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Supplement of

Evaluation of the accuracy of thermal dissociation CRDS and LIF techniques for atmospheric measurement of reactive nitrogen species

Caroline C. Womack et al.

Correspondence to: Steven S. Brown (steven.s.brown@noaa.gov)

Supporting information

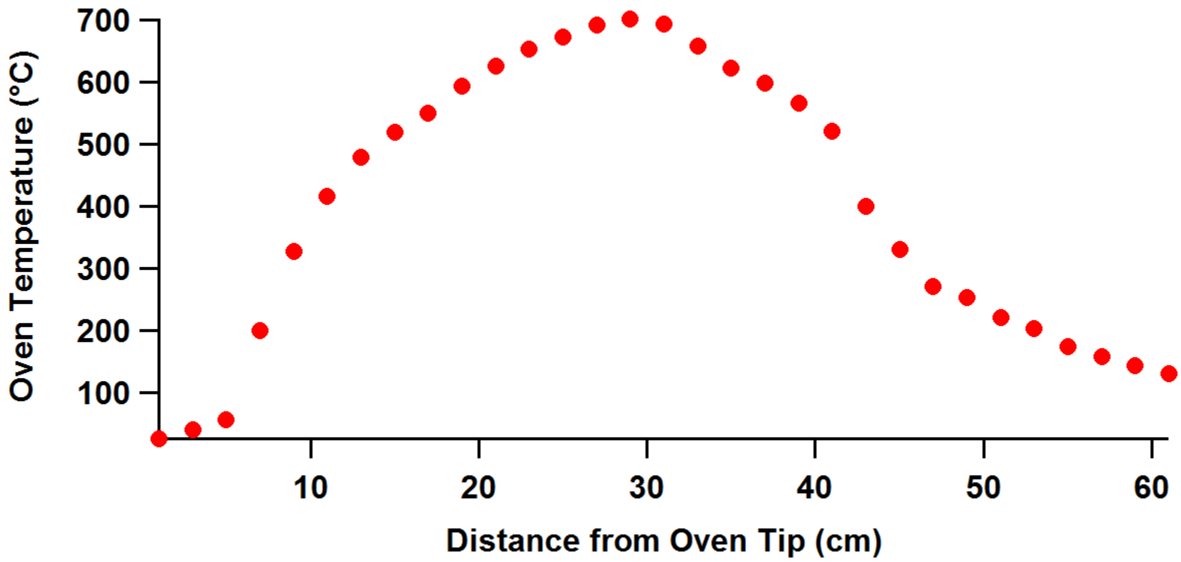

Figure S1. A sample oven temperature profile measured with a 2.0 slpm flow rate through the TD oven inlet, while the oven was set at 650 °C. Distance is measured from end of the quartz tube. The first ~5 cm are not heated, and the heated portion stretched from approximately 5 – 42 cm, with a cooling region from 42 – 63 cm.

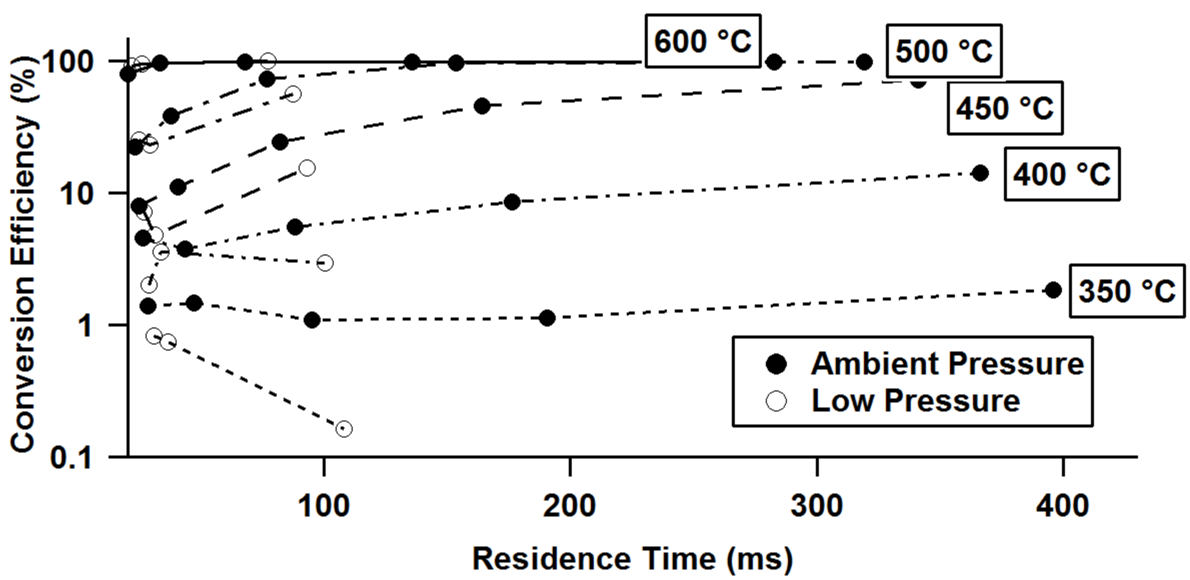

Figure S2. Log scale plot of conversion efficiency vs residence time. This plot is similar to the linear plot in Fig. 3, but is presented in log space to highlight small differences in the low conversion efficiency region.

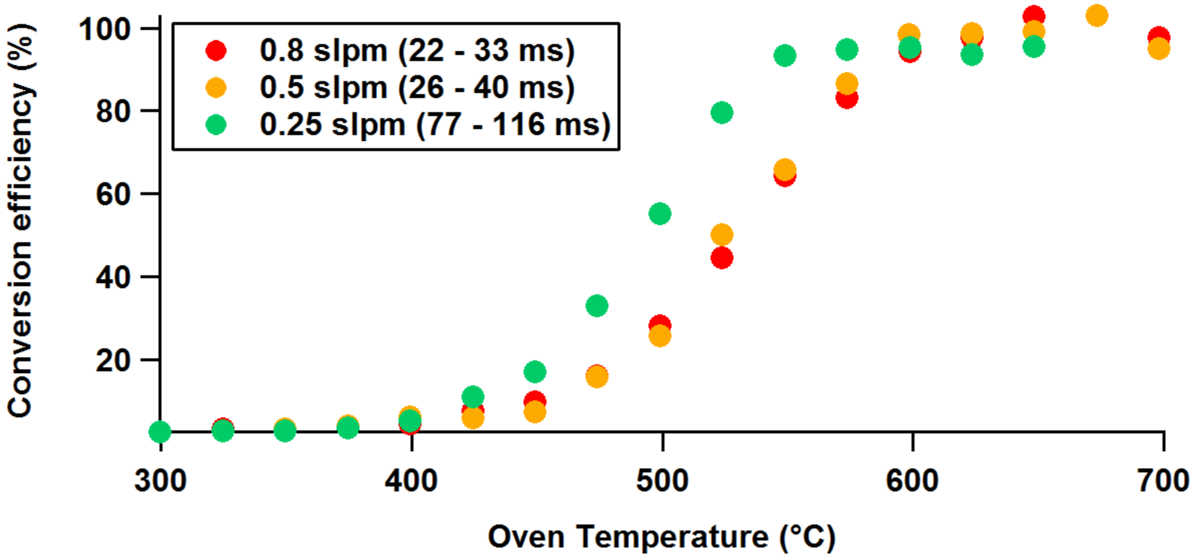

Figure S3. HNO_3 thermograms taken at low oven pressure (~250 mbar). As in Fig. 2, the onset of signal shifts to higher temperatures at faster flow rates.

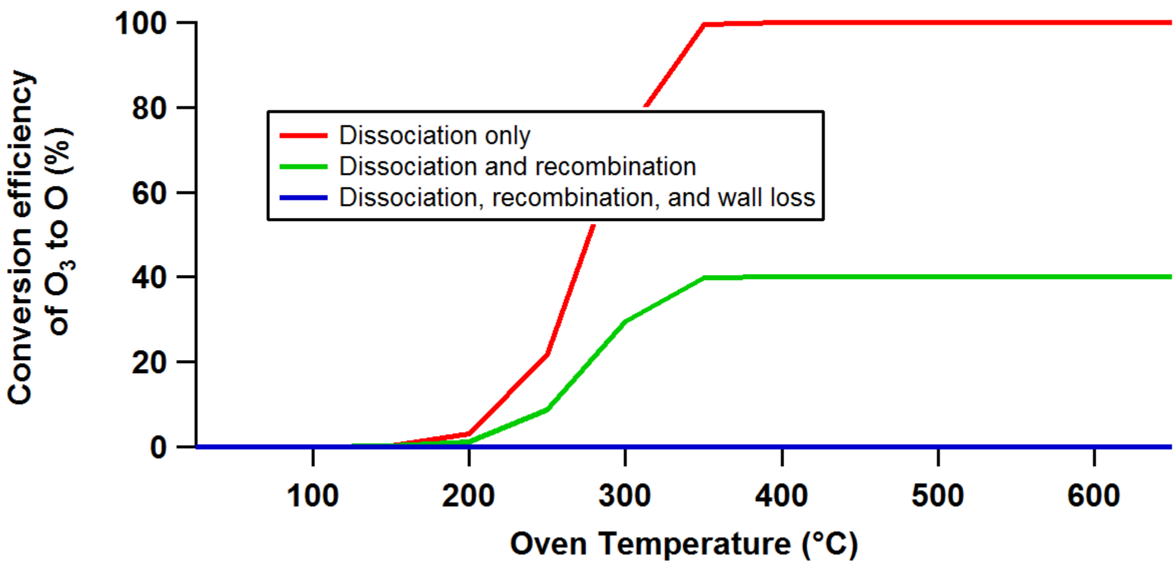

Figure S4. A simulated O_3 dissociation curve to O. These results indicate that O_3 dissociates to form O at the entire temperature range relevant for AN and HNO_3 TD ovens, but that if allowed to recombine, only ~40% will remain as O_2 + O. If wall loss is permitted, nearly all O atoms would be lost to reactions with the wall.

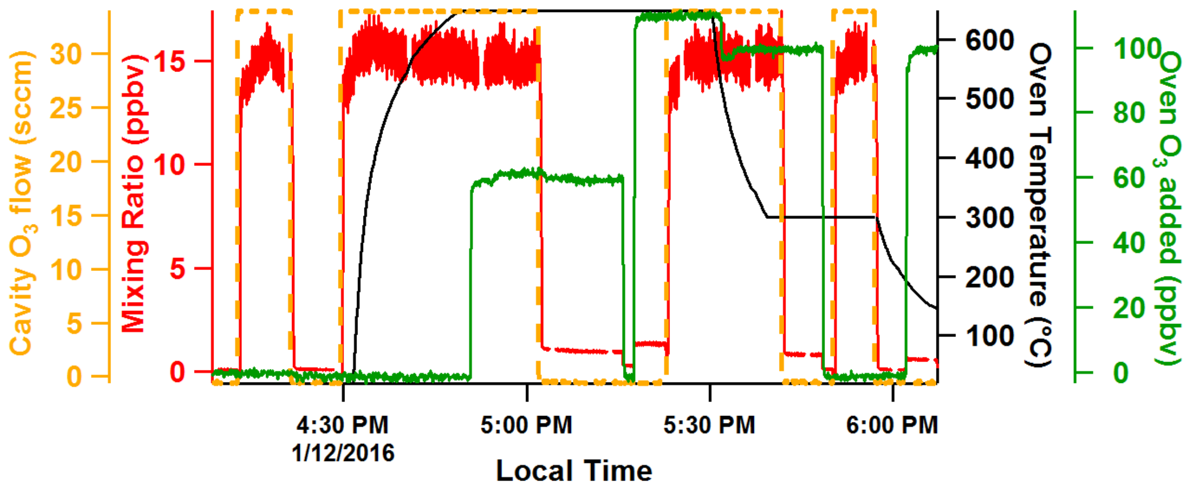

Figure S5. The measured NO_2 mixing ratios as ~15 ppbv NO in zero air is introduced to the NOy thermal dissociation inlet is shown in red. The green and yellow lines represent the addition of O_3 in two places: ppbv levels before the NO sample enters the TD inlet (green) and ppmv levels in the mixing volume just prior to entering the CRDS cavity (yellow). The mixing volume O_3 converts any NO to NO_2 prior to detection, so when this O_3 is added (such as between 4:30 and 5pm), the measured NO_2 is ~15 ppbv, as expected. When O_3 is not added to either the TD inlet or the mixing volume (such as between 4:20 and 4:30pm), no NO_2 signal is observed. However, when O_3 is added to the TD inlet, but not to the mixing volume, and the oven is at 650 °C, (such as between 5:05 and 5:15), approximately 2.25 ppbv NO_2 is observed, indicating that this NO_2 is formed by reaction of O_3 and NO in the oven. This has no effect on this TD-CRDS instrument, as any NO would be converted to NO_2 in the mixing volume region immediately following the TD oven. But techniques such as TD-LIF or TD-CRDS in which NO is not converted to NO_2 would see a ~15% conversion of ambient NO to NO_2, which must be accounted for.

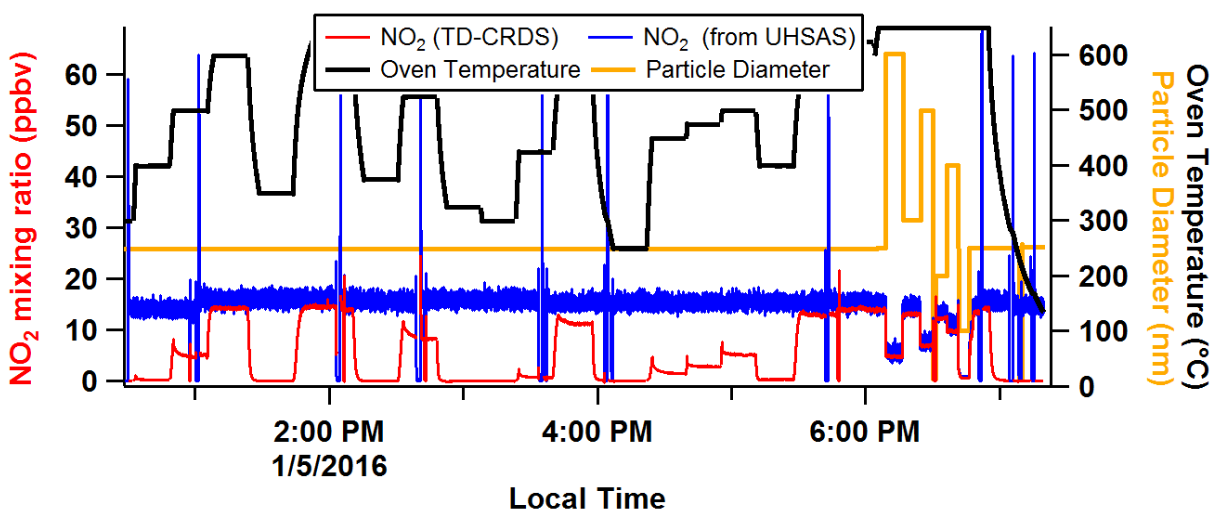

Figure S6. NO_2 signal (red) detected in the NOy channel of the TD-CRDS instrument when NH_4NO_3 aerosol is introduced to the inlets on two separate occasions. The blue trace is the expected NH_4NO_3 concentrations derived from the UHSAS measurement of the particle size distribution. The yellow indicates set DMA diameter.

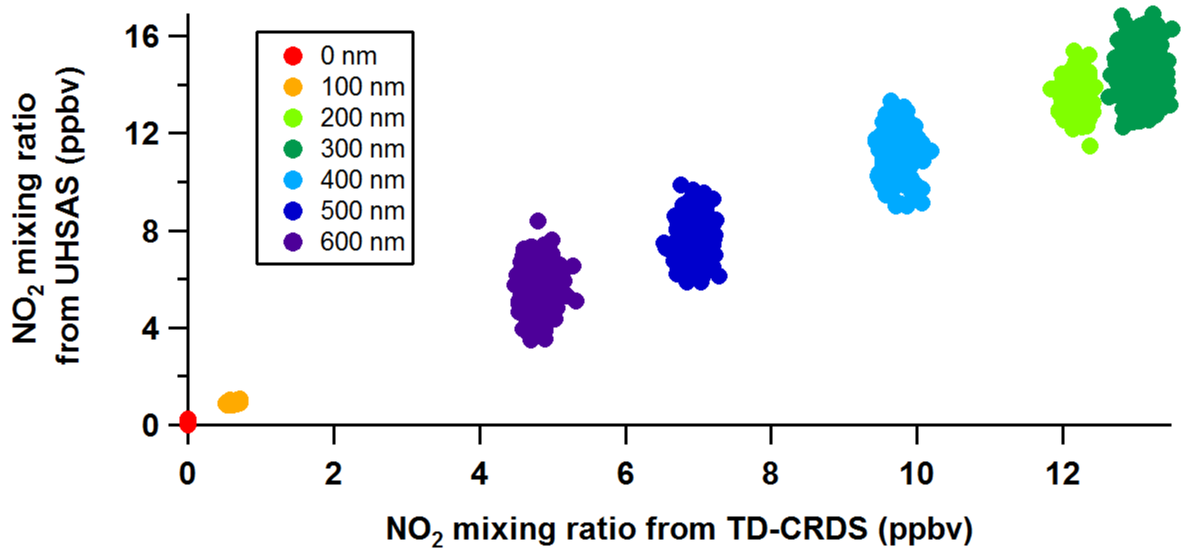

Figure S7. NO_2 mixing ratios as measured by the TD-CRDS instrument, and derived NO_2 mixing ratios from the UHSAS size distribution of NH_4NO_3 particles, colored by DMA selected diameter. Here, "0 nm" refers to setting the DMA voltage to 0, which nominally does not allow any particles through. A linear trend is shown in the scatter plot, with no dependence on particle size, emphasizing that complete conversion of the NH_4NO_3 particles is observed in the TD oven.

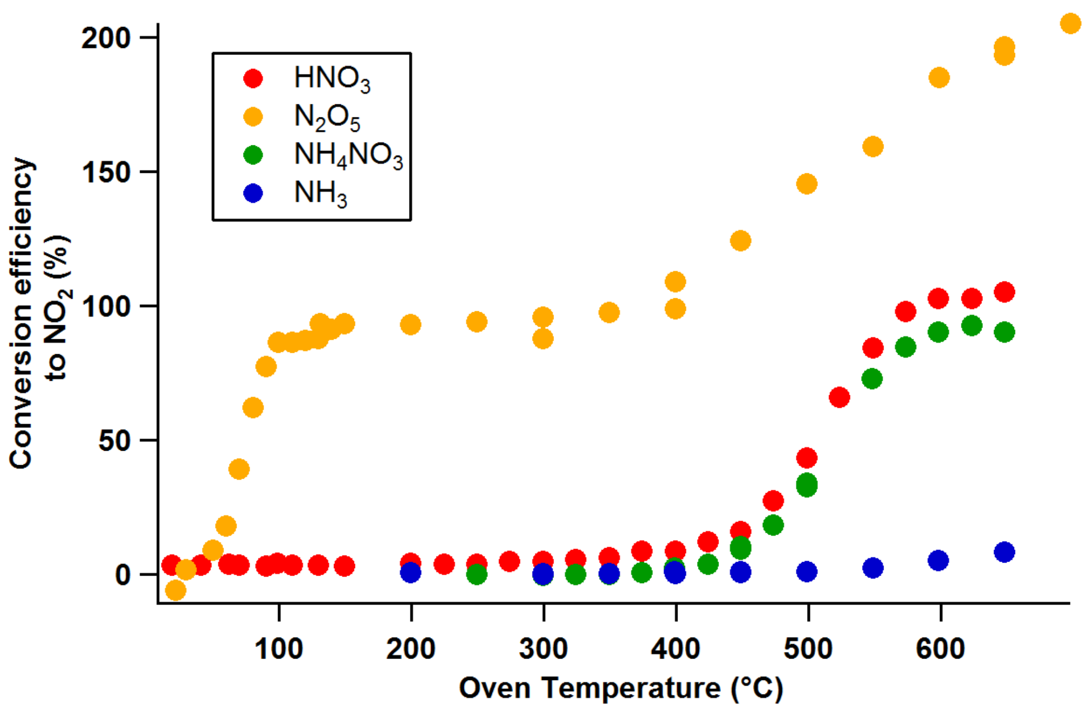

Figure S8. A representative thermogram for each of the four major species studied. All were at ambient pressure and a flow rate of 1.9 slpm, except for the high temperature region of the N_2O_5 trace, which was taken at 1 slpm. The NH_3 thermogram was taken with 100 ppbv of O_3 in the TD inlet.

Table S1. Reactions used in HNO_3 box model

Rate laws are presented in table form, where the parameters listed can be inserted into the equation $k(T) = A(298/T)^{n}e^{-(Ea/RT)}$. For third order equations, a high pressure limit is also given. For third order reactions, a value of $F_c = 0.6$ was used. Ea/R is in units of K^{-1}. A is in units of cm^3 $molec^{-1}$ s^{-1} for second order reactions and cm^6 $molec^{-2}$ s^{-1} for third order reactions. The rate expression at 298 and 950 K (max and min temperatures used in each thermogram) are given. The technique (experimental, theoretical, combination/review) is given, along with the temperature range and reaction order. Temperature ranges with approximates are based on JPL combinations of multiple studies and are thus approximate.

Reactions used in HNO_3 box model

Reaction	**Rate Expression**											
	A_0	n_0	Ea/R_0	A_∞	n_∞	Ea/R_∞	**Ref.**	**k(298K)**	**k(950K)**	**Technique**	**Temp range**	**Order**
$HNO_3 \rightarrow NO_2 + OH$	1.83e-4	-1.98	24054	1.26e-15	0	24054	[1]	5.51e-21	409.81	Expt	295-1200	2
$NO_3 \rightarrow NO_2 + O$	*See main text*											
$NO_3 + NO_2 \rightarrow N_2O_5$	2.0e-30	-4.4	0	1.4e-12	-0.7	0	[2]	1.15e-12	5.66e-14	Expt	~250-400	3
$NO_2 + O \rightarrow NO_3$	2.50e-31	-1.8	0	2.2e-11	-0.7	0	[2]	2.74e-12	1.72e-13	Expt	~200-400	3
$NO_2 + OH \rightarrow HNO_3$	1.80e-30	-3	0	2.80e-11	0	0	[2]	9.28e-12	3.29e-13	Expt	~200-600	3
$NO_2 + HO_2 \rightarrow HO_2NO_2$	2.00e-31	-3.4	0	2.90e-12	-1.1	0	[2]	2.53e-12	2.45e-14	Expt	~200-350	3
$NO + O \rightarrow NO_2$	9.00e-32	-1.5	0	3.00e-11	0	0	[2]	1.32e-12	9.33e-14	Expt	~200-500	3
$NO + OH \rightarrow HONO$	7.00e-31	-2.6	0	3.60e-11	-0.1	0	[2]	6.31e-12	2.06e-13	Expt	~200-500	3
$NO + H \rightarrow HNO$	1.22e-31	-1.17	211.6	N/A	N/A	N/A	[3]	1.13e-12	1.57e-13	Review	230-4200	3
$O_3 \rightarrow O + O_2$	7.16e-10	0	11200	N/A	N/A	N/A	[4]	6.49e-7	10000	Review	300-3000	2
$O_2 + H \rightarrow HO_2$	4.40e-32	-1.3	0	7.50e-11	0.2	0	[2]	7.37e-13	5.88e-14	Theory	300-3000	3
$O + H \rightarrow OH$	4.36e-32	-1	0	N/A	N/A	N/A	[5]	8.20e-13	8.55e-14	Review	300-2500	3
$2OH \rightarrow H_2O_2$	6.90e-31	-1	0	2.60e-11	0	0	[2]	5.42e-12	1.06e-12	Expt	~200-700	3
$OH + H \rightarrow H_2O$	4.38e-30	-2	0	N/A	N/A	N/A	[6]	8.28e-11	2.79e-12	Review	300-3000	3
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	3.00e-13	0	-460	N/A	N/A	N/A	[2]	0.0858	0.00343	Expt	~250-1200	3
$N_2O_3 \rightarrow NO + NO_2$	1.90e-7	-8.7	4800	4.7e15	0.4	4880	[7]	10000	10000	Review	225-300	2
$HO_2NO_2 \rightarrow HO_2 + NO_2$	4.10e-5	0	10650	4.8e15	0	11170	[8]	0.0738	10000	Expt	260-300	2
$HONO \rightarrow OH + NO$	1.98e-3	-3.8	25257	1.09e16	-1.23	25016	[3]	1.41e-21	171.88	Review	300-2500	2
$HNO \rightarrow NO + H$	5.48e-7	-1.24	25257	N/A	N/A	N/A	[3]	1.67e-24	1.07634	Review	300-2500	2
$H_2O_2 \rightarrow 2OH$	2.03e-3	-4.86	26820	N/A	N/A	N/A	[5]	3.34e-27	0.00125	Review	500-2500	2
$N_2O_5 \rightarrow NO_2 + NO_3$	1.30e-3	-3.5	11000	9.7e14	0.1	11080	[8]	0.0498	10000	Expt	200-400	2
$HNO_3 + OH \rightarrow H_2O + NO_3$	6.50e-34	0	-1335	2.70e-17	0	-2199	[2]**	1.12e-13	3.95e-14	Expt	~200-350	3
$2NO_3 \rightarrow 2NO_2 + O_2$	8.5e-13	0	2450				[2]	2.29e-16	5.98e-14	Expt	298-329	2
$NO_3 + NO \rightarrow 2NO_2$	1.79e-11	0	-109.45				[9]	2.58e-11	2.02e-11	Review	220-4400	2
$NO_3 + O \rightarrow O_2 + NO_2$	1.00e-17	0	0				[2]	1e-11	1e-11	Expt	298	2
$NO_3 + OH \rightarrow HO_2 + NO_2$	2.2e-11	0	0				[2]	2.2e-11	2e-11	Expt	298	2
$NO_3 + HO_2 \rightarrow O_2 + HNO_3$	3.5e-12	0	0				[2]	3.5e-12	3.5e-12	Expt	298	2
$NO_3 + H \rightarrow NO_2 + OH$	9.4e-11	0	0				[10]	9.4e-11	9.4e-11	Expt	298	2

$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2e-13	0	2450				[2]	3.24e-17	8.44e-15	Expt	~250-350	2
$NO_2 + O \rightarrow NO + O_2$	5.10e-12	0	-210				[2]	1.03e-11	6.40e-12	Expt	~200-350	2
$NO_2 + HNO \rightarrow HONO + NO$	1e-12	0	1000				[3]	3.49e-14	3.38e-13	Review	300-2500	2
$NO_2 + H \rightarrow NO + OH$	4.00e-10	0	340				[2]	1.28e-10	2.77e-10	Expt	~200-500	2
$NO + O_3 \rightarrow NO_2 + O_2$	3.00e-12	0	1500				[2]	1.96e-14	5.91e-13	Expt	~200-400	2
$NO + HO_2 \rightarrow NO_2 + OH$	3.30e-12	0	-270				[2]	8.16e-12	4.42e-12	Expt	~200-400	2
$O_3 + O \rightarrow 2O_2$	8.00e-12	0	2060				[2]	7.99e-15	8.59e-13	Expt	~250-350	2
$O_3 + OH \rightarrow HO_2 + O_2$	1.70e-12	0	940				[2]	7.26e-14	6.14e-13	Expt	~200-450	2
$O_3 + HNO \rightarrow HONO + O_2$	2.56e-15	3.59	-396.9				[11]	9.48e-15	2.23e-13	Theory	150-1000	2
$O_3 + H \rightarrow O_2 + OH$	1.40e-10	0	470.26				[12]	2.89e-11	8.41e-11	Review	200-300	2
$O_2 + H \rightarrow OH + O$	1.22e-11	0.96	6157.9				[13]	1.30e-20	4.55e-14	Review	950-3550	2
$O + OH \rightarrow O_2 + H$	1.80e-11	0	-180				[2]	3.29e-11	2.19e-11	Expt	~150-500	2
$O + HO_2 \rightarrow OH + O_2$	3.00e-11	0	-200				[2]	5.87e-11	3.72e-11	Expt	~250-400	2
$O + N_2O_3 \rightarrow$ Products	4.30e-13	0	0				[14]	4.30e-13	4.30e-13	Theory	199	2
$O + HO_2NO_2 \rightarrow$ Products	7.8e-11	0	3400				[2]	8.70e-16	1.96e-12	Expt	225-300	2
$O + HONO \rightarrow OH + NO_2$	2.01e-11	0	3000				[3]	8.58e-16	7.80e-13	Review	300-2500	2
$O + HNO \rightarrow OH + NO$	6.00e-11	0	0				[3]	6.00e-11	6.00e-11	Review	300-2500	2
$O + H_2O_2 \rightarrow HO_2 + OH$	1.40e-12	0	2000				[2]	1.71e-15	1.60e-13	Expt	~275-375	2
$2OH \rightarrow H_2O + O$	1.80e-12	0	0				[2]	1.80e-12	1.80e-12	Expt	250-580	2
$OH + HO_2 \rightarrow H_2O + O_2$	4.80e-11	0	-250				[2]	1.11e-10	6.29e-11	Expt	250-380	2
$OH + HO_2NO_2 \rightarrow H_2O_2 + NO_3$	1.30e-12	0	-380				[2]	4.65e-12	1.96e-12	Expt	~250-325	2
$OH + HO_2NO_2 \rightarrow HO_2 + HNO_3$	1.30e-12	0	-380				[2]	4.65e-12	1.96e-12	Expt	~250-325	2
$OH + HONO \rightarrow H_2O + NO_2$	1.80e-11	0	390				[2]	4.87e-12	1.18e-11	Expt	~275-375	2
$OH + HNO \rightarrow H_2O + NO$	8.00e-11	0	500				[3]	1.50e-11	4.65e-11	Review	300-2000	2
$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2.90e-12	0	160				[8]	1.70e-12	2.44e-12	Expt	240-460	2
$HO_2 + H_2O_2 \rightarrow OH + H_2O + O_2$	1.00e-13	0	0				[15]	1.00e-13	1.00e-13	Theory	825-875	2
$HO_2 + H \rightarrow H_2O + O$	5.00e-11	0	865.95				[6]	2.74e-12	1.96e-11	Review	300-1000	2
$HO_2 + H \rightarrow 2OH$	2.81e-10	0	440.19				[6]	6.42e-12	1.74e-11	Review	300-1000	2
$HO_2 + H \rightarrow O_2 + H_2$	7.11e-11	0	709.6				[6]	6.57e-12	3.29e-11	Review	300-1000	2
$HO_2NO_2 + H \rightarrow$ Products	2.46e-14	0	0				[16]	2.46e-14	2.46e-14	Expt	248-315	2
$HONO + H \rightarrow H_2O + NO$	6.39e-13	1.89	1940				[17]	9.43e-16	6.54e-13	Theory	300-3500	2
$HONO + H \rightarrow OH + HNO$	1.26e-11	0.86	2500				[17]	2.86e-15	2.21e-12	Theory	300-3500	2
$HNO + H \rightarrow H_2 + NO$	3.01e-11	0	500				[3]	5.63e-12	1.75e-11	Review	298-2000	2
$H_2O_2 + H \rightarrow OH + H_2O$	1.69e-11	0	1800				[6]	4.04e-14	2.40e-12	Review	300-1000	2
$H_2O_2 + H \rightarrow H_2 + HO_2$	2.81e-12	0	1889.5				[6]	4.96e-15	3.63e-13	Review	300-1000	2
$OH \rightarrow$ Wall	$46\ s^{-1}$						**See main text					
$O \rightarrow$ Wall	$70\ s^{-1}$						**See main text					
$C_3H_8 + O \rightarrow C_3H_7 + OH$	1.37e-12	2.68	1870.2				[18]	2.54e-15	3.67e-12	Review	300-2500	2
$C_3H_8 + H \rightarrow C_3H_7 + H_2$	4.23e-12	2.54	3400				[18]	4.64e-17	1.85e-12	Review	298-2500	2
$C_3H_8 + NO_3 \rightarrow C_3H_7 + HNO_3$	4.17e-12	0	3260.6				[19]	7.44e-17	1.22e-13	Theory	298	2
$C_3H_8 + NO_2 \rightarrow C_3H_7 + HONO$	4.00e-13	0	11400				[20]	9.89e-30	1.73e-18	Expt	423-498	2
$C_3H_8 + O_3 \rightarrow$ Products	2.74e-13	0	7270				[21]	7.05e-24	1.04e-16	Expt	273-333	2
$C_3H_8 + OH \rightarrow C_3H_7 + H_2O$	1.44e-12	1	130				[22]	9.25e-13	3.85e-12	Review	300-1000	2

$C_3H_7 + O \rightarrow$ Products	1.6e-10	0	0				[18]	1.60e-10	1.60e-10	Review	300-2500	2
$CO + O \rightarrow CO_2$	1.70e-33	0	1509	1e-14	0	1629	[5]	8.86e-18	5.55e-16	Review	300-2500	3

**See discussion of more complicated rate expression that was used in the original reference

Reactions used in N_2O_5 box model

Reaction	**Rate Expression**											
	A_0	n_0	Ea/R_0	A_∞	n_∞	Ea/R_∞	**Ref.**	**k(298K)**	**k(950K)**	**Technique**	**Temp range**	**Order**
$NO_3 + NO_2 \rightarrow N_2O_5$	2.0e-30	-4.4	0	1.4e-12	-0.7	0	[2]	1.17e-12	5.66e-14	Expt	~250-400	3
$NO_2 + O \rightarrow NO_3$	2.50e-31	-1.8	0	2.2e-11	-0.7	0	[2]	2.84e-12	1.72e-13	Expt	~200-400	3
$NO + O \rightarrow NO_2$	9.00e-32	-1.5	0	3.00e-11	0	0	[2]	1.36e-12	9.33e-14	Expt	~200-500	3
$O_2 + O \rightarrow O_3$	6.00e-34	-2.4	0	0	0	0	[2]	1.21e-14	2.44e-16	Expt	~200-270	3
$O + O \rightarrow O_2$	5.21e-35	0	-900				[5]	2.13e-14	8.33e-16	Review	200-4000	3
$N_2O_5 \rightarrow NO_2 + NO_3$	1.30e-3	-3.5	11000	9.7e14	0.1	11080	[8]	0.0267	10000	Expt	200-400	2
$NO_3 + NO \rightarrow 2NO_2$	1.79e-11	0	-109.45				[9]	2.60e-11	2.02e-11	Review	220-4400	2
$NO_3 + O \rightarrow O_2 + NO_2$	1.00e-17	0	0				[2]	1.00e-11	1.00e-11	Expt	298	2
$NO_2 + O \rightarrow NO + O_2$	5.10e-12	0	-210				[2]	1.04e-11	6.40e-12	Expt	~200-350	2
$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2e-13	0	2450				[2]	2.82e-17	8.44e-15	Expt	~250-350	2
$NO + O_3 \rightarrow NO_2 + O_2$	3.00e-12	0	1500				[2]	1.80e-14	5.91e-13	Expt	~200-450	2
$O_3 \rightarrow O + O_2$	7.16e-10	0	11200	N/A	N/A	N/A	[4]	3.48e-07	10000	Review	300-3000	2
$O \rightarrow$ Walls	70 s^{-1}						*see main text*					
$NO_3 \rightarrow NO_2 + O$	*see main text*											

Reactions used in NH_3 box model

Reaction	**Rate Expression**											
	A_0	n_0	Ea/R_0	A_∞	n_∞	Ea/R_∞	**Ref.**	**k(298K)**	**j(950K)**	**Technique**	**Temp range**	**Order**
$HNO \rightarrow NO + H$	5.48e-7	-1.24	25257	N/A	N/A	N/A	[3]	9.75e-32	1.076	Review	300-2500	2
$NH_3 + O \rightarrow NH_2 + OH$	2.87e-13	2.1	0				[23]	6.04e-18	3.00e-13	Review	298-2000	2
$NH_3 + OH \rightarrow NH_2 + H_2O$	4.48e-13	1.8	0				[24]	1.16e-13	2.58e-12	Review	225-2350	2
$NH_2 + O_3 \rightarrow NH_2O + O_2$	4.9e-12	0	1000				[25]	8.71e-14	1.66e-12	Review	250-380	2
$NH_2 + O \rightarrow HNO + H$	7.47e-11	0	0				[23]	7.47e-11	7.47e-11	Review	298-3000	2
$NH_2 + O \rightarrow OH + NH$	1.16e-11	0	0				[23]	1.16e-11	1.16e-11	Review	298-3000	2
$NH_2 + O \rightarrow NO + H_2$	8.30e-12	0	0				[23]	8.30e-12	8.30e-12	Review	298-3000	2
$NH_2 + NH_2 \rightarrow N_2H_4$	1.96e-29	-3.9	0	N/A	N/A	N/A	[26]	1.12e-10	1.60e-10	Expt	200-400	3
$NH_2 + OH \rightarrow NH_2OH$	6.77e-10	-3.23	673				[27]	8.30e-11	8.65e-12	Theory	200-3000	2
$NH_2 + OH \rightarrow NH + H_2O$	7.69e-13	1.5	-230				[23]	1.46e-12	5.33e-12	Review	250-3000	2
$NH_2 + OH \rightarrow NH_3 + O$	4.95e-15	2.6	-870				[23]	1.01e-13	2.36e-13	Review	298-2000	2
$NH_2 + NH \rightarrow N_2H_2 + H$	1.5e-10	-0.27	-38.4				[28]	1.84e-10	1.15e-10	Theory	200-2500	2
$NH_2 + NH_2OH \rightarrow NH_3 + NH_2O$	1.42e-15	4	-13.03				[28]	7.01e-16	1.29e-13	Theory	300-2500	2
$NH_2O + O_3 \rightarrow$ Products	2.01e-14	0	0				[29]	2.01e-14	2.01e-14	Expt	298	2
$NH_2O + OH \rightarrow H_2O + HNO$	1.66e-12	0	0				[30]	1.66e-12	1.66e-12	Theory	80-420	2

$NH_2OH \rightarrow OH + NH_2$	0.16	-5.96	33555				[28]	2.09e-40	0.195	Theory	450-2500	2
$NH + OH \rightarrow HNO + H$	3.32e-11	0	0				[23]	3.32e-11	3.32e-11	Review	298-3000	2
$NH_2OH + NH \rightarrow NH_2 + NH_2O$	3.73e-16	4.4	786.6				[28]	6.82e-18	2.24e-14	Theory	400-2500	2
$NO + O \rightarrow NO_2$	9.00e-32	-1.5	0	3.00e-11	0	0	[2]	1.93e-12	9.33e-14	Expt	~200-500	3
$NO + O_3 \rightarrow NO_2 + O_2$	3.00e-12	0	1500				[2]	7.11e-15	5.91e-13	Expt	~200-400	2
$NO_2 + O \rightarrow NO_3$	5.10e-12	0	-210				[2]	4.00e-12	4.00e-12	Expt	~200-400	3
$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2e-13	0	2450				[2]	6.19e-18	8.44e-15	Expt	~250-350	2
$NO_3 \rightarrow NO_2 + O$	**See main text											
$NO + H \rightarrow HNO$	1.22e-31	-1.17	211.6	N/A	N/A	N/A	[2]	1.46e-12	1.57e-13	Expt	230-4200	3
$O_3 \rightarrow O + O_2$	7.16e-10	0	11200	N/A	N/A	N/A	[4]	4.02e-10	10000	Review	300-3000	2
$NO_3 + NO \rightarrow NO_2 + NO_2$	1.79e-11	0	-109.45				[9]	2.78e-11	2.02e-11	Review	220-4400	2
$NO_3 + O \rightarrow O_2 + NO_2$	1.00e-17	0	0				[2]	1.00e-11	1.00e-11	Expt	298	2
$NO_3 + OH \rightarrow HO_2 + NO_2$	2.2e-11	0	0				[2]	2.20e-11	2.20e-11	Expt	298	2
$HNO + H \rightarrow NH_2 + O$	1.05e-9	-0.3	14673				[23]	2.32e-35	9.37e-17	Review	550-3000	2
$HNO + H \rightarrow OH + NH$	2.41e-9	-0.5	9009				[23]	4.66e-25	8.19e-14	Review	350-3000	2
$HNO + H \rightarrow H_2 + NO$	3.01e-11	0	500				[3]	4.01e-12	1.75e-11	Review	298-2000	2
$O + HNO \rightarrow OH + NO$	6.00e-11	0	0				[3]	6.00e-11	6.00e-11	Review	298-2000	2
$OH + HNO \rightarrow H_2O + NO$	8.00e-11	0	500				[3]	1.07e-11	4.65e-11	Review	300-2000	2
$NH_2 + NO \rightarrow N_2 + H_2O$	5.96e-11	-2.37	436				[31]	1.61e-11	2.59e-12	Review	400-1900	2
$NH_2 + NO_2 \rightarrow N_2O + H_2O$	7e-12	-1.44	135				[32]	5.34e-12	1.20e-12	Expt	300-910	2
$NH_2 + NO_2 \rightarrow NO + NH_2O$	5.81e-12	0	0				[33]	5.81e-12	5.81e-12	Expt	850-1350	2
$O \rightarrow$ Walls	~70 s^{-1}						**See main text					
$OH \rightarrow$ Walls	~46 s^{-1}						**See main text					

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