

Supplementary Information for the Paper:

Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations

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Numerical values of all data points in the Figures of the main manuscript

Table of Figure 1: Determination of the N₂O decomposition order over monocuclear iron sites of Fe-ZSM-5 at 650 K. The N₂O decomposition rate was determined at a gas composition of 1 ppb NO (solid symbols), 100 ppm NO (open symbols), varying amounts of N₂O in He (10,000 – 50,000 ppm N₂O), and 0.1 ppm (diamond) / 1 ppm H₂O (square).

	0.1 ppb NO 1 ppm H ₂ O	0.1 ppb NO 0.1 ppm H ₂ O	100 ppm NO 1 ppm H ₂ O	100 ppm NO 0.1 ppm H ₂ O
Ln(p _{N₂O} /bar)	Ln(-R _{N₂O} / (mol _{N₂O} s ⁻¹ mol _{Fe} ⁻¹))			
-4.61	-8.80	-6.66	-6.07	-6.07
-4.20	-8.40	-6.25	-5.67	-5.67
-3.91	-8.12	-5.96	-5.38	-5.38
-3.69	-7.90	-5.73	-5.16	-5.15
-3.51	-7.72	-5.55	-4.97	-4.97
-3.35	-7.57	-5.39	-4.82	-4.82
-3.22	-7.43	-5.26	-4.69	-4.68
-3.10	-7.32	-5.14	-4.57	-4.57
-3.00	-7.21	-5.03	-4.46	-4.46

Table of Figure 2: Arrhenius plot of the N₂O decomposition over monocuclear iron sites of Fe-ZSM-5 in the presence of varying amounts of nitric oxide, 0.1 (top) / 1 (bottom) ppm H₂O, and 15,000 ppm N₂O in He.

	1 ppm H ₂ O			
	0.1 ppb NO	10 ppb NO	1 ppm NO	100 ppm NO
1000 K / T	Ln(k _{app} / (mol _{N₂O} s ⁻¹ mol _{Fe} ⁻¹ bar _{N₂O} ⁻¹))			
1.67	-7.45E+00	-3.76E+00	-2.94E+00	-2.92E+00
1.60	-6.09E+00	-3.39E+00	-2.16E+00	-2.14E+00
1.54	-4.20E+00	-2.97E+00	-1.51E+00	-1.47E+00
1.48	-2.24E+00	-1.97E+00	-8.78E-01	-8.15E-01
1.43	-4.61E-01	-4.46E-01	-2.39E-01	-2.06E-01
1.38	1.04E+00	1.03E+00	5.91E-01	3.66E-01
1.33	2.22E+00	2.21E+00	1.73E+00	9.17E-01
1.29	3.08E+00	3.08E+00	2.83E+00	1.49E+00
1.25	3.75E+00	3.75E+00	3.65E+00	2.19E+00
	0.1 ppm H ₂ O			
1.67	-6.27E+00	-3.73E+00	-2.94E+00	-2.92E+00
1.60	-4.04E+00	-3.12E+00	-2.16E+00	-2.14E+00
1.54	-2.05E+00	-1.93E+00	-1.49E+00	-1.47E+00
1.48	-2.84E-01	-3.14E-01	-7.32E-01	-8.11E-01
1.43	1.04E+00	1.03E+00	3.16E-01	-1.91E-01
1.38	1.99E+00	1.98E+00	1.58E+00	4.20E-01
1.33	2.70E+00	2.70E+00	2.56E+00	1.11E+00
1.29	3.30E+00	3.30E+00	3.26E+00	2.02E+00
1.25	3.84E+00	3.84E+00	3.83E+00	3.10E+00

Tables of Figure 3: Left: Steady-state turnover frequency of monocular iron sites in Fe-ZSM-5 for the formation of NO, NO₂, and N₂O versus temperature. The turnover frequencies are determined at a gas composition of 1 ppm NO, 0.1 ppm H₂O, and 15,000 ppm N₂O in He. Right: Partial pressures of NO, NO₂, and the sum of NO and NO₂ versus temperature during catalytic decomposition of N₂O in 15,000 ppm N₂O and 2000 ppm NO (0.1 ppb H₂O, residence time: 0.112 sec).

Left:

T / K	R _{N₂O} / (mol _{N₂O} s ⁻¹ mol _{Fe} ⁻¹)	R _{NO} / (mol _{NO} s ⁻¹ mol _{Fe} ⁻¹)	R _{NO₂} / (mol _{NO₂} s ⁻¹ mol _{Fe} ⁻¹)	R _{NO} + R _{NO₂}
650	-3.40E-03	-3.30E-03	3.30E-03	-8.90E-07
675	-7.21E-03	-6.00E-03	6.00E-03	-2.15E-06
700	-2.06E-02	-9.23E-03	9.23E-03	-4.07E-06
725	-7.25E-02	-9.93E-03	9.93E-03	-4.87E-06
750	-1.95E-01	-7.04E-03	7.03E-03	-3.19E-06
775	-3.92E-01	-4.42E-03	4.42E-03	-1.26E-06
800	-6.92E-01	-3.26E-03	3.26E-03	-9.20E-08

Right:

T / K	P _{NO} / mbar	P _{NO₂} / mbar	P _{NO} + P _{NO₂}
660	8.95E-02	1.11E-01	2.00E-01
680	8.04E-02	1.20E-01	2.00E-01
700	1.11E-01	8.92E-02	2.00E-01
720	1.47E-01	5.32E-02	2.00E-01
740	1.69E-01	3.05E-02	2.00E-01
760	1.81E-01	1.90E-02	2.00E-01
780	1.87E-01	1.31E-02	2.00E-01
800	1.90E-01	9.96E-03	2.00E-01

Table of Figure 4: Steady-state surface fraction of $Z^-[\text{Fe}(\text{OH})_2]^+$, $Z^-[\text{FeO}_2]^+$, $Z^-[\text{FeO}]^+$, $Z^-[\text{FeOH}]^+$, $Z^-[\text{OFeOH}]^+$, and the sum of $Z^-[\text{FeONO}]^+$, $Z^-[\text{FeO}_2\text{N}]^+$, $Z^-[\text{FeO}_2\text{NO}]^+$ in Fe-ZSM-5 versus temperature. The surface composition was determined at a gas composition with varying amounts of NO, 0.1 ppm H_2O , and 15,000 ppm N_2O in He.

T / K	Surface fraction					
	$Z^-[\text{FeO}]^+$	$Z^-[\text{FeO}_2]^+$	$Z^-[\text{Fe}(\text{OH})_2]^+$	$Z^-[\text{FeOH}]^+$	$Z^-[\text{OFeOH}]^+$	$Z^-[\text{FeONO}]^+$ $Z^-[\text{FeO}_2\text{N}]^+$ $Z^-[\text{FeO}_2\text{NO}]^+$
0.1 ppb NO						
550	0.00	0.00	0.95	0.03	0.0211	0.0000
575	0.00	0.00	0.96	0.02	0.0217	0.0000
600	0.01	0.00	0.96	0.01	0.0235	0.0000
625	0.02	0.01	0.94	0.00	0.0237	0.0000
650	0.08	0.03	0.86	0.00	0.0216	0.0000
675	0.22	0.10	0.66	0.00	0.0166	0.0000
700	0.39	0.20	0.38	0.00	0.0094	0.0000
725	0.51	0.29	0.17	0.00	0.0043	0.0000
750	0.56	0.34	0.07	0.00	0.0017	0.0000
775	0.56	0.38	0.03	0.00	0.0007	0.0000
800	0.55	0.40	0.01	0.00	0.0003	0.0000
1 ppb NO						
550	0.00	0.00	0.73	0.26	0.0168	0.0000
575	0.00	0.00	0.84	0.14	0.0202	0.0000
600	0.00	0.00	0.90	0.07	0.0219	0.0000
625	0.02	0.01	0.91	0.04	0.0224	0.0000
650	0.08	0.03	0.85	0.02	0.0210	0.0000
675	0.21	0.10	0.66	0.01	0.0164	0.0000
700	0.39	0.20	0.38	0.00	0.0095	0.0000
725	0.51	0.29	0.17	0.00	0.0043	0.0000
750	0.56	0.34	0.07	0.00	0.0017	0.0000
775	0.56	0.38	0.03	0.00	0.0007	0.0000
800	0.55	0.40	0.01	0.00	0.0003	0.0000
10 ppb NO						
550	0.00	0.00	0.23	0.76	0.0050	0.0000
575	0.00	0.00	0.37	0.62	0.0091	0.0000
600	0.00	0.00	0.55	0.43	0.0134	0.0000
625	0.02	0.01	0.69	0.27	0.0170	0.0000
650	0.07	0.03	0.73	0.16	0.0181	0.0000
675	0.20	0.09	0.61	0.07	0.0153	0.0000
700	0.38	0.19	0.37	0.03	0.0093	0.0000
725	0.51	0.28	0.17	0.01	0.0042	0.0000
750	0.56	0.34	0.07	0.00	0.0017	0.0000
775	0.56	0.38	0.03	0.00	0.0007	0.0000
800	0.55	0.40	0.01	0.00	0.0003	0.0000

1 ppm NO						
550	0.00	0.00	0.00	1.00	0.0001	0.0000
575	0.00	0.00	0.01	0.99	0.0001	0.0000
600	0.00	0.00	0.01	0.99	0.0003	0.0000
625	0.00	0.00	0.02	0.97	0.0006	0.0001
650	0.00	0.00	0.04	0.95	0.0011	0.0001
675	0.02	0.01	0.07	0.89	0.0018	0.0002
700	0.11	0.05	0.10	0.73	0.0026	0.0004
725	0.30	0.17	0.10	0.42	0.0025	0.0004
750	0.47	0.29	0.06	0.15	0.0014	0.0003
775	0.54	0.36	0.03	0.04	0.0006	0.0001
800	0.55	0.40	0.01	0.01	0.0003	0.0001
10 ppm NO						
550	0.00	0.00	0.00	1.00	0.0000	0.0000
575	0.00	0.00	0.00	1.00	0.0000	0.0000
600	0.00	0.00	0.00	1.00	0.0000	0.0000
625	0.00	0.00	0.00	1.00	0.0001	0.0001
650	0.00	0.00	0.00	0.99	0.0001	0.0001
675	0.00	0.00	0.01	0.99	0.0002	0.0002
700	0.01	0.01	0.01	0.96	0.0003	0.0005
725	0.06	0.03	0.02	0.88	0.0005	0.0008
750	0.20	0.11	0.02	0.65	0.0006	0.0011
775	0.39	0.25	0.02	0.32	0.0005	0.0010
800	0.50	0.34	0.01	0.11	0.0003	0.0006
100 ppm NO						
550	0.00	0.00	0.00	1.00	0.0000	0.0000
575	0.00	0.00	0.00	1.00	0.0000	0.0000
600	0.00	0.00	0.00	1.00	0.0000	0.0000
625	0.00	0.00	0.00	1.00	0.0000	0.0001
650	0.00	0.00	0.00	1.00	0.0000	0.0001
675	0.00	0.00	0.00	1.00	0.0000	0.0003
700	0.00	0.00	0.00	1.00	0.0000	0.0005
725	0.01	0.00	0.00	0.99	0.0001	0.0010
750	0.03	0.01	0.00	0.95	0.0001	0.0017
775	0.10	0.04	0.00	0.84	0.0001	0.0026
800	0.26	0.12	0.01	0.59	0.0001	0.0031

Table of Figure 5: Degree of thermodynamic rate control of $Z^-[\text{FeO}]^+$, $Z^-[\text{FeO}_2]^+$, $Z^-[\text{FeOH}]^+$, and $Z^-[\text{HOFeOH}]^+$ species in Fe-ZSM-5 versus temperature for various amounts of NO, 0.1 ppm H_2O , and 15,000 ppm N_2O in He.

T / K	X_{TRC}			
	$Z^-[\text{FeO}]^+$	$Z^-[\text{FeO}_2]^+$	$Z^-[\text{HOFeOH}]^+$	$Z^-[\text{FeOH}]^+$
0.1 ppb NO				
622.5	-0.02	-0.01	-0.97	0.00
642.5	-0.06	-0.03	-0.92	0.00
662.5	-0.14	-0.06	-0.81	0.00
682.5	-0.28	-0.13	-0.60	0.00
702.5	-0.43	-0.22	-0.37	0.00
722.5	-0.53	-0.29	-0.19	0.00
742.5	-0.57	-0.34	-0.09	0.00
762.5	-0.58	-0.38	-0.04	0.00
782.5	-0.58	-0.40	-0.02	0.00
800.0	-0.57	-0.42	-0.01	0.00
1 ppb NO				
622.5	-0.02	-0.01	-0.94	-0.04
642.5	-0.06	-0.02	-0.90	-0.02
662.5	-0.14	-0.06	-0.80	-0.01
682.5	-0.28	-0.13	-0.60	-0.01
702.5	-0.43	-0.22	-0.37	0.00
722.5	-0.53	-0.29	-0.19	0.00
742.5	-0.57	-0.34	-0.09	0.00
762.5	-0.58	-0.38	-0.04	0.00
782.5	-0.58	-0.40	-0.02	0.00
800.0	-0.57	-0.42	-0.01	0.00
10 ppb NO				
622.5	-0.02	-0.01	-0.70	-0.29
642.5	-0.05	-0.02	-0.75	-0.20
662.5	-0.13	-0.05	-0.72	-0.12
682.5	-0.27	-0.12	-0.57	-0.06
702.5	-0.42	-0.21	-0.36	-0.02
722.5	-0.52	-0.29	-0.19	-0.01
742.5	-0.57	-0.34	-0.09	0.00
762.5	-0.58	-0.38	-0.04	0.00
782.5	-0.58	-0.40	-0.02	0.00
800.0	-0.57	-0.42	-0.01	0.00
1 ppm NO				
622.5	0.00	0.00	-0.02	-1.00
642.5	0.00	0.00	-0.04	-0.98
662.5	-0.01	0.00	-0.06	-0.95
682.5	-0.04	-0.02	-0.09	-0.88
702.5	-0.13	-0.07	-0.11	-0.73

722.5	-0.29	-0.16	-0.11	-0.47
742.5	-0.45	-0.27	-0.07	-0.23
762.5	-0.54	-0.34	-0.04	-0.09
782.5	-0.57	-0.39	-0.02	-0.03
800.0	-0.57	-0.41	-0.01	-0.01
	10 ppm NO			
622.5	0.00	0.00	0.00	-1.02
642.5	0.00	0.00	0.00	-1.02
662.5	0.00	0.00	-0.01	-1.02
682.5	0.00	0.00	-0.01	-1.01
702.5	-0.02	-0.01	-0.02	-0.98
722.5	-0.06	-0.03	-0.02	-0.92
742.5	-0.16	-0.09	-0.03	-0.76
762.5	-0.31	-0.19	-0.02	-0.50
782.5	-0.45	-0.29	-0.02	-0.25
800.0	-0.52	-0.36	-0.01	-0.12
	100 ppm NO			
622.5	0.00	0.00	0.00	-1.03
642.5	0.00	0.00	0.00	-1.03
662.5	0.00	0.00	0.00	-1.02
682.5	0.00	0.00	0.00	-1.02
702.5	0.00	0.00	0.00	-1.02
722.5	-0.01	0.00	0.00	-1.01
742.5	-0.02	-0.01	0.00	-0.99
762.5	-0.06	-0.02	0.00	-0.94
782.5	-0.15	-0.06	-0.01	-0.81
800.0	-0.27	-0.13	-0.01	-0.62

Table of Figure 6: Determination of the N₂O reaction order for the N₂O decomposition over mononuclear iron sites of Fe-ZSM-5 at low temperatures. The N₂O decomposition rate was determined at a gas composition of 1 ppm H₂O and varying amounts of N₂O and NO in He (P_{N₂O} = 10,000 – 50,000 ppm, P_{N₂O}/P_{NO} = 10⁷).

Ln(p _{N₂O} /bar)	Ln(-R _{N₂O} /(mol _{N₂O} s ⁻¹ mol _{Fe} ⁻¹))		
	@ 550 K	@ 570 K	@ 590 K
-4.61	-1.03E+01	-1.01E+01	-9.85E+00
-4.20	-9.85E+00	-9.64E+00	-9.44E+00
-3.91	-9.54E+00	-9.33E+00	-9.16E+00
-3.69	-9.31E+00	-9.13E+00	-8.94E+00
-3.51	-9.18E+00	-8.94E+00	-8.75E+00
-3.35	-9.07E+00	-8.78E+00	-8.60E+00
-3.22	-8.88E+00	-8.65E+00	-8.46E+00
-3.10	-8.82E+00	-8.54E+00	-8.34E+00
-3.00	-8.64E+00	-8.44E+00	-8.24E+00

Table of Figure 7: Surface composition of the most abundant surface species in Fe-ZSM-5 at a temperature of 590 K. The steady state surface composition was determined at a gas composition of 1 ppm H₂O and varying amounts of N₂O and fixed P_{N₂O}/P_{N₂O} ratio of 10⁷ in He.

p _{N₂O} / bar	Surface fraction		
	Z ⁻ [HOF ₂ OH] ⁺	Z ⁻ [FeOH] ⁺	Z ⁻ [OF ₂ OH] ⁺
1.00E-02	0.847	0.132	0.021
1.50E-02	0.847	0.132	0.021
2.00E-02	0.848	0.131	0.021
2.50E-02	0.849	0.130	0.020
3.00E-02	0.847	0.132	0.021
3.50E-02	0.848	0.131	0.021
4.00E-02	0.847	0.132	0.021
4.50E-02	0.847	0.132	0.021
5.00E-02	0.848	0.131	0.021

Table of Figure 8: Determination of the reaction order of the N₂O decomposition over mononuclear iron sites in Fe-ZSM-5 at low temperatures. The N₂O decomposition rate was determined at a gas composition of 1 ppb NO, 1 ppm H₂O, and varying amounts of N₂O in He.

Ln(p _{N₂O} /bar)	Ln(-R _{N₂O} /(mol _{N₂O} s ⁻¹ mol _{Fe} ⁻¹))		
	@ 550 K	@ 570 K	@ 590 K
-4.61	-1.029E+01	-1.005E+01	-9.848E+00
-4.20	-1.019E+01	-9.962E+00	-9.812E+00
-3.91	-1.005E+01	-9.903E+00	-9.775E+00
-3.69	-1.004E+01	-9.894E+00	-9.771E+00
-3.51	-1.005E+01	-9.880E+00	-9.739E+00
-3.35	-9.990E+00	-9.875E+00	-9.731E+00
-3.22	-9.908E+00	-9.871E+00	-9.713E+00
-3.10	-9.978E+00	-9.825E+00	-9.699E+00
-3.00	-9.976E+00	-9.853E+00	-9.695E+00

Table of Figure 9: Surface composition of the most abundant surface species in Fe-ZSM-5 at a temperature of 590 K. The steady-state surface composition was determined at a gas composition of 1 ppb NO, 1 ppm H₂O, and varying amounts of N₂O in He.

p _{N₂O} / bar	Surface fraction		
	Z ⁻ [HOF ₂ OH] ⁺	Z ⁻ [FeOH] ⁺	Z ⁻ [OF ₂ OH] ⁺
1.00E-02	0.847	0.132	0.021
1.50E-02	0.888	0.091	0.021
2.00E-02	0.907	0.070	0.022
2.50E-02	0.922	0.056	0.022
3.00E-02	0.929	0.048	0.023
3.50E-02	0.936	0.041	0.023
4.00E-02	0.940	0.037	0.023
4.50E-02	0.944	0.033	0.023
5.00E-02	0.947	0.029	0.023

Table of Figure 10: Steady-state turnover frequency of mononuclear iron sites in Fe-ZSM-5 for the formation of nitric oxide at low temperatures. The NO formation rate was determined at a gas composition of 0.1 ppb NO, 1 ppm H₂O, and varying amounts of N₂O in He.

550 K		570 K		590 K	
P _{N₂O} /bar	R _{NO}	P _{N₂O} /bar	R _{NO}	P _{N₂O} /bar	R _{NO}
1.00E-06	-6.77E-09	1.00E-06	-1.85E-08	1.00E-06	-3.04E-08
1.00E-05	-8.84E-08	1.00E-05	-1.59E-07	1.00E-05	-3.22E-07
1.00E-04	-5.70E-07	1.00E-04	-1.16E-06	1.00E-04	-2.13E-06
1.00E-03	-3.25E-06	1.00E-03	-4.01E-06	1.00E-03	-4.94E-06
2.00E-03	-4.36E-06	2.00E-03	-4.87E-06	2.00E-03	-5.48E-06
1.00E-02	-4.70E-06	1.00E-02	-5.37E-06	1.00E-02	-5.55E-06
1.00E-01	-7.07E-06	9.60E-02	-6.76E-06	9.80E-02	-5.48E-06
2.20E-01	-5.54E-06	2.20E-01	-4.33E-06	2.20E-01	-2.57E-06
9.00E-01	-2.42E-06	8.00E-01	-7.92E-07	7.00E-01	6.38E-07
4.97E+00	2.77E-06	3.40E+00	8.83E-06	2.00E+00	1.64E-05
7.37E+00	6.65E-06	5.20E+00	1.42E-05	3.00E+00	4.34E-05
1.80E+01	1.56E-05	6.15E+00	1.86E-05	4.40E+00	6.19E-05
		9.97E+00	6.25E-05	9.80E+00	2.22E-04

* The rates are in (mol_{NO} s⁻¹ mol_{Fe}⁻¹).

Table of Figure 11: Degree of rate control of reactions 39, 40, 42, 126, and 127 versus temperature for various amounts of NO, 0.1 ppm H₂O, and 15,000 ppm N₂O in He.

T / K	X _{RC}				
	R39	R40	R42	R126	R127
0.1 ppb NO					
624.5	0.28	0.67	0.03	0.00	0.02
642.5	0.28	0.68	0.04	0.01	0.02
661.0	0.27	0.66	0.06	0.01	-0.01
664.0	0.27	0.65	0.07	0.00	0.00
684.0	0.25	0.61	0.14	0.00	0.00
704.5	0.22	0.55	0.22	0.00	0.00
724.5	0.20	0.50	0.29	0.00	0.00
744.5	0.19	0.46	0.33	0.00	0.00
764.5	0.18	0.44	0.36	0.00	0.00
784.5	0.17	0.42	0.39	0.00	0.00
800.0	0.16	0.41	0.40	0.00	0.00
1 ppb NO					
624.5	0.22	0.53	0.03	0.03	0.19
642.5	0.27	0.64	0.04	0.02	0.04
664.0	0.27	0.65	0.07	0.01	0.00
684.0	0.25	0.60	0.13	0.01	0.00
704.5	0.22	0.55	0.22	0.00	0.00
724.5	0.20	0.50	0.29	0.00	0.00
744.5	0.19	0.46	0.33	0.00	0.00
764.5	0.18	0.44	0.36	0.00	0.00
784.5	0.17	0.42	0.39	0.00	0.00
800.0	0.16	0.41	0.40	0.00	0.00
10 ppb NO					
605.0	0.02	0.04	0.00	0.38	0.54
624.5	0.07	0.18	0.01	0.26	0.46
642.5	0.18	0.42	0.03	0.18	0.19
664.0	0.24	0.59	0.06	0.10	-0.01
684.0	0.24	0.59	0.13	0.05	-0.03
704.5	0.22	0.54	0.21	0.02	-0.02
724.5	0.20	0.50	0.28	0.01	-0.01
744.5	0.19	0.46	0.33	0.00	0.00
764.5	0.18	0.44	0.36	0.00	0.00
784.5	0.17	0.42	0.39	0.00	0.00
800.0	0.16	0.41	0.40	0.00	0.00
1 ppm NO					
605.0	0.00	0.00	0.00	0.97	0.01
624.5	0.00	0.00	0.00	0.96	0.02
642.5	0.00	0.01	0.00	0.94	0.02
664.0	0.02	0.05	0.01	0.91	-0.01

684.0	0.08	0.19	0.03	0.83	-0.14
704.5	0.16	0.40	0.08	0.67	-0.32
724.5	0.20	0.49	0.17	0.42	-0.30
744.5	0.19	0.48	0.27	0.19	-0.16
764.5	0.18	0.45	0.34	0.07	-0.06
784.5	0.17	0.43	0.38	0.03	-0.02
800.0	0.16	0.42	0.39	0.01	-0.01
	10 ppm NO				
605.0	0.00	0.00	0.00	0.98	0.00
624.5	0.00	0.00	0.00	0.98	0.00
642.5	0.00	0.00	0.00	0.98	0.00
664.0	0.00	0.01	0.00	0.98	-0.01
684.0	0.01	0.02	0.01	0.97	-0.03
704.5	0.04	0.09	0.02	0.94	-0.11
724.5	0.10	0.24	0.06	0.87	-0.28
744.5	0.17	0.42	0.12	0.70	-0.41
764.5	0.19	0.48	0.21	0.45	-0.34
784.5	0.18	0.46	0.30	0.22	-0.18
800.0	0.17	0.44	0.35	0.11	-0.10
	100 ppm NO				
605.0	0.00	0.00	0.00	0.99	0.00
624.5	0.00	0.00	0.00	0.98	0.00
642.5	0.00	0.00	0.00	0.98	0.00
664.0	0.00	0.00	0.00	0.98	0.00
684.0	0.00	0.00	0.00	0.98	-0.01
704.5	0.00	0.01	0.01	0.98	-0.02
724.5	0.01	0.03	0.02	0.97	-0.05
744.5	0.04	0.10	0.04	0.95	-0.14
764.5	0.09	0.24	0.09	0.89	-0.30
784.5	0.16	0.40	0.15	0.75	-0.43
800.0	0.19	0.48	0.20	0.58	-0.42