Supplemental Material Section

Table S1: Vibrational frequencies of N_2O_5.

Table S2: $\Delta S°_{rxn}(T)$ for $NO_2+NO_3 \rightarrow N_2O_5$.

Table S3: $C_{p,rxn}(T)$ for $NO_2+NO_3 \rightarrow N_2O_5$.

Table S4: $\Delta H°_{rxn}(T)$ for $NO_2+NO_3 \rightarrow N_2O_5$.

Table S5: $\Delta H°_{rxn}(298K)$ for $NO_2+NO_3 \rightarrow N_2O_5$.

Table S6: $\Delta H°_f(N_2O_5, 298K)$.

Table S1: Vibrational frequencies (in cm^{-1}) of N_2O_5. Only 10 of the 15 modes, some of which are internal rotations, have been assigned.

Obs.	**G3 MP2B3**	**MP2 6-311G***	**MP2 DZ+P**	**DFT**	**MP2 6-31G**	**DFT PW/P**	**DFT VWN**	**DFT B/P**	**NIST JANAF**
1	2	3	4	4	5	6	6	6	7
1720	1857	1879	1958	1725	1966	1764	1874	1785	1728
1720	1812	1861	1941	1679	1947	1716	1827	1738	1728
1338	1412	1303	1346	1315	1360	1344	1409	1354	1338
1246	1313	1224	1262	1222	1275	1249	1316	1261	1247
860	886	822	834	820	840	834	868	837	860
?	804	767	766	717	781	726	779	742	743
743	750	719	719	698	725	716	734	716	743
?	726	690	690	652	703	661	715	678	614
614	675	631	644	630	648	638	687	650	614
557	571	519	520	475	520	470	519	477	577
353	385	347	348	336	357	340	373	342	353
?	360	226	220	258	229	186	258	209	353
?	227	213	205	197	227	186	227	196	85
50	62	64	61	62	63	77	81	77	55*
?	48	18	42	48	34	51	64	55	8*

* estimated

Table S2: $\Delta S°_{rxn}$ (J mol^{-1} K^{-1}) calculated using frequencies in Table S1. NASA-JPL recommends -(143±8) J mol^{-1} K^{-1}. Rotational constant of N_2O_5 are from Ref. [8]. A correction of +1.95 J mol^{-1} K^{-1} was applied for the anharmonicity of the internal rotors of N_2O_5.[2]

T (K)	G3MP2 B3	MP2 6-311G*	MP2 DZ+P	DFT	MP2 6-31G	DFT PW/P	DFT B/P	DFT VWN	NIST JANAF
Ref.	2	3	4	4	5	6	6	6	7
271.0	-156.18	-145.01	-151.31	-152.17	-151.29	-151.86	-154.09	-159.97	-132.99
272.5	-156.16	-144.98	-151.28	-152.13	-151.27	-151.82	-154.06	-159.96	-132.97
274.0	-156.15	-144.95	-151.26	-152.10	-151.25	-151.79	-154.03	-159.94	-132.94
275.5	-156.13	-144.93	-151.23	-152.06	-151.23	-151.75	-154.00	-159.92	-132.92
277.0	-156.11	-144.90	-151.21	-152.03	-151.21	-151.72	-153.97	-159.91	-132.89
278.6	-156.10	-144.87	-151.18	-151.99	-151.18	-151.68	-153.94	-159.89	-132.87
280.1	-156.08	-144.84	-151.15	-151.95	-151.16	-151.64	-153.91	-159.87	-132.84
281.7	-156.06	-144.81	-151.12	-151.92	-151.13	-151.61	-153.87	-159.86	-132.81
283.3	-156.04	-144.78	-151.09	-151.88	-151.11	-151.57	-153.84	-159.84	-132.78
284.9	-156.02	-144.75	-151.06	-151.84	-151.08	-151.53	-153.80	-159.82	-132.75
286.5	-156.00	-144.71	-151.03	-151.80	-151.05	-151.49	-153.77	-159.80	-132.73
288.2	-155.98	-144.68	-151.00	-151.76	-151.03	-151.45	-153.73	-159.78	-132.69
289.9	-155.95	-144.65	-150.97	-151.71	-151.00	-151.41	-153.69	-159.75	-132.66
291.5	-155.93	-144.61	-150.94	-151.67	-150.97	-151.37	-153.66	-159.73	-132.63
293.3	-155.91	-144.58	-150.90	-151.63	-150.94	-151.32	-153.62	-159.71	-132.60
295.0	-155.88	-144.54	-150.87	-151.58	-150.91	-151.28	-153.58	-159.69	-132.56
296.7	-155.86	-144.50	-150.83	-151.54	-150.88	-151.23	-153.54	-159.66	-132.53
298.5	-155.83	-144.46	-150.80	-151.49	-150.85	-151.19	-153.50	-159.64	-132.49
278.1	-156.10	-144.88	-151.19	-152.00	-151.19	-151.69	-153.95	-159.90	-132.88
298.2	-155.84	-144.47	-150.80	-151.50	-150.85	-151.20	-153.50	-159.64	-132.50
308.2	-155.68	-144.25	-150.59	-151.23	-150.66	-150.93	-153.27	-159.49	-132.29
314.8	-155.57	-144.10	-150.45	-151.05	-150.53	-150.76	-153.11	-159.39	-132.15
321.5	-155.45	-143.94	-150.30	-150.87	-150.40	-150.58	-152.94	-159.28	-132.00

Table S3: $C_{p,rxn}$ (J mol^{-1} K^{-1}) calculated using frequencies in Table S1.

T (K)	G3MP2 B3	MP2 6-311G*	MP2 DZ+P	DFT	MP2 6-31G	DFT PW/P	DFT B/P	DFT VWN	NIST JANAF
Ref.	[2]	[3]	[4]	[4]	[5]	[6]	[6]	[6]	[7]
271.0	2.65	4.79	4.52	6.10	3.84	6.13	5.37	2.63	4.30
272.5	2.76	4.89	4.61	6.20	3.93	6.22	5.47	2.72	4.40
274.0	2.86	4.98	4.71	6.30	4.02	6.31	5.56	2.82	4.50
275.5	2.97	5.08	4.80	6.40	4.12	6.40	5.65	2.91	4.60
277.0	3.07	5.18	4.89	6.50	4.21	6.49	5.74	3.01	4.70
278.6	3.19	5.28	4.98	6.60	4.31	6.59	5.84	3.11	4.80
280.1	3.29	5.37	5.07	6.70	4.40	6.68	5.93	3.20	4.90
281.7	3.40	5.47	5.17	6.80	4.49	6.77	6.02	3.30	5.00
283.3	3.51	5.56	5.26	6.90	4.59	6.86	6.11	3.39	5.10
284.9	3.61	5.66	5.35	7.00	4.68	6.95	6.21	3.49	5.20
286.5	3.72	5.76	5.44	7.10	4.77	7.04	6.30	3.58	5.30
288.2	3.83	5.86	5.54	7.20	4.87	7.13	6.39	3.68	5.41
289.9	3.94	5.96	5.63	7.30	4.96	7.23	6.49	3.78	5.51
291.5	4.05	6.05	5.72	7.40	5.05	7.31	6.58	3.88	5.61
293.3	4.16	6.15	5.82	7.50	5.15	7.41	6.68	3.98	5.71
295.0	4.27	6.25	5.91	7.60	5.25	7.50	6.77	4.07	5.82
296.7	4.37	6.34	6.00	7.70	5.34	7.59	6.86	4.17	5.91
298.5	4.48	6.44	6.09	7.80	5.43	7.68	6.95	4.27	6.02
278.1	3.15	5.24	4.95	6.57	4.28	6.56	5.81	3.08	4.77
298.2	4.47	6.43	6.08	7.78	5.42	7.67	6.94	4.25	6.00
308.2	5.06	6.96	6.58	8.32	5.93	8.17	7.44	4.78	6.56
314.8	5.43	7.29	6.89	8.66	6.25	8.48	7.76	5.11	6.91
321.5	5.80	7.61	7.20	8.99	6.56	8.78	8.07	5.43	7.25

Table S4: $\Delta H°_{rxn}$ (kJ mol^{-1}) calculated using frequencies in Table S1.

T (K)	G3MP2 B3	MP2 6-311G*	MP2 DZ+P	DFT	MP2 6-31G	DFT PW/P	DFT B/P	DFT VWN	NIST JANAF
Ref.	[2]	[3]	[4]	[4]	[5]	[6]	[6]	[6]	[7]
271.0	-96.5	-93.4	-95.1	-95.4	-95.1	-95.3	-95.9	-97.5	-90.2
272.5	-97.0	-94.0	-95.7	-95.9	-95.7	-95.8	-96.4	-98.0	-90.7
274.0	-96.6	-93.5	-95.2	-95.4	-95.2	-95.4	-96.0	-97.6	-90.2
275.5	-96.8	-93.7	-95.4	-95.6	-95.4	-95.6	-96.2	-97.8	-90.4
277.0	-97.2	-94.1	-95.8	-96.1	-95.8	-96.0	-96.6	-98.2	-90.8
278.6	-97.4	-94.3	-96.0	-96.2	-96.0	-96.2	-96.8	-98.4	-90.9
280.1	-97.4	-94.3	-96.1	-96.3	-96.1	-96.2	-96.8	-98.5	-90.9
281.7	-97.4	-94.3	-96.0	-96.3	-96.0	-96.2	-96.8	-98.5	-90.9
283.3	-97.8	-94.6	-96.4	-96.7	-96.4	-96.6	-97.2	-98.9	-91.2
284.9	-97.1	-93.9	-95.7	-95.9	-95.7	-95.8	-96.5	-98.2	-90.5
286.5	-97.3	-94.1	-95.9	-96.1	-95.9	-96.0	-96.7	-98.4	-90.7
288.2	-97.2	-93.9	-95.8	-96.0	-95.8	-95.9	-96.5	-98.3	-90.5
289.9	-97.0	-93.7	-95.6	-95.8	-95.6	-95.7	-96.4	-98.1	-90.3
291.5	-97.1	-93.8	-95.7	-95.9	-95.7	-95.8	-96.5	-98.2	-90.3
293.3	-97.0	-93.7	-95.5	-95.7	-95.5	-95.6	-96.3	-98.1	-90.2
295.0	-97.3	-93.9	-95.8	-96.0	-95.8	-95.9	-96.6	-98.4	-90.4
296.7	-97.5	-94.1	-96.0	-96.2	-96.0	-96.1	-96.8	-98.6	-90.5
298.5	-96.8	-93.4	-95.3	-95.5	-95.3	-95.4	-96.1	-97.9	-89.8
278.1	-97.2	-94.1	-95.8	-96.0	-95.8	-95.9	-96.6	-98.2	-90.7
298.2	-97.4	-94.0	-95.9	-96.1	-95.9	-96.0	-96.7	-98.5	-90.4
308.2	-97.6	-94.0	-96.0	-96.2	-96.0	-96.1	-96.8	-98.7	-90.4
314.8	-97.5	-93.9	-95.9	-96.1	-96.0	-96.0	-96.8	-98.7	-90.2
321.5	-97.6	-93.9	-96.0	-96.2	-96.0	-96.1	-96.8	-98.9	-90.1

Table S5: $\Delta H°_{rxn}(298K)$ (kJ mol^{-1}) calculated using frequencies in Table S1. NASA-JPL recommends -94.6 kJ mol^{-1};[9] IUPAC recommends -95.6 kJ mol^{-1}.[10]

T (K)	G3MP2 B3	MP2 6-311G*	MP2 DZ+P	DFT	MP2 6-31G	DFT PW/P	DFT B/P	DFT VWN	NIST JANAF
Ref.	[2]	[3]	[4]	[4]	[5]	[6]	[6]	[6]	[7]
271.0	-96.6	-93.6	-95.3	-95.6	-95.3	-95.5	-96.1	-97.6	-90.3
272.5	-97.1	-94.1	-95.8	-96.1	-95.8	-96.0	-96.6	-98.1	-90.8
274.0	-96.6	-93.6	-95.3	-95.6	-95.3	-95.5	-96.1	-97.7	-90.3
275.5	-96.9	-93.8	-95.5	-95.8	-95.5	-95.7	-96.3	-97.9	-90.5
277.0	-97.3	-94.2	-96.0	-96.2	-95.9	-96.1	-96.7	-98.3	-90.9
278.6	-97.5	-94.4	-96.1	-96.4	-96.1	-96.3	-96.9	-98.5	-91.0
280.1	-97.5	-94.4	-96.2	-96.4	-96.1	-96.3	-96.9	-98.6	-91.0
281.7	-97.5	-94.4	-96.1	-96.4	-96.1	-96.3	-96.9	-98.6	-91.0
283.3	-97.9	-94.7	-96.5	-96.8	-96.5	-96.7	-97.3	-99.0	-91.3
284.9	-97.1	-94.0	-95.8	-96.0	-95.7	-95.9	-96.5	-98.2	-90.5
286.5	-97.4	-94.2	-96.0	-96.2	-96.0	-96.1	-96.8	-98.5	-90.7
288.2	-97.2	-94.0	-95.8	-96.1	-95.8	-96.0	-96.6	-98.3	-90.5
289.9	-97.0	-93.8	-95.6	-95.8	-95.6	-95.8	-96.4	-98.1	-90.3
291.5	-97.2	-93.9	-95.7	-95.9	-95.7	-95.8	-96.5	-98.3	-90.4
293.3	-97.0	-93.7	-95.6	-95.8	-95.6	-95.7	-96.4	-98.1	-90.2
295.0	-97.3	-94.0	-95.8	-96.0	-95.8	-95.9	-96.6	-98.4	-90.4
296.7	-97.5	-94.1	-96.0	-96.2	-96.0	-96.1	-96.8	-98.6	-90.6
298.5	-96.8	-93.4	-95.3	-95.5	-95.3	-95.4	-96.1	-97.9	-89.8
278.1	-97.2	-94.2	-95.9	-96.2	-95.9	-96.1	-96.7	-98.3	-90.8
298.2	-97.4	-94.0	-95.9	-96.1	-95.9	-96.0	-96.7	-98.5	-90.4
308.2	-97.5	-94.0	-95.9	-96.1	-96.0	-96.0	-96.8	-98.7	-90.3
314.8	-97.5	-93.8	-95.8	-96.0	-95.9	-95.9	-96.6	-98.7	-90.1
321.5	-97.5	-93.8	-95.8	-96.0	-95.9	-95.9	-96.6	-98.7	-89.9

Table S6: $\Delta H°_f(N_2O_5, 298K)$ (kJ mol^{-1}) calculated using N_2O_5 frequencies in Table S1.

$\Delta H°_f(NO_3+NO_2, 298K)$=(107.9±1.9) kJ mol^{-1}; NASA/JPL recommends 13.3 kJ mol^{-1}.[9]

Neglecting the DFT/VWN[6] and NIST-JANAF[7] results, $\Delta H°_f(N_2O_5, 298K)$ equals

(12±1) kJ mol^{-1}.

	G3MP2 B3	**MP2 6-311G***	**MP2 DZ+P**	**DFT**	**MP2 6-31G**	**DFT PW/P**	**DFT B/P**	**DFT VWN**	**NIST JANAF**
Ref.	[2]	[3]	[4]	[4]	[5]	[6]	[6]	[6]	[7]
lab	10.5	13.9	12.0	11.8	12.0	11.9	11.2	9.3	17.6
field	10.7	13.9	12.1	11.8	12.1	11.9	11.3	9.6	17.3

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