Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Appraisal of Individual Hydrogen Bond Strengths and Cooperativity in Ammonia Clusters via Molecular Tailoring Approach

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Table S1: Molecular energies (in a.u.) of various species in the MTA calculation of ammonia tetramer, $(NH_3)_4$ at MP2(full)/aug-cc-pvTZ level of theory. See text for details.

Species	Energy
Ammonia Tetramer (E_m)	-225.940105
Fragment F1 (E_{F1})	-169.446144
Fragment F2 (E_{F2})	-169.446144
Fragment F3 (E_{F3})	-112.9603633
Ammonia dimer ($E_{N1\ldots N2}^{dimer}$)	-112.9603633
Ammonia monomer (E_{N1})	-56.477293
Ammonia monomer (E_{N2})	-56.477293

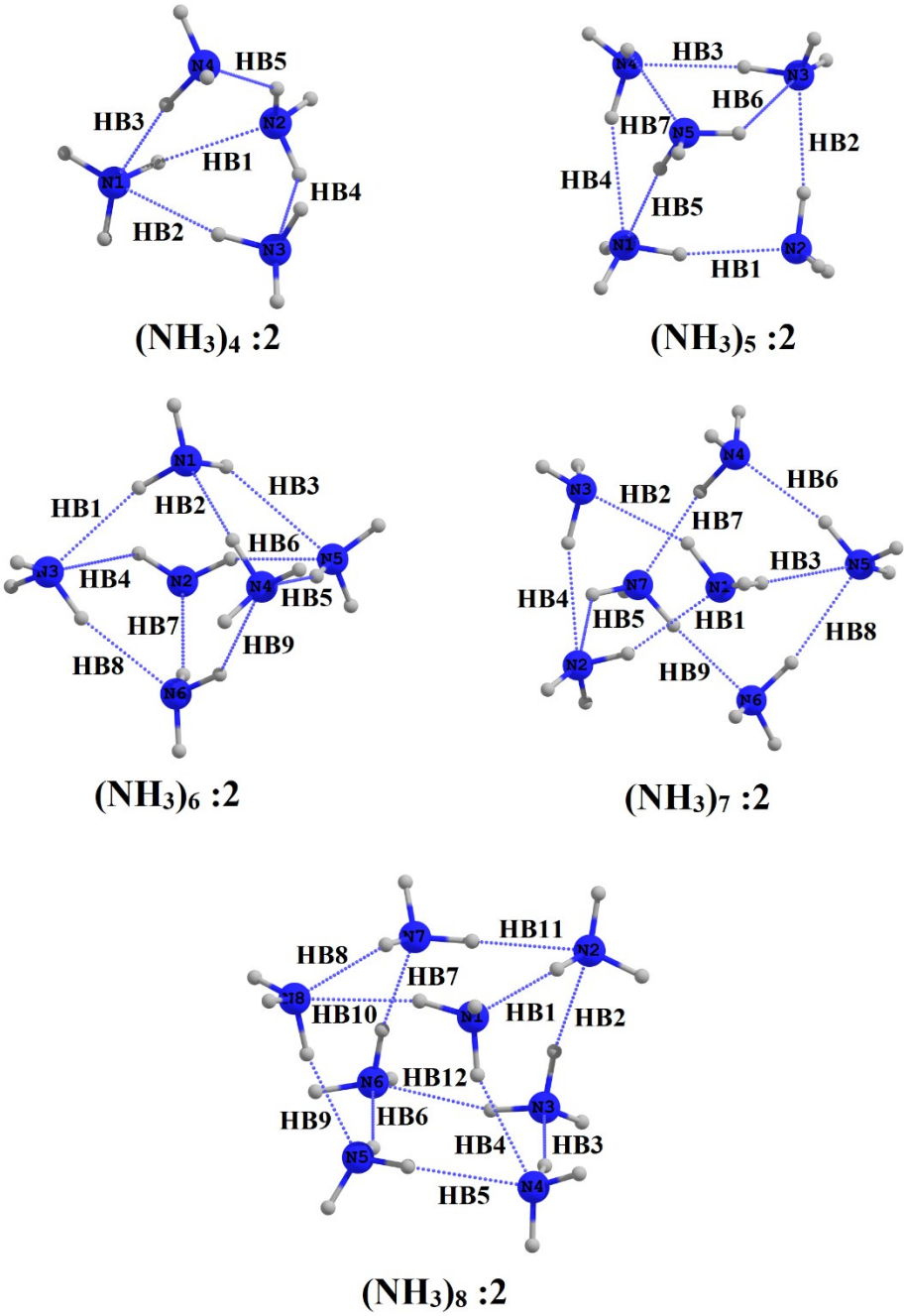

Figure S1: The MP2-optimized geometries of various ammonia clusters $(NH_3)_n$:2. Also see Figures 1 and S2.

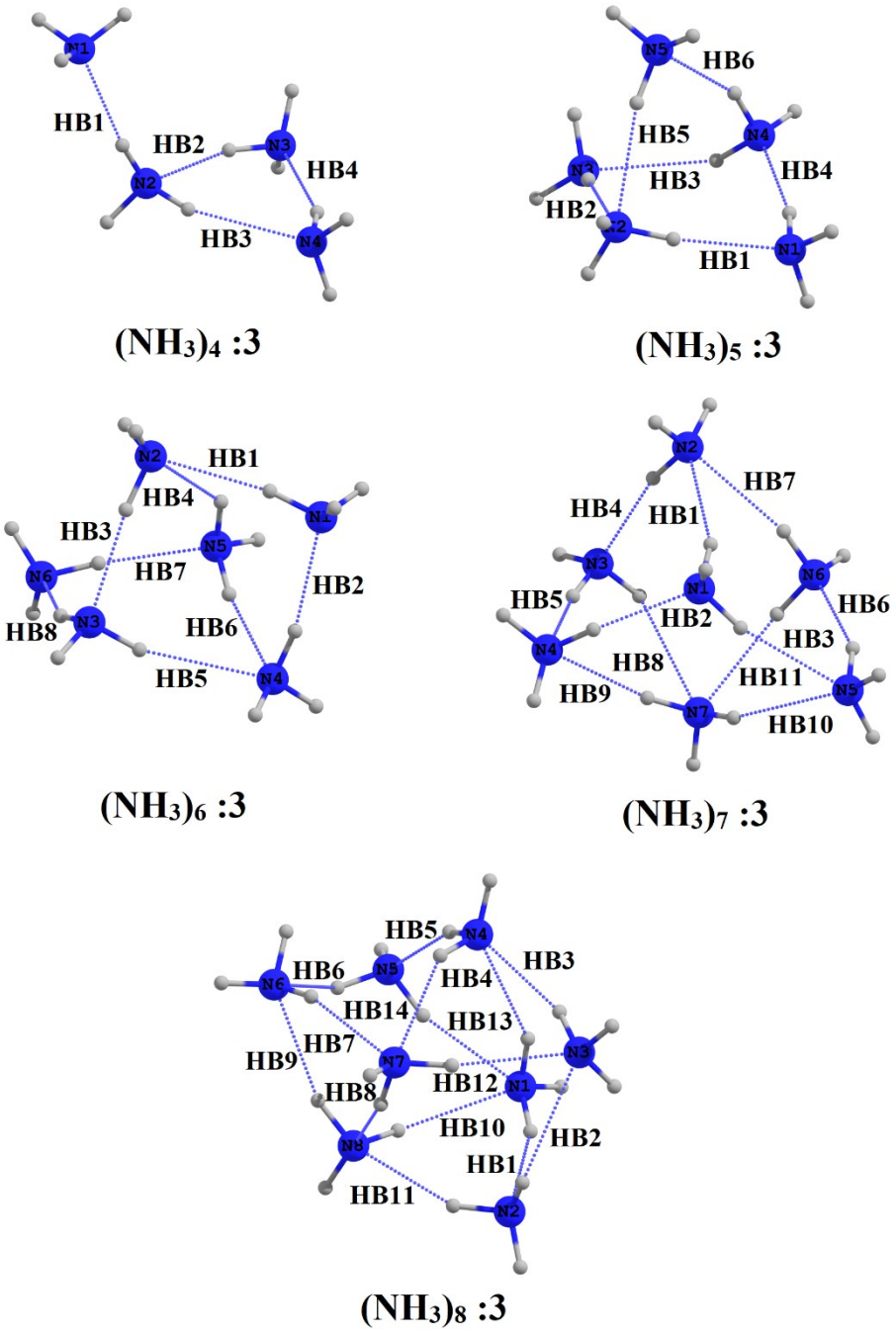

Figure S2: The MP2-optimized geometries of various ammonia clusters $(NH_3)_n$:3. Also see Figures 1 and S1.

Table S2: The HB energies in ammonia clusters $(NH_3)_n$:1 n=7, 8, calculated at MP2(full)/aug-cc-pVTZ level, along with the cooperativity contribution.

HB label	HB Distance (in Å)	HB Angles (in degrees)	HB energy byMTA (in kcal/mol)	HB energy in Dimer (in kcal/mol)	Cooperativity (in kcal/mol)
			$(NH_3)_7$:1		
HB1	2.12	170	5.32	3.56	1.76
HB2	2.30	160	3.94	3.34	0.60
HB3	2.30	160	3.94	3.34	0.60
HB4	2.28	161	3.90	3.38	0.53
HB5	2.12	158	5.01	3.51	1.50
HB6	2.12	158	5.01	3.51	1.50
HB7	2.28	161	3.90	3.38	0.53
HB8	2.39	162	3.79	3.14	0.65
HB9	2.45	140	3.70	3.19	0.51
HB10	2.45	140	3.70	3.19	0.51
HB11	2.39	162	3.79	3.14	0.65
			$(NH_3)_8$:1		
HB1	2.30	163	4.00	3.36	0.64
HB2	2.30	163	4.00	3.36	0.64
HB3	2.30	163	4.00	3.36	0.64
HB4	2.30	163	4.00	3.36	0.64
HB5	2.10	169	5.34	3.53	1.81
HB6	2.30	163	4.00	3.36	0.64
HB7	2.30	163	4.00	3.36	0.64
HB8	2.30	163	4.00	3.36	0.64
HB9	2.30	163	4.00	3.36	0.64
HB10	2.10	169	5.34	3.53	1.81
HB11	2.10	169	5.34	3.53	1.81
HB12	2.10	169	5.34	3.53	1.81

Table S3: The HB energies in the second most stable conformers of ammonia clusters, $(NH_3)_n$:2 (n=3-8) calculated at MP2(full)/aug-cc-pVTZ level of theory, along with cooperativity contribution.

HB label	HB Distance (in Å)	HB Angles (in degrees)	HB energy with MTA (in kcal/mol)	HB energy in Dimer (in kcal/mol)	Cooperativity (in kcal/mol)
			$(NH_3)_4$:2		
HB1	2.15	150	4.84	3.44	1.41
HB2	2.42	151	3.54	3.09	0.45
HB3	2.29	158	3.94	3.21	0.73
HB4	2.43	129	2.67	2.39	0.28
HB5	2.42	140	3.76	3.21	0.55
			$(NH_3)_5$:2		
HB1	2.13	167	5.04	3.59	1.45
HB2	2.15	170	5.02	3.59	1.44
HB3	2.13	165	4.86	3.34	1.51
HB4	2.34	157	3.79	3.00	0.79
HB5	2.39	168	2.17	2.31	-0.13
HB6	2.84	124	2.53	2.19	0.35
HB7	2.47	120	1.65	1.70	-0.04
			$(NH_3)_6$:2		
HB1	2.22	163	4.32	3.58	0.73
HB2	2.13	158	4.87	3.49	1.37
HB3	2.57	137	3.49	2.96	0.53
HB4	2.58	137	3.33	2.76	0.57
HB5	2.25	165	4.31	3.35	0.96
HB6	2.27	153	3.84	3.45	0.38
HB7	2.22	150	3.55	3.07	0.48
HB8	2.16	159	4.86	3.47	1.39
HB9	2.42	147	3.31	3.10	0.20
			$(NH_3)_7$:2		
HB1	2.17	152	4.92	3.64	1.28
HB2	2.30	158	4.27	3.59	0.68
HB3	2.42	176	1.50	2.04	-0.54
HB4	2.26	160	4.56	3.60	0.97
HB5	2.57	129	1.18	1.59	-0.40
HB6	2.09	166	5.19	3.48	1.70
HB7	2.15	168	4.99	3.60	1.39
HB8	2.21	168	4.55	3.47	1.07
HB9	2.19	168	4.73	3.57	1.16
			$(NH_3)_8$:2		
HB1	2.11	167	5.19	3.49	1.70
HB2	2.30	156	3.90	3.40	0.50
HB3	2.11	167	5.19	3.49	1.70
HB4	2.30	156	3.90	3.40	0.50
HB5	2.30	165	2.29	2.48	-0.19
HB6	2.30	156	3.90	3.40	0.50
HB7	2.11	167	5.19	3.49	1.70
HB8	2.30	156	3.90	3.40	0.50
HB9	2.11	167	5.19	3.49	1.70
HB10	2.30	165	2.29	2.48	-0.19
HB11	2.30	165	2.29	2.48	-0.19
HB12	2.30	165	2.29	2.48	-0.19

Table S4: The HB energies in the third most stable conformers of ammonia clusters, $(NH_3)_n$:3 (n=3-8) calculated at MP2(full)/aug-cc-pVTZ level of theory, along with cooperativity contribution.

HB label	HB Distance (in Å)	HB Angles (in degrees)	HB energy with MTA (in kcal/mol)	HB energy in Dimer (in kcal/mol)	Cooperativity (in kcal/mol)
			$(NH_3)_4$:3		
HB1	2.27	172	3.49	3.60	-0.11
HB2	2.16	157	5.11	3.65	1.47
HB3	2.30	151	4.37	3.61	0.76
HB4	2.22	157	4.86	3.68	1.18
			$(NH_3)_5$:3		
HB1	2.11	169	5.42	3.55	1.88
HB2	2.33	165	3.63	3.12	0.51
HB3	2.36	137	2.48	2.30	0.18
HB4	2.10	166	5.31	3.54	1.77
HB5	2.25	168	3.62	3.01	0.61
HB6	2.28	152	3.84	3.35	0.49
			$(NH_3)_6$:3		
HB1	2.18	169	4.81	3.48	1.33
HB2	2.14	167	5.03	3.61	1.41
HB3	2.10	169	5.19	3.35	1.84
HB4	2.55	136	3.01	2.61	0.40
HB5	2.37	159	3.23	2.83	0.40
HB6	2.30	165	2.76	2.58	0.18
HB7	2.17	164	4.81	3.59	1.22
HB8	2.21	157	3.73	3.13	0.60
			$(NH_3)_7$:3		
HB1	2.31	159	3.95	3.37	0.58
HB2	2.10	167	5.24	3.49	1.76
HB3	2.29	165	2.41	2.49	-0.07
HB4	2.12	166	5.08	3.56	1.51
HB5	2.25	161	4.34	3.43	0.90
HB6	2.12	156	4.99	3.44	1.56
HB7	2.33	165	2.40	2.48	-0.08
HB8	2.73	120	0.65	1.06	-0.41
HB9	2.37	164	1.95	2.29	-0.33
HB10	2.41	153	3.75	3.13	0.62
HB11	2.31	147	3.87	3.42	0.45
			$(NH_3)_8$:3		
HB1	2.21	157	4.07	3.38	0.69
HB2	2.53	132	3.02	2.85	0.17
HB3	2.22	159	4.47	3.44	1.03
HB4	2.42	151	3.87	3.23	0.64
HB5	2.20	160	4.18	3.35	0.83
HB6	2.52	133	3.03	2.88	0.15
HB7	2.25	159	4.39	3.42	0.97
HB8	2.31	151	4.17	3.46	0.71
HB9	2.31	156	4.06	3.47	0.59
HB10	2.34	154	4.15	3.37	0.78
HB11	2.35	149	3.99	3.32	0.67
HB12	2.29	160	4.15	3.46	0.69
HB13	2.31	150	4.03	3.37	0.66
HB14	2.39	148	3.92	3.35	0.57

Table S5: Error in the estimation of total energy of the second most stable conformer $(NH_3)_n$:2 at MP2(full)/aug-cc-pVTZ level of theory. See text for details

Ammonia Clusters	$\sum E_{HB}$¶ (in a.u.)	$\sum E_{monomers}$‡ (in a.u.)	$E_{calculated}$[a] (in a.u.)	E_{actual} (in a.u.)	Error (in a.u.)	Error (in kcal/ mol)	Error per H-bond (in kcal/mol)
$(NH_3)_4$:2	0.02988	-225.90932	-225.93919	-225.93608	0.003112	1.95	0.39
$(NH_3)_5$:2	0.03995	-282.38647	-282.42642	-282.42570	0.000729	0.46	0.07
$(NH_3)_6$:2	0.05715	-338.86383	-338.92098	-338.91528	0.005699	3.58	0.40
$(NH_3)_7$:2	0.05718	-395.34111	-395.39830	-395.40498	-0.006680	-4.19	-0.47
$(NH_3)_8$:2	0.07252	-451.81824	-451.89076	-451.89626	-0.005502	-3.45	-0.29

[a] E (calculated) = $\sum E_{monomers}$ - $\sum E_{HB}$

¶ $\sum E_{HB}$ is sum of HB energy by MTA. $\sum E_{HB}$ is subtracted from sum of monomers energy is because of by definition E_{HB} is taken as positive.

‡ Monomer energies were calculated from the respective monomer geometries as in the clusters.

Table S6: Error in the estimation of total energy of the third most stable conformer $(NH_3)_n$:3 at MP2(full)/aug-cc-pVTZ level of theory. See text for details

Ammonia Clusters	$\sum E_{HB}$¶ (in a.u.)	$\sum E_{monomers}$‡ (in a.u.)	$E_{calculated}$[a] (in a.u.)	E_{actual} (in a.u.)	Error (in a.u.)	Error (kcal/ mol)	Error per H-bond (kcal/mol)
$(NH_3)_4$:3	0.02842	-225.90933	-225.93775	-225.93397	0.003775	2.37	0.59
$(NH_3)_5$:3	0.03873	-282.38648	-282.42521	-282.42558	-0.000377	-0.24	-0.08
$(NH_3)_6$:3	0.05188	-338.86372	-338.91560	-338.91541	0.000190	0.12	0.02
$(NH_3)_7$:3	0.06158	-395.34103	-395.40261	-395.40542	-0.002808	-1.76	-0.16
$(NH_3)_8$:3	0.07578	-451.81857	-451.89436	-451.89538	-0.001022	-0.64	-0.05

[a] E (calculated) = $\sum E_{monomers}$ - $\sum E_{HB}$

¶ $\sum E_{HB}$ is sum of HB energy by MTA. $\sum E_{HB}$ is subtracted from sum of monomers energy is because of by definition E_{HB} is taken as positive.
‡ Monomer energies were calculated from the respective monomer geometries as in the clusters.

Table S7: The comparison of sum of hydrogen bond energy and the dissociation energy (ΔE)[#] in $(NH_3)_n$:m (n=3 to 8 and m=1,3) calculated at MP2(full)/aug-cc-pVTZ level.

Ammonia Cluster	Sum of HB Energy by MTA	Dissociation Energy (ΔE)
$(NH_3)_3$:1	14.55	11.84
$(NH_3)_4$:1	20.52	18.91
$(NH_3)_5$:1	24.88	24.24
$(NH_3)_6$:1	31.98	31.03
$(NH_3)_7$:1	46.00	39.59
$(NH_3)_8$:1	56.36	48.13
$(NH_3)_4$:2	18.75	16.39
$(NH_3)_5$:2	25.06	24.00
$(NH_3)_6$:2	35.88	31.58
$(NH_3)_7$:2	35.89	39.24
$(NH_3)_8$:2	45.52	47.90
$(NH_3)_4$:3	17.83	15.07
$(NH_3)_5$:3	24.30	23.92
$(NH_3)_6$:3	32.57	31.66
$(NH_3)_7$:3	38.63	39.52
$(NH_3)_8$:3	55.50	47.34

[#] $\Delta E = n*E_{monomer} - E_{cluster}$. Here, n is number of monomers in a cluster. $E_{cluster}$ and $E_{monomer}$ are the energies of a clusters and the free monomer, respectively.

Cartesian Coordinates of Ammonia Clusters Optimized at MP2/6-31++G(d,p) level of theory along with Single point energy at MP2(full)/aug-cc-pVTZ level

$(NH_3)_3$: 1
MP2(full)/aug-cc-pVTZ = -169.45134 a.u.

N	-0.727259000	1.677926000	-0.000011000
H	-1.073226000	2.174029000	0.813451000
H	-1.144814000	0.747171000	-0.000070000
H	-1.073274000	2.174162000	-0.813372000
N	1.816773000	-0.209147000	0.000020000
H	2.419656000	-0.157526000	0.813285000
H	1.219490000	0.617841000	0.000086000
H	2.419273000	-0.157650000	-0.813537000
N	-1.089508000	-1.468777000	-0.000003000
H	-1.346166000	-2.016554000	-0.813392000
H	-1.346314000	-2.016415000	0.813432000
H	-0.074668000	-1.365074000	0.000079000

$((NH_3)_4$: 1
MP2(full)/aug-cc-pVTZ = -225.94010 a.u.

N	2.134740000	-0.618723000	-0.151696000
H	2.805893000	-0.922624000	0.545324000
H	2.549015000	-0.822702000	-1.054751000
H	1.305745000	-1.209996000	-0.056885000
N	-0.618721000	-2.134731000	0.151697000
H	-1.210002000	-1.305742000	0.056889000
H	-0.822690000	-2.549011000	1.054752000
H	-0.922617000	-2.805886000	-0.545325000
N	-2.134741000	0.618716000	-0.151696000
H	-2.549021000	0.822692000	-1.054750000
H	-1.305747000	1.209989000	-0.056890000
H	-2.805891000	0.922622000	0.545326000
N	0.618722000	2.134739000	0.151696000
H	0.922627000	2.805887000	-0.545329000
H	1.209990000	1.305741000	0.056888000
H	0.822705000	2.549018000	1.054749000

$(NH_3)_5$: 1
MP2(full)/aug-cc-pVTZ = -282.42609 a.u.

N	2.148530000	-0.781362000	0.964641000
H	1.839127000	-0.554926000	1.903526000
H	3.020593000	-1.289640000	1.062369000
H	1.460839000	-1.423309000	0.563333000
N	-0.076250000	-2.496942000	-0.458428000
H	-0.901442000	-1.903219000	-0.343140000
H	-0.329824000	-3.427812000	-0.145345000
H	0.104595000	-2.569729000	-1.453879000
N	-2.533337000	-0.548740000	-0.020680000
H	-3.159642000	-0.434650000	-0.810541000
H	-2.116913000	0.366886000	0.166431000
H	-3.119714000	-0.776587000	0.775216000
N	-1.105717000	2.226533000	0.511881000
H	-0.861578000	2.392600000	1.482406000
H	-1.554625000	3.074350000	0.182212000
H	-0.228101000	2.126277000	-0.004035000
N	1.588532000	1.612729000	-0.996322000
H	2.359049000	2.265974000	-1.085638000
H	1.439083000	1.214307000	-1.916893000
H	1.896249000	0.853954000	-0.383662000

$(NH_3)_6$: 1
MP2(full)/aug-cc-pVTZ = -338.91440 a.u.

N	-1.440681000	-0.741528000	-1.693160000
H	-1.518983000	-1.128188000	-0.752695000
H	-0.586597000	-1.118516000	-2.090397000
H	-2.211285000	-1.102329000	-2.245289000
N	1.440792000	1.095555000	-1.488680000
H	1.519087000	0.087758000	-1.353303000
H	2.211429000	1.393314000	-2.077164000
H	0.586737000	1.251081000	-2.013825000
N	1.440798000	-1.837019000	-0.204354000
H	0.586741000	-2.369581000	-0.076529000
H	1.519031000	-1.215880000	0.600741000
H	2.211440000	-2.495532000	-0.167925000
N	-1.440792000	-1.095558000	1.488676000
H	-1.519084000	-0.087761000	1.353300000
H	-0.586741000	-1.251086000	2.013827000
H	-2.211433000	-1.393318000	2.077153000
N	-1.440802000	1.837017000	0.204352000
H	-0.586747000	2.369584000	0.076527000
H	-2.211447000	2.495526000	0.167923000
H	-1.519031000	1.215878000	-0.600743000
N	1.440684000	0.741533000	1.693166000
H	2.211288000	1.102334000	2.245296000
H	0.586600000	1.118520000	2.090402000
H	1.518988000	1.128194000	0.752701000

$(NH_3)_7$: 1
MP2(full)/aug-cc-pVTZ = -395.40553 a.u.

N	-0.000010000	2.133193000	-1.499358000
H	-0.811861000	2.550783000	-1.942808000
H	0.811834000	2.550789000	-1.942814000
H	-0.000007000	1.136262000	-1.736344000
N	-0.000002000	-0.982290000	-1.845757000
H	-0.821273000	-1.286201000	-1.325920000
H	0.821272000	-1.286200000	-1.325921000
H	-0.000002000	-1.490641000	-2.723794000
N	-2.821501000	-1.251285000	-0.226263000
H	-3.436018000	-1.772137000	0.390702000
H	-3.299765000	-1.190095000	-1.119049000
H	-2.736328000	-0.303132000	0.148814000
N	-1.827794000	1.355673000	1.101098000
H	-1.238191000	0.771442000	1.688035000
H	-2.223550000	2.085028000	1.683658000
H	-1.209703000	1.802785000	0.427119000
N	1.827797000	1.355681000	1.101085000
H	1.209700000	1.802789000	0.427109000
H	1.238201000	0.771452000	1.688030000
H	2.223557000	2.085040000	1.683638000
N	2.821503000	-1.251282000	-0.226265000
H	2.736331000	-0.303126000	0.148803000
H	3.299757000	-1.190100000	-1.119058000
H	3.436030000	-1.772125000	0.390698000
N	0.000005000	-1.341010000	1.613079000
H	0.000007000	-2.022729000	2.364789000
H	0.815345000	-1.535319000	1.035487000
H	-0.815334000	-1.535323000	1.035488000

$(NH_3)_8$: 1
MP2(full)/aug-cc-pVTZ = -451.89663 a.u.

N	-2.109504000	1.726363000	1.261954000
H	-3.067935000	1.462392000	1.466698000
H	-2.040322000	2.717953000	1.467270000
H	-1.966549000	1.609821000	0.253791000
N	1.125441000	1.375173000	1.703012000
H	1.494154000	1.825752000	2.533881000
H	1.376005000	0.390004000	1.761470000
H	0.110179000	1.426298000	1.761222000
N	2.108586000	-1.726831000	1.262704000
H	2.039121000	-2.718481000	1.467634000
H	3.066912000	-1.463068000	1.468204000
H	1.966354000	-1.609927000	0.254480000
N	-1.126643000	-1.375777000	1.701985000
H	-1.377238000	-0.390629000	1.760664000
H	-1.495891000	-1.826680000	2.532440000
H	-0.111418000	-1.426924000	1.760821000
N	-1.726176000	-2.108774000	-1.263200000
H	-2.717715000	-2.039302000	-1.468666000
H	-1.462345000	-3.067145000	-1.468405000
H	-1.609804000	-1.966380000	-0.254937000
N	1.376054000	-1.125773000	-1.702266000
H	1.427226000	-0.110523000	-1.760647000
H	1.827031000	-1.494655000	-2.532845000
H	0.390907000	-1.376324000	-1.761153000
N	1.727100000	2.109242000	-1.261454000
H	2.718791000	2.039848000	-1.466211000
H	1.609979000	1.966501000	-0.253327000
H	1.463409000	3.067680000	-1.466528000
N	-1.374845000	1.126394000	-1.702733000
H	-0.389667000	1.376983000	-1.760941000
H	-1.825319000	1.495521000	-2.533475000
H	-1.425962000	0.111162000	-1.761451000

$(NH_3)_4$: 2
MP2(full)/aug-cc-pVTZ = -225.93608 a.u.

N	-0.540719000	-1.476443000	1.149284000
H	-1.406509000	-1.975887000	1.322649000
H	0.175604000	-1.951239000	1.688557000
H	-0.304517000	-1.587434000	0.160923000
N	0.360852000	-0.769719000	-1.712072000
H	1.271592000	-0.495550000	-1.353536000
H	-0.218096000	0.065716000	-1.678320000
H	0.472403000	-1.039906000	-2.682217000
N	1.785119000	0.858567000	0.598655000
H	2.443538000	1.156136000	1.308760000
H	1.023180000	0.370880000	1.059965000
H	1.392712000	1.689186000	0.170686000
N	-1.538968000	1.349978000	-0.111810000
H	-1.490417000	2.207915000	0.425936000
H	-1.320551000	0.578498000	0.515810000
H	-2.502937000	1.245008000	-0.407615000

$(NH_3)_5$: 2
MP2(full)/aug-cc-pVTZ = -282.42570 a.u.

N	-0.695861000	-2.082414000	0.623687000
H	-1.349458000	-1.303387000	0.511691000
H	-0.646568000	-2.294974000	1.614717000
H	-1.107452000	-2.896768000	0.179967000
N	-2.327672000	0.546283000	0.107120000
H	-2.730764000	0.627561000	-0.820182000
H	-1.527573000	1.181638000	0.150901000
H	-3.027442000	0.893148000	0.754353000
N	0.339132000	2.224858000	0.387285000
H	0.961515000	1.469942000	0.687205000
H	0.261446000	2.878168000	1.159892000
H	0.822723000	2.721976000	-0.353680000
N	2.092005000	-0.330166000	0.822992000
H	1.400711000	-1.074589000	0.874670000
H	2.888799000	-0.597665000	1.389391000
H	2.389201000	-0.301601000	-0.147985000
N	0.689731000	-0.365669000	-1.944432000
H	0.309274000	-1.006834000	-1.253222000
H	0.505775000	-0.746423000	-2.865152000
H	0.168461000	0.499557000	-1.859133000

$(NH_3)_6$: 2
MP2(full)/aug-cc-pVTZ = -338.91528 a.u.

N	0.312385000	0.866601000	-1.928297000
H	0.651877000	-0.089536000	-1.886221000
H	0.272922000	1.135124000	-2.905177000
H	-0.642142000	0.868001000	-1.568780000
N	-1.213243000	-2.045925000	-0.268723000
H	-0.234603000	-2.015823000	-0.547384000
H	-1.693292000	-1.294945000	-0.754398000
H	-1.607360000	-2.923008000	-0.588799000
N	-2.404279000	1.128626000	-0.248908000
H	-2.545947000	2.130089000	-0.328901000
H	-1.905557000	0.953217000	0.626192000
H	-3.326545000	0.716718000	-0.151967000
N	1.915155000	1.599688000	0.621652000
H	1.422616000	1.616884000	-0.275041000
H	2.835776000	2.000911000	0.477086000
H	1.423147000	2.226300000	1.250079000
N	1.953334000	-1.534851000	-0.209514000
H	1.947964000	-2.200686000	0.556404000
H	2.021435000	-0.605303000	0.205158000
H	2.812105000	-1.695836000	-0.725402000
N	-0.604489000	-0.012173000	2.052063000
H	-0.684751000	-0.150091000	3.053107000
H	0.365836000	0.207486000	1.846950000
H	-0.825510000	-0.893265000	1.589190000

$(NH_3)_7$: 2
MP2(full)/aug-cc-pVTZ = -395.40498 a.u.

N	0.079424000	0.236460000	1.908837000
H	0.599083000	-0.602764000	1.656600000
H	-0.833045000	0.171819000	1.465894000
H	-0.076180000	0.213657000	2.911057000
N	2.374318000	1.524615000	0.193279000
H	1.597521000	1.360743000	0.836154000
H	3.125397000	1.963727000	0.714830000
H	2.061292000	2.198722000	-0.496971000
N	2.234180000	-1.694252000	0.456099000
H	2.027129000	-2.165734000	-0.417703000
H	3.068475000	-2.127925000	0.836656000
H	2.467061000	-0.729075000	0.224696000
N	-1.025340000	-2.260197000	-0.512089000
H	-1.297802000	-3.061439000	-1.071275000
H	-0.379117000	-2.596372000	0.194559000
H	-0.498358000	-1.621362000	-1.112307000
N	-3.031258000	-0.125833000	0.499082000
H	-3.777954000	0.024663000	-0.171683000
H	-3.481617000	-0.382006000	1.371663000
H	-2.492718000	-0.936639000	0.179153000
N	-1.118511000	2.274851000	-0.463434000
H	-1.804131000	1.617693000	-0.090342000
H	-1.624047000	3.086016000	-0.803675000
H	-0.562053000	2.582368000	0.327265000
N	0.489115000	0.029494000	-2.078444000
H	-0.043773000	0.809958000	-1.689465000
H	0.458158000	0.114245000	-3.089276000
H	1.453186000	0.183746000	-1.799136000

$(NH_3)_8$: 2
MP2(full)/aug-cc-pVTZ = -451.89626 a.u.

N	1.148330000	-2.084689000	0.010668000
H	1.283427000	-1.568777000	-0.856539000
H	1.520234000	-3.017432000	-0.134688000
H	0.144280000	-2.184349000	0.144848000
N	2.140591000	-0.095341000	2.187823000
H	2.211711000	-0.521316000	3.105980000
H	3.059210000	0.278552000	1.973037000
H	1.940404000	-0.839790000	1.512882000
N	1.148337000	2.084685000	-0.010671000
H	1.520246000	3.017426000	0.134685000
H	0.144288000	2.184350000	-0.144849000
H	1.283434000	1.568773000	0.856537000
N	2.140588000	0.095336000	-2.187825000
H	1.940403000	0.839786000	-1.512884000
H	3.059207000	-0.278559000	-1.973040000
H	2.211708000	0.521311000	-3.105982000
N	-1.148335000	-0.010668000	-2.084684000
H	-0.144287000	-0.144849000	-2.184350000
H	-1.283428000	0.856536000	-1.568764000
H	-1.520244000	0.134698000	-3.017424000
N	-2.140586000	2.187831000	0.095339000
H	-3.059207000	1.973050000	-0.278554000
H	-1.940402000	1.512889000	0.839789000
H	-2.211700000	3.105988000	0.521314000
N	-1.148332000	0.010671000	2.084686000
H	-1.520238000	-0.134685000	3.017429000
H	-0.144283000	0.144847000	2.184347000
H	-1.283432000	-0.856536000	1.568774000
N	-2.140593000	-2.187825000	-0.095338000
H	-1.940408000	-1.512885000	-0.839788000
H	-3.059212000	-1.973041000	0.278557000
H	-2.211711000	-3.105983000	-0.521312000

$(NH_3)_4$: 3
MP2(full)/aug-cc-pVTZ = -225.93397 a.u.

N	-3.330840000	-0.062771000	0.442178000
H	-3.932424000	0.718558000	0.208667000
H	-3.058247000	0.046709000	1.412054000
H	-3.892759000	-0.903796000	0.380352000
N	-0.441691000	0.064164000	-1.098729000
H	-1.369220000	-0.031511000	-0.690399000
H	0.123241000	-0.727395000	-0.795480000
H	-0.549283000	-0.005683000	-2.104415000
N	1.890320000	1.581699000	0.332849000
H	2.464085000	2.166181000	-0.264573000
H	1.622201000	2.151504000	1.127214000
H	1.041660000	1.341784000	-0.183886000
N	1.976961000	-1.595148000	0.262485000
H	2.753866000	-1.992265000	-0.253335000
H	1.947880000	-2.068094000	1.158430000
H	2.185754000	-0.611602000	0.433887000

$(NH_3)_5$: 3
MP2(full)/aug-cc-pVTZ = -282.42558 a.u.

N	-2.559960000	-0.114417000	-0.263497000
H	-3.212218000	-0.245656000	0.502118000
H	-1.878512000	-0.878405000	-0.223929000
H	-3.095340000	-0.227989000	-1.117608000
N	-0.304684000	2.045427000	-0.255844000
H	-1.127535000	1.434740000	-0.264253000
H	-0.203775000	2.418204000	-1.194754000
H	-0.523807000	2.840729000	0.335788000
N	1.987606000	-0.071293000	-1.404516000
H	2.668136000	-0.411399000	-0.734893000
H	1.409198000	0.616552000	-0.928735000
H	2.496839000	0.406299000	-2.139017000
N	-0.142009000	-2.052515000	-0.122060000
H	0.423045000	-1.772454000	-0.920522000
H	-0.098081000	-3.063142000	-0.052713000
H	0.330017000	-1.662086000	0.692065000
N	1.000550000	0.086921000	1.992895000
H	0.330578000	0.132002000	2.752570000
H	0.717433000	0.771597000	1.293736000
H	1.893510000	0.382144000	2.371301000

$(NH_3)_6$: 3
MP2(full)/aug-cc-pVTZ = -338.91541 a.u.

N	2.948206000	-0.531780000	0.345813000
H	3.243923000	-0.635141000	1.310603000
H	3.710163000	-0.880357000	-0.225904000
H	2.150071000	-1.153648000	0.203156000
N	0.343110000	-2.213198000	-0.384504000
H	-0.097695000	-1.477961000	-0.947345000
H	-0.398188000	-2.652173000	0.152437000
H	0.678798000	-2.923922000	-1.026877000
N	-0.987466000	0.244440000	-1.743953000
H	-1.132062000	0.488659000	-2.717457000
H	-0.445481000	0.992377000	-1.318704000
H	-1.899711000	0.239303000	-1.287608000
N	1.400343000	2.118960000	-0.340143000
H	1.697075000	2.904965000	0.228798000
H	1.539663000	2.400020000	-1.305185000
H	2.037351000	1.340927000	-0.152695000
N	-0.457825000	0.305293000	1.685869000
H	-0.266253000	0.600842000	2.637126000
H	-0.026871000	0.986646000	1.063063000
H	0.046031000	-0.563060000	1.533724000
N	-3.329382000	0.091793000	0.384191000
H	-3.807214000	-0.774695000	0.603919000
H	-3.952662000	0.846931000	0.646438000
H	-2.495835000	0.151726000	0.971599000

$(NH_3)_7$: 3
MP2(full)/aug-cc-pVTZ = -395.40542 a.u.

N	-0.352090000	0.418144000	1.879527000
H	-1.233477000	0.623385000	1.412744000
H	-0.544914000	0.410487000	2.875777000
H	-0.091185000	-0.531436000	1.619466000
N	1.265364000	-2.290210000	0.980775000
H	1.749607000	-1.765376000	0.247300000
H	1.331605000	-3.275907000	0.749041000
H	1.785850000	-2.165822000	1.842993000
N	2.306986000	-0.429437000	-1.302554000
H	3.150096000	-0.513192000	-1.860087000
H	2.321889000	0.484485000	-0.852041000
H	1.521433000	-0.409539000	-1.945138000
N	1.908894000	2.136816000	0.609877000
H	2.795871000	2.035126000	1.092392000
H	1.196926000	1.647961000	1.161699000
H	1.686689000	3.126745000	0.628521000
N	-3.218933000	0.503003000	0.272620000
H	-2.854688000	-0.387482000	-0.075363000
H	-3.789000000	0.312337000	1.089692000
H	-3.844558000	0.876915000	-0.433166000
N	-1.400450000	-1.692013000	-0.912882000
H	-0.996941000	-0.924564000	-1.446725000
H	-0.699633000	-1.980534000	-0.234135000
H	-1.554563000	-2.471224000	-1.542797000
N	-0.538983000	1.333823000	-1.543269000
H	0.295885000	1.637197000	-1.048559000
H	-1.313106000	1.403294000	-0.886781000
H	-0.709308000	2.006257000	-2.283503000

$(NH_3)_8$: 3
MP2(full)/aug-cc-pVTZ = -451.89538 a.u.

N	-0.644833000	-0.143185000	2.194329000
H	-0.542288000	0.761956000	1.740743000
H	-0.867232000	0.028281000	3.169438000
H	-1.452653000	-0.603218000	1.773132000
N	-2.634772000	-1.614962000	0.203407000
H	-3.358700000	-2.324144000	0.178208000
H	-2.898353000	-0.879176000	-0.444324000
H	-1.774118000	-2.030357000	-0.145429000
N	-2.610078000	1.636695000	-0.372078000
H	-1.705056000	1.942343000	-0.013281000
H	-3.143318000	1.294033000	0.420294000
H	-3.094770000	2.458011000	-0.718401000
N	0.502423000	2.205780000	0.098057000
H	0.495761000	1.732423000	-0.802961000
H	1.279859000	1.816497000	0.633694000
H	0.714379000	3.183731000	-0.071419000
N	2.513884000	0.341319000	1.696447000
H	3.202512000	0.372289000	2.439794000
H	2.864602000	-0.280701000	0.974892000
H	1.664266000	-0.076438000	2.070104000
N	2.726205000	-0.252264000	-1.539242000
H	3.251620000	-0.573062000	-2.345672000
H	3.197492000	0.576754000	-1.192659000
H	1.807392000	0.042959000	-1.868701000
N	-0.421150000	0.018111000	-2.185714000
H	-0.609148000	-0.178762000	-3.163463000
H	-1.250203000	0.475693000	-1.808618000
H	-0.335504000	-0.875762000	-1.704228000
N	0.566555000	-2.209660000	-0.050200000
H	0.756246000	-3.185483000	0.153650000
H	0.385807000	-1.742575000	0.836879000
H	1.423772000	-1.808121000	-0.426719000