THE JOURNAL OF PHYSICAL CHEMISTRY A
J. Phys. Chem. A, 1997, 101(17), 3143-3151, DOI:10.1021/jp9624358

Table S.I. Calculated energies at points along the NH_3 enhanced inversion potential surface in Hartrees with q in degrees.[a]

	MP2	QCISD(T)			
	6-311++G**	APNO		CBSB5	
q	Opt.	Uncorr.	CBS	Uncorr.	CBS
0	-56.42678	-56.45423	-56.55157	-56.47833	-56.57567
1	-56.42682	-56.45426	-56.55161	-56.47837	-56.57572
2	-56.42693	-56.45437	-56.55173	-56.47848	-56.57584
3	-56.42710	-56.45455	-56.55191	-56.47867	-56.57603
4	-56.42735	-56.45480	-56.55215	-56.47894	-56.57628
5	-56.42766	-56.45511	-56.55244	-56.47927	-56.57660
6	-56.42803	-56.45548	-56.55280	-56.47966	-56.57698
7	-56.42845	-56.45591	-56.55322	-56.48010	-56.57742
8	-56.42891	-56.45638	-56.55369	-56.48060	-56.57791
9	-56.42942	-56.45689	-56.55419	-56.48114	-56.57844
10	-56.42995	-56.45743	-56.55473	-56.48170	-56.57900
11	-56.43051	-56.45800	-56.55528	-56.48229	-56.57957
12	-56.43107	-56.45857	-56.55584	-56.48290	-56.58016
13	-56.43164	-56.45915	-56.55641	-56.48350	-56.58076
14	-56.43219	-56.45972	-56.55699	-56.48410	-56.58136
15	-56.43272	-56.46027	-56.55755	-56.48467	-56.58195
16	-56.43321	-56.46078	-56.55807	-56.48521	-56.58250
17	-56.43365	-56.46125	-56.55855	-56.48571	-56.58300
18	-56.43403	-56.46166	-56.55896	-56.48615	-56.58345
19	-56.43434	-56.46200	-56.55930	-56.48652	-56.58383
20	-56.43455	-56.46225	-56.55956	-56.48681	-56.58413

Table S.I. Continued.

	MP2	QCISD(T)			
	6-311++G**	APNO		CBSB5	
q	Opt.	Uncorr.	CBS	Uncorr.	CBS
21	-56.43467	-56.46240	-56.55972	-56.48701	-56.58433
22	-56.43466	-56.46244	-56.55978	-56.48710	-56.58444
23	-56.43453	-56.46236	-56.55974	-56.48706	-56.58445
24	-56.43426	-56.46213	-56.55957	-56.48690	-56.58433
25	-56.43384	-56.46176	-56.55925	-56.48659	-56.58409
26	-56.43324	-56.46122	-56.55879	-56.48613	-56.58370
27	-56.43248	-56.46050	-56.55815	-56.48549	-56.58314
28	-56.43152	-56.45959	-56.55733	-56.48468	-56.58242
29	-56.43038	-56.45848	-56.55632	-56.48368	-56.58152
30	-56.42904	-56.45716	-56.55513	-56.48248	-56.58044
31	-56.42749	-56.45562	-56.55372	-56.48107	-56.57917
32	-56.42575	-56.45385	-56.55210	-56.47944	-56.57769
33	-56.42382	-56.45185	-56.55024	-56.47759	-56.57598
34	-56.42168	-56.44960	-56.54815	-56.47549	-56.57403
35	-56.41936	-56.44711	-56.54581	-56.47313	-56.57183
40	-56.40440	-56.43080	-56.52991	-56.45718	-56.55629
45	-56.38177	-56.40702	-56.50592	-56.43316	-56.53206
50	-56.34889	-56.37368	-56.47226	-56.39950	-56.49809
55	-56.30391	-56.32870	-56.42715	-56.35438	-56.45284
60	-56.24460	-56.27041	-56.36882	-56.29612	-56.39453

a. QCISD(T) calculations utilized the MP2/6-311++G** optimized geometries.

Table S.II. Values of the inversional kinetic energy terms for $^{14}NH_3$ and $^{15}NH_3$ calculated from the MP2/6-311++G** optimized geometries. Reduced mass $\mu(q)$ is in m_e Bohr^2/deg^2, the determinant of the **G** matrix in deg^2/m_e^4 Bohr^8, the $f_1(q)$ term in Hartrees and q in degrees.

	$^{14}NH_3$			$^{15}NH_3$		
q	$\mu(q)$	det **G**	$f_1(q)$	$\mu(q)$	det **G**	$f_1(q)$
0	4.9120	1.0798E-13	7.9170E-05	4.9708	1.0671E-13	8.7352E-05
5	4.9245	1.0693E-13	7.0613E-05	4.9828	1.0565E-13	7.8506E-05
10	4.9719	1.0374E-13	4.6308E-05	5.0291	1.0244E-13	5.3380E-05
15	5.0599	9.8795E-14	1.0029E-05	5.1154	9.7476E-14	1.5856E-05
20	5.1644	9.3215E-14	-3.2534E-05	5.2175	9.1873E-14	-2.8231E-05
25	5.3031	8.7301E-14	-7.4439E-05	5.3533	8.5942E-14	-7.1772E-05
30	5.4640	8.1735E-14	-1.0828E-04	5.5104	8.0366E-14	-1.0721E-04
35	5.6517	7.6867E-14	-1.2708E-04	5.6938	7.5491E-14	-1.2747E-04
40	5.8751	7.2413E-14	-1.2496E-04	5.9129	7.1037E-14	-1.2656E-04
45	6.1675	6.7685E-14	-9.8391E-05	6.2006	6.6335E-14	-1.0094E-04
50	6.5431	6.2604E-14	-4.7839E-05	6.5718	6.1300E-14	-5.1023E-05
55	7.0537	5.6398E-14	2.0137E-05	7.0778	5.5186E-14	1.6617E-05
60	7.8204	4.7918E-14	8.9885E-05	7.8405	4.6860E-14	8.6314E-05

Table S.III. Values of the inversional kinetic energy terms for $^{14}ND_3$ and $^{15}ND_3$ calculated from the MP2/6-311++G** optimized geometries. Reduced mass $\mu(q)$ is in m_e Bohr^2/deg^2, the determinant of the **G** matrix in deg^2/m_e^4 Bohr^8, the $f_1(q)$ term in Hartrees and q in degrees.

	$^{14}ND_3$			$^{15}ND_3$		
q	$\mu(q)$	det **G**	$f_1(q)$	$\mu(q)$	det **G**	$f_1(q)$
0	8.3383	4.6435E-15	-2.9219E-05	8.5087	7.8102E-15	-1.6138E-05
5	8.3733	4.6631E-15	-3.3992E-05	8.5427	7.7488E-15	-2.1368E-05
10	8.4949	4.7308E-15	-4.7472E-05	8.6611	7.5590E-15	-3.6162E-05
15	8.7122	4.8518E-15	-6.7216E-05	8.8737	7.2609E-15	-5.7924E-05
20	8.9833	5.0028E-15	-8.9309E-05	9.1376	6.9269E-15	-8.2532E-05
25	9.3370	5.1997E-15	-1.0897E-04	9.4823	6.5702E-15	-1.0495E-04
30	9.7507	5.4301E-15	-1.2074E-04	9.8855	6.2346E-15	-1.1947E-04
35	10.2304	5.6973E-15	-1.1933E-04	10.3531	5.9432E-15	-1.2059E-04
40	10.7905	6.0092E-15	-1.0009E-04	10.9001	5.6722E-15	-1.0348E-04
45	11.4913	6.3995E-15	-6.0331E-05	11.5875	5.3660E-15	-6.5343E-05
50	12.3555	6.8807E-15	-8.2012E-07	12.4387	5.0187E-15	-6.9186E-06
55	13.4887	7.5118E-15	7.2034E-05	13.5589	4.5650E-15	6.5322E-05
60	15.1240	8.4225E-15	1.4336E-04	15.1822	3.9110E-15	1.3631E-04

Table S.IV. Values of the inversional kinetic energy terms for $^{14}NT_3$ and $^{15}NT_3$ calculated from the MP2/6-311++G** optimized geometries. Reduced mass $\mu(q)$ is in m_e Bohr^2/deg^2, the determinant of the **G** matrix in deg^2/m_e^4 Bohr^8, the $f_1(q)$ term in Hartrees and q in degrees.

	$^{14}NT_3$			$^{15}NT_3$		
q	$\mu(q)$	det **G**	$f_1(q)$	$\mu(q)$	det **G**	$f_1(q)$
0	10.8581	1.8226E-15	-1.1728E-04	11.1491	1.7751E-15	-1.0086E-04
5	10.9219	1.8107E-15	-1.1890E-04	11.2108	1.7632E-15	-1.0309E-04
10	11.1335	1.7734E-15	-1.2332E-04	11.4171	1.7260E-15	-1.0924E-04
15	11.5049	1.7145E-15	-1.2909E-04	11.7802	1.6673E-15	-1.1769E-04
20	11.9791	1.6501E-15	-1.3370E-04	12.2422	1.6027E-15	-1.2565E-04
25	12.5927	1.5821E-15	-1.3418E-04	12.8407	1.5343E-15	-1.2980E-04
30	13.3140	1.5199E-15	-1.2688E-04	13.5440	1.4713E-15	-1.2613E-04
35	14.1476	1.4684E-15	-1.0814E-04	14.3569	1.4185E-15	-1.1064E-04
40	15.1113	1.4211E-15	-7.4596E-05	15.2984	1.3697E-15	-7.9704E-05
45	16.2893	1.3634E-15	-2.4186E-05	16.4534	1.3110E-15	-3.1179E-05
50	17.7082	1.2931E-15	4.2611E-05	17.8501	1.2404E-15	3.4300E-05
55	19.5295	1.1916E-15	1.2107E-04	19.6492	1.1403E-15	1.1146E-04
60	22.0917	1.0332E-15	1.9991E-04	22.1910	9.8663E-16	1.8791E-04

Table S.V. Values of the inversional energy levels of ammonia calculated from a cubic spline interpolation of the potential surface at various levels of ab initio theory. Functions for $\mu(q)$ and $f_1(q)$ calculated at the MP2/6-311++G** level. E is in Hartrees. All other energy units are cm^{-1}.

	HF			MP2	
	6-31G*			6-311++G**	
Lit.	Opt.	Fix Eq.[a]	Fix Ts.[b]	Opt.	Fix Eq.
E_{eq}	-56.18436	-56.18436	-56.18383	-56.43468	-56.43468
E_{ts}	-56.17399	-56.17340	-56.17399	-56.42678	-56.42622
Barrier	2276	2403	2159	1733	1857
ZPE	575.63	589.99	575.22	506.69	524.74
0.00	0.00	0.00	0.00	0.00	0.00
0.79	0.79	0.77	1.23	2.18	1.74
932.43	1044.94	1079.53	1028.67	874.96	918.25
968.12	1082.04	1110.82	1080.95	951.79	984.45
1598.47	1792.16	1860.84	1758.80	1507.70	1573.09
1882.18	2102.73	2152.37	2116.90	1885.33	1939.71
2384.17	2664.06	2724.40	2690.23	2405.17	2469.68
2895.61	3235.18	3295.60	3287.50	2955.61	3027.79
3448	3870.29	3936.63	3943.92	3549.37	3633.01
4045	4546.08	4619.02	4641.84	4175.60	4272.63
	5259.84	5340.77	5377.82	4830.65	4943.09

a. NH bond length held constant at the equilibrium value.

b. NH bond length held constant at the planar transition state value.

Table S.VI. Inversional energy levels for ammonia calculated from the enhanced CBS-QCI/CBSB5 PES using different values of reduced mass $\mu(q)$. Function $f_1(q)$ calculated from the MP2/6-311++G** geometries. Reduced mass given in m_e $Bohr^2/deg^2$ with function coefficients in corresponding units. Energy units are cm^{-1}.

	MP2					HF
	6-311++G**			6-31+G**		6-31G*
	Opt.	Eq.	TS	Opt.	Eq.	Eq.
μ_0	4.910	5.203	4.910	4.902	5.177	5.100
μ_1	6.669E-04			6.730E-04		
μ_2	-7.937E-08			-9.542E-08		
μ_3	2.089E-11			2.859E-11		
μ_4	3.348E-15			1.628E-15		
ZPE	498.11	498.61	512.60	498.46	499.81	503.40
0+	0.00	0.00	0.00	0.00	0.00	0.00
0-	0.99	0.86	1.12	1.00	0.88	0.94
1+	905.50	905.45	923.09	906.01	906.99	911.58
1-	946.84	944.54	971.26	947.59	946.81	953.64
2+	1553.20	1546.74	1576.07	1554.05	1549.19	1556.60
2-	1852.91	1843.26	1903.69	1854.64	1848.36	1863.75
3+	2353.99	2340.64	2421.80	2356.31	2347.47	2368.11
3-	2869.27	2855.37	2963.54	2872.38	2864.51	2892.08
4+	3439.37	3425.64	3560.44	3443.28	3437.04	3471.42
4-	4046.53	4034.92	4197.75	4051.29	4048.70	4090.24
5+	4687.78	4680.11	4871.98	4693.45	4696.36	4745.33