ± 0.05				5.86 ± 0.11	9.75E-04 ± 5.38E-05	0.24 ± 0.07	4.0E-05 ± 1.2E-05	0.04 ± 0.01	0.32 ± 0.11	5.3E-05 ± 1.8E-05	0.06 ± 0.01	1.0E-05 ± 1.1E-06	0.19 ± 0.07
27	01.09.2016	GR 1	Pole	214 ± 20	5.16 ± 0.27	0.52 ± 0.03	1.0E-01 ± 7.2E-03	3.35 ± 0.17	0.65 ± 0.05	1.16 ± 0.21	2.2E-04 ± 4.3E-05	3.5E-04 ± 6.5E-05	4.97 ± 0.08	9.63E-04 ± 5.27E-05	0.94 ± 0.10	1.8E-04 ± 2.2E-05	0.19 ± 0.02	0.36 ± 0.08	7.0E-05 ± 1.7E-05	0.12 ± 0.01	2.3E-05 ± 2.1E-06	0.32 ± 0.08
28	02.09.2016	GR 1	San Pedro Rim	720 ± 50						0.07 ± 0.10			0.35 ± 0.02		0.26 ± 0.05		0.72 ± 0.14	0.05 ± 0.02				0.75 ± 0.29
29	03.09.2016	GR 1	Nindirí Rim	740 ± 50	0.22 ± 0.01	0.17 ± 0.01	5.0E-02 ± 3.6E-03	0.64 ± 0.03	2.94 ± 0.22	0.55 ± 0.12	2.5E-03 ± 5.7E-04	8.5E-04 ± 1.9E-04	0.75 ± 0.02	3.45E-03 ± 2.07E-04	0.47 ± 0.06	2.2E-03 ± 3.0E-04	0.63 ± 0.08	0.05 ± 0.02	2.4E-04 ± 1.0E-04	0.01 ± 0.00	4.0E-05 ± 1.2E-05	0.17 ± 0.09
30	03.09.2016	GR 1	Pole	214 ± 20	3.31 ± 0.17			2.27 ± 0.12	0.69 ± 0.05	0.20 ± 0.12	6.1E-05 ± 3.7E-05	8.9E-05 ± 5.4E-05	3.27 ± 0.26	9.89E-04 ± 9.28E-05	0.36 ± 0.06	1.1E-04 ± 2.0E-05	0.11 ± 0.02	0.24 ± 0.26	7.3E-05 ± 7.7E-05	0.06 ± 0.00	1.9E-05 ± 1.8E-06	0.25 ± 0.27
31	03.09.2016	UAV	Nindirí Crater	351 ± 50	3.32 ± 0.14					1.42 ± 1.71	4.3E-04 ± 5.2E-04				1.04 ± 0.76	3.1E-04 ± 2.3E-04						
32	03.09.2016	UAV	Nindirí Crater	337 ± 50	11.04 ± 0.29					2.48 ± 1.35	2.2E-04 ± 1.2E-04				3.36 ± 0.77	3.0E-04 ± 7.0E-05				0.11 ± 0.03	9.8E-06 ± 2.8E-06	
33	03.09.2016	UAV	Nindirí Crater	337 ± 50	11.04 ± 0.29										1.32 ± 0.55	1.2E-04 ± 5.0E-05				0.13 ± 0.03	1.1E-05 ± 2.8E-06	
34	04.09.2016	GR 1	Nindirí Rim	740 ± 50	0.31 ± 0.02			1.02 ± 0.05	3.27 ± 0.24				1.08 ± 0.02	3.45E-03 ± 1.88E-04				0.05 ± 0.02	1.6E-04 ± 5.7E-05			
35	04.09.2016	GR 1	Lookout (night)	231 ± 20	0.85 ± 0.04			0.75 ± 0.04	0.88 ± 0.06	7.58 ± 0.83	8.9E-03 ± 1.1E-03	1.0E-02 ± 1.2E-03	0.60 ± 0.06	7.01E-04 ± 7.59E-05	0.23 ± 0.07	2.7E-04 ± 8.7E-05	0.38 ± 0.13	0.11 ± 0.06	1.2E-04 ± 6.7E-05	0.04 ± 0.00	4.3E-05 ± 5.5E-06	0.35 ± 0.19
36	05.09.2016	GR 1	Cerro Ventarrón	2800 ± 200						0.75 ± 0.13			0.29 ± 0.02		0.22 ± 0.05		0.76 ± 0.20	0.03 ± 0.02		0.02 ± 0.00		0.92 ± 0.67

Table S 3: Overview on the HSC output and species and their mixing ratios at different volume ratios of atmospheric and magmatic gas at 1000°C

Temperature	1000°C							
VA:VM	0:100	1:99	2:98	5:95	10:90	15:85	35:65	50:50
H2O(g)	9.30E-01	9.21E-01	9.11E-01	8.83E-01	8.37E-01	7.90E-01	3.25E-01	4.65E-01
N2(g)	0.00E+00	7.80E-03	1.56E-02	3.90E-02	7.80E-02	1.17E-01	5.07E-01	3.90E-01
O2(g)	6.43E-06	2.04E-03	4.12E-03	1.04E-02	2.08E-02	3.13E-02	1.37E-01	1.05E-01
CO2(g)	4.39E-02	4.34E-02	4.30E-02	4.17E-02	3.95E-02	3.74E-02	1.56E-02	2.21E-02
CH4(g)	1.37E-24	1.32E-29	3.14E-30	4.52E-31	9.53E-32	3.56E-32	1.32E-34	6.51E-34
CO(g)	1.53E-06	8.48E-08	5.92E-08	3.62E-08	2.42E-08	1.87E-08	3.73E-09	6.04E-09
O3(g)	6.55E-18	3.72E-14	1.07E-13	4.25E-13	1.21E-12	2.23E-12	2.03E-11	1.36E-11
CH3OH(g)	1.14E-24	1.95E-28	6.61E-29	1.51E-29	4.51E-30	2.07E-30	1.60E-32	6.91E-32
SO2(g)	1.49E-02	1.47E-02	1.45E-02	1.40E-02	1.31E-02	1.24E-02	4.95E-03	7.12E-03
HCl(g)	1.03E-02	1.02E-02	1.01E-02	9.76E-03	9.25E-03	8.73E-03	3.59E-03	5.13E-03
HBr(g)	1.06E-05	9.11E-06	8.75E-06	8.07E-06	7.24E-06	6.59E-06	1.98E-06	3.16E-06
HF(g)	1.05E-03	1.04E-03	1.03E-03	9.99E-04	9.46E-04	8.93E-04	3.68E-04	5.26E-04
HI(g)	3.22E-08	7.64E-09	6.30E-09	4.76E-09	3.67E-09	3.03E-09	5.58E-10	1.01E-09
Br(g)	4.77E-07	1.75E-06	2.01E-06	2.37E-06	2.61E-06	2.70E-06	1.83E-06	2.28E-06
Cl(g)	1.42E-06	5.95E-06	7.06E-06	8.74E-06	1.01E-05	1.09E-05	1.01E-05	1.13E-05
I(g)	6.57E-07	6.62E-07	6.54E-07	6.31E-07	5.95E-07	5.60E-07	2.33E-07	3.30E-07
F(g)	6.34E-13	2.66E-12	3.16E-12	3.92E-12	4.54E-12	4.88E-12	4.53E-12	5.07E-12
BrO(g)	1.66E-12	1.09E-10	1.78E-10	3.33E-10	5.17E-10	6.58E-10	9.29E-10	1.02E-09
ClO(g)	1.13E-10	8.45E-09	1.43E-08	2.80E-08	4.59E-08	6.05E-08	1.17E-07	1.15E-07
IO(g)	1.39E-12	2.49E-11	3.49E-11	5.35E-11	7.14E-11	8.25E-11	7.15E-11	8.89E-11
Cl2(g)	2.12E-08	3.75E-07	5.28E-07	8.09E-07	1.09E-06	1.26E-06	1.08E-06	1.35E-06
Br2(g)	4.34E-11	5.84E-10	7.71E-10	1.07E-09	1.29E-09	1.39E-09	6.35E-10	9.92E-10
I2(g)	2.62E-12	2.65E-12	2.59E-12	2.41E-12	2.14E-12	1.90E-12	3.27E-13	6.60E-13
BrCl(g)	2.05E-09	3.16E-08	4.31E-08	6.30E-08	8.01E-08	8.93E-08	5.59E-08	7.81E-08
HOCl(g)	6.56E-09	1.16E-07	1.63E-07	2.50E-07	3.36E-07	3.89E-07	3.34E-07	4.17E-07
H2(g)	1.91E-05	1.06E-06	7.41E-07	4.52E-07	3.03E-07	2.33E-07	4.59E-08	7.50E-08
H(g)	3.16E-09	7.44E-10	6.21E-10	4.86E-10	3.97E-10	3.49E-10	1.55E-10	1.98E-10
H2SO4(g)	7.94E-09	1.38E-07	1.91E-07	2.84E-07	3.58E-07	3.91E-07	1.34E-07	2.42E-07
OClO(g)	9.98E-14	9.27E-14	2.22E-13	6.92E-13	1.61E-12	2.60E-12	1.05E-11	8.99E-12
OH(g)	1.73E-06	7.27E-06	8.62E-06	1.07E-05	1.24E-05	1.33E-05	1.24E-05	1.38E-05
H2O2(g)	1.06E-10	1.87E-09	2.63E-09	4.04E-09	5.42E-09	6.28E-09	5.39E-09	6.75E-09
HO2(g)	9.80E-11	7.34E-09	1.24E-08	2.43E-08	3.99E-08	5.27E-08	1.02E-07	9.99E-08
O(g)	2.73E-10	4.88E-09	6.93E-09	1.10E-08	1.56E-08	1.91E-08	3.99E-08	3.49E-08
NO(g)	0.00E+00	3.56E-06	7.15E-06	1.79E-05	3.59E-05	5.40E-05	2.35E-04	1.80E-04
NO2(g)	0.00E+00	4.34E-09	1.24E-08	4.93E-08	1.40E-07	2.58E-07	2.34E-06	1.57E-06
NO3(g)	0.00E+00	1.30E-16	5.29E-16	3.34E-15	1.34E-14	3.03E-14	5.75E-13	3.38E-13
HNO3(g)	0.00E+00	5.18E-14	1.75E-13	8.66E-13	2.85E-12	5.64E-12	4.75E-11	3.57E-11
N2O5(g)	0.00E+00	1.75E-28	2.03E-27	5.09E-26	5.81E-25	2.41E-24	4.16E-22	1.65E-22
N2O(g)	0.00E+00	2.18E-11	6.19E-11	2.46E-10	6.96E-10	1.28E-09	1.16E-08	7.80E-09
HNO(g)	0.00E+00	1.13E-12	1.90E-12	3.72E-12	6.09E-12	8.03E-12	1.55E-11	1.52E-11
HNO2(g)	0.00E+00	3.00E-10	7.15E-10	2.23E-09	5.16E-09	8.34E-09	3.36E-08	2.89E-08

Ar(g)	0.00E+00	1.00E-04	2.00E-04	5.00E-04	1.00E-03	1.50E-03	6.50E-03	5.00E-03
BrBrO(g)	4.38E-21	1.05E-18	1.97E-18	4.35E-18	7.43E-18	9.79E-18	9.34E-18	1.28E-17
BrF(g)	9.89E-15	1.52E-13	2.08E-13	3.04E-13	3.86E-13	4.31E-13	2.71E-13	3.78E-13
BrOBr(g)	9.20E-20	2.20E-17	4.14E-17	9.14E-17	1.56E-16	2.06E-16	1.96E-16	2.68E-16
BrOO(g)	6.85E-17	7.98E-14	1.85E-13	5.50E-13	1.21E-12	1.89E-12	5.57E-12	5.33E-12
CH3(g)	4.53E-27	1.84E-31	5.26E-32	9.68E-33	2.50E-33	1.06E-33	8.87E-36	3.43E-35
Cl2O(g)	1.45E-17	4.57E-15	9.14E-15	2.22E-14	4.22E-14	5.98E-14	1.07E-13	1.17E-13
ClClO(g)	0.00E+00	1.39E-14	2.77E-14	6.74E-14	1.28E-13	1.82E-13	3.25E-13	3.56E-13
ClF(g)	2.30E-14	4.05E-13	5.71E-13	8.77E-13	1.18E-12	1.36E-12	1.17E-12	1.46E-12
ClO2(g)	3.34E-17	4.47E-14	1.07E-13	3.33E-13	7.74E-13	1.25E-12	5.06E-12	4.33E-12
ClOCl(g)	4.38E-17	1.38E-14	2.76E-14	6.70E-14	1.27E-13	1.81E-13	3.24E-13	3.54E-13
ClOO(g)	3.30E-16	4.41E-13	1.06E-12	3.29E-12	7.65E-12	1.24E-11	5.00E-11	4.28E-11
COCl(g)	1.46E-14	3.40E-15	2.81E-15	2.13E-15	1.65E-15	1.37E-15	2.53E-16	4.58E-16
COCl2(g)	8.15E-17	7.98E-17	7.85E-17	7.34E-17	6.58E-17	5.88E-17	1.01E-17	2.04E-17
COOH(g)	1.91E-13	4.45E-14	3.68E-14	2.79E-14	2.16E-14	1.80E-14	3.32E-15	6.02E-15
COS(g)	1.40E-14	2.40E-18	8.17E-19	1.92E-19	5.99E-20	2.91E-20	5.31E-22	1.61E-21
CS(g)	6.48E-25	6.24E-30	1.50E-30	2.21E-31	4.88E-32	1.93E-32	1.69E-34	5.86E-34
CS2(g)	1.04E-27	3.10E-35	3.62E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
H2S(g)	5.56E-12	9.56E-16	3.25E-16	7.63E-17	2.38E-17	1.15E-17	2.08E-19	6.37E-19
H2S2(g)	3.71E-21	1.97E-27	3.28E-28	2.95E-29	4.31E-30	1.31E-30	2.16E-33	1.24E-32
HClCO(g)	7.97E-17	4.38E-18	3.03E-18	1.79E-18	1.13E-18	8.26E-19	6.77E-20	1.57E-19
HCN(g)	0.00E+00	1.72E-23	9.98E-24	4.75E-24	2.59E-24	1.76E-24	1.55E-25	3.21E-25
HCO(g)	2.03E-17	2.65E-19	1.55E-19	7.38E-20	4.04E-20	2.74E-20	2.42E-21	5.01E-21
HCOOH(g)	9.24E-13	5.07E-14	3.50E-14	2.08E-14	1.32E-14	9.59E-15	7.87E-16	1.82E-15
HIO(g)	2.15E-09	9.10E-09	1.07E-08	1.28E-08	1.39E-08	1.41E-08	5.43E-09	8.63E-09
HNCO(g)	0.00E+00	1.15E-18	9.47E-19	7.15E-19	5.53E-19	4.59E-19	8.46E-20	1.54E-19
HS(g)	5.29E-13	3.86E-16	1.57E-16	4.72E-17	1.80E-17	9.94E-18	4.04E-19	9.69E-19
HSO3Cl(g)	3.23E-12	5.61E-11	7.77E-11	1.15E-10	1.45E-10	1.59E-10	5.44E-11	9.78E-11
HSO3F(g)	2.30E-12	3.99E-11	5.54E-11	8.24E-11	1.04E-10	1.13E-10	3.89E-11	7.00E-11
IBr(g)	0.00E+00	1.36E-10	1.55E-10	1.76E-10	1.82E-10	1.78E-10	4.99E-11	8.86E-11
ICl(g)	1.74E-09	7.34E-09	8.61E-09	1.03E-08	1.12E-08	1.14E-08	4.37E-09	6.94E-09
IF(g)	3.13E-13	1.32E-12	1.55E-12	1.86E-12	2.03E-12	2.06E-12	7.92E-13	1.26E-12
IOO(g)	3.56E-17	1.14E-14	2.27E-14	5.52E-14	1.04E-13	1.48E-13	2.68E-13	2.91E-13
N(g)	0.00E+00	5.80E-18	8.20E-18	1.30E-17	1.83E-17	2.25E-17	4.68E-17	4.10E-17
N2O2(g)	0.00E+00	1.36E-18	5.51E-18	3.47E-17	1.39E-16	3.14E-16	5.93E-15	3.50E-15
N2O3(g)	0.00E+00	4.72E-20	2.71E-19	2.70E-18	1.54E-17	4.25E-17	1.68E-15	8.66E-16
NBr(g)	0.00E+00	3.68E-17	5.99E-17	1.12E-16	1.74E-16	2.20E-16	3.10E-16	3.40E-16
NH2(g)	0.00E+00	1.74E-17	1.72E-17	1.66E-17	1.57E-17	1.48E-17	6.05E-18	8.68E-18
NH2OH(g)	0.00E+00	8.53E-19	9.97E-19	1.19E-18	1.31E-18	1.33E-18	5.04E-19	8.09E-19
NH3(g)	0.00E+00	1.40E-14	1.15E-14	8.69E-15	6.72E-15	5.56E-15	1.01E-15	1.85E-15
NO2Cl(g)	0.00E+00	1.64E-15	5.54E-15	2.73E-14	8.97E-14	1.78E-13	1.50E-12	1.12E-12
NOBr(g)	0.00E+00	5.88E-13	1.36E-12	4.02E-12	8.84E-12	1.38E-11	4.05E-11	3.88E-11
NOCl(g)	0.00E+00	5.82E-11	1.39E-10	4.31E-10	9.99E-10	1.61E-09	6.50E-09	5.57E-09
NOF(g)	0.00E+00	1.18E-14	2.80E-14	8.73E-14	2.02E-13	3.27E-13	1.32E-12	1.13E-12
NOI(g)	0.00E+00	1.34E-14	2.67E-14	6.46E-14	1.22E-13	1.73E-13	3.11E-13	3.39E-13
NS(g)	0.00E+00	1.82E-19	1.26E-19	7.64E-20	5.05E-20	3.88E-20	7.39E-21	1.22E-20

OBrO(g)	1.33E-19	1.55E-16	3.60E-16	1.07E-15	2.35E-15	3.67E-15	1.08E-14	1.04E-14
OIO(g)	1.05E-19	3.37E-17	6.71E-17	1.63E-16	3.09E-16	4.37E-16	7.92E-16	8.62E-16
S(g)	3.84E-14	1.19E-16	5.80E-17	2.23E-17	1.04E-17	6.54E-18	5.98E-19	1.12E-18
S2(g)	4.46E-16	4.27E-21	1.02E-21	1.50E-22	3.28E-23	1.29E-23	1.08E-25	3.82E-25
S2Br2(g)	2.58E-27	3.32E-31	1.04E-31	2.15E-32	5.64E-33	2.39E-33	9.15E-36	5.04E-35
S2Cl(g)	2.64E-20	1.07E-24	3.01E-25	5.50E-26	1.39E-26	5.89E-27	4.57E-29	1.80E-28
S2Cl2(g)	5.62E-24	9.52E-28	3.19E-28	7.21E-29	2.11E-29	9.63E-30	6.92E-32	3.05E-31
S2O(g)	5.38E-15	9.19E-19	3.11E-19	7.28E-20	2.25E-20	1.09E-20	1.90E-22	5.88E-22
S3(g)	3.22E-25	9.57E-33	1.11E-33	6.30E-35	6.43E-36	1.59E-36	1.00E-36	1.00E-36
S4(g)	2.89E-34	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
S5(g)	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
S6(g)	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36	1.00E-36
SBr2(g)	2.54E-17	1.06E-18	6.82E-19	3.65E-19	2.05E-19	1.39E-19	5.79E-21	1.70E-20
SCl(g)	2.57E-15	3.34E-17	1.93E-17	9.20E-18	4.98E-18	3.36E-18	2.85E-19	5.98E-19
SCl2(g)	1.44E-15	7.88E-17	5.41E-17	3.19E-17	2.00E-17	1.45E-17	1.14E-18	2.67E-18
SF(g)	7.85E-18	1.02E-19	5.91E-20	2.82E-20	1.52E-20	1.03E-20	8.74E-22	1.84E-21
SO(g)	2.72E-08	1.50E-09	1.04E-09	6.34E-10	4.20E-10	3.23E-10	6.18E-11	1.02E-10
SO2Cl2(g)	5.82E-16	1.01E-14	1.40E-14	2.08E-14	2.61E-14	2.85E-14	9.78E-15	1.76E-14
SO2ClF(g)	5.95E-16	1.03E-14	1.43E-14	2.13E-14	2.68E-14	2.92E-14	1.01E-14	1.81E-14
SO3(g)	5.66E-06	9.94E-05	1.39E-04	2.13E-04	2.83E-04	3.28E-04	2.74E-04	3.45E-04
SOCl(g)	7.07E-11	1.64E-11	1.35E-11	1.02E-11	7.80E-12	6.46E-12	1.14E-12	2.10E-12
SOCl2(g)	4.44E-14	4.33E-14	4.23E-14	3.95E-14	3.50E-14	3.12E-14	5.12E-15	1.05E-14
SOF(g)	4.70E-11	1.09E-11	8.96E-12	6.78E-12	5.19E-12	4.30E-12	7.63E-13	1.40E-12

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