Reliable Predictions of the Thermochemistry of Boron-Nitrogen Hydrogen Storage Compounds: $B_xN_xH_y$, $x = 2, 3$

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Supporting Information Available: CCSD(T) energies (E_h); calculated MP2/cc-pVTZ frequencies; enthalpies (kcal/mol) as a function of method, entropies (cal/mol·K) and free energies (kcal/mol) of reactions 20-52; and cartesian coordinates for $B_xN_xH_y$ compounds.

Table S1: CCSD(T)/aVnZ ($n = D, T, Q$) and CBS energies (E_h) for $B_xN_xH_y$ compounds.

Molecule	CCSD(T)			
	aVDZ	aVTZ	aVQZ	CBS
2a	-245.528353	-245.763033	-245.825890	-245.860246
2b	-245.526248	-245.761005	-245.823989	-245.858429
3	-242.025660	-242.242606	-242.304885	-242.339469
4	-163.664337	-163.822483	-163.864803	-163.887929
5	-243.157902	-243.380504	-243.442726	-243.477073
6	-243.132772	-243.354844	-243.416855	-243.451078
7	-244.332234	-244.560749	-244.623302	-244.657668
8a	-164.810183	-164.972839	-165.015817	-165.039231
8b	-164.829982	-164.992929	-165.035864	-165.059239
9a	-246.641097	-246.881495	-246.945332	-246.980151
9b	-246.680803	-246.921027	-246.984719	-247.019447
10	-163.645389	-163.803274	-163.845829	-163.869123
11	-245.467768	-245.703157	-245.766496	-245.801153
12	-165.995673	-166.163630	-166.207333	-166.231052
13	-241.807083	-242.020821	-242.082426	-242.116666
14	-243.161744	-243.383755	-243.446418	-243.481085

Table S2: MP2/cc-pVTZ frequencies for B_xN_xH_y compounds.^a

Molecule		Vibrational modes									
2a	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	111.55	218.66	225.37	355.26	377.17	467.68	638.89	668.96	694.77	745.99
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	752.65	804.45	810.45	878.20	886.36	894.36	913.86	946.12	990.21	1057.10
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1090.56	1100.94	1119.78	1187.50	1187.97	1220.04	1228.43	1234.20	1245.18	1248.45
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1265.41	1270.84	1276.57	1616.00	1618.33	1638.00	2503.99	2505.30	2520.88	2550.19
2b	Symmetry	a	a	a	a	a	a	a	a		
	ω (cm ⁻¹)	2550.38	2564.44	3509.24	3509.60	3520.37	3588.65	3589.22	3592.63		
	Symmetry	e	e	a	e	e	a	e	e	a	e
	ω (cm ⁻¹)	167.30	167.30	289.74	351.13	351.13	450.22	652.26	652.26	681.41	740.54
	Symmetry	e	e	e	a	a	e	e	a	a	a
	ω (cm ⁻¹)	740.54	812.76	812.76	861.44	883.22	904.32	904.32	926.92	989.85	1069.09
	Symmetry	e	e	e	e	a	a	e	e	e	e
	ω (cm ⁻¹)	1088.22	1088.22	1150.32	1150.32	1215.79	1233.46	1238.08	1238.08	1248.15	1248.15
	Symmetry	a	e	e	e	e	a	e	e	a	e

	ω (cm ⁻¹)	1261.06	1280.60	1280.60	1617.56	1617.56	1638.75	2495.77	2495.77	2507.43	2578.18
	Symmetry	e	a	a	e	e	a	e	e		
	ω (cm ⁻¹)	2578.18	2592.20	3493.87	3496.39	3496.39	3570.03	3572.04	3572.04		
4	Symmetry	b _{1u}	a _g	b _{3g}	b _{1u}	b _{1g}	b _{2g}	b _{3u}	b _{2u}	a _u	a _g
	ω (cm ⁻¹)	51.14	593.81	628.62	670.28	725.19	730.31	787.99	788.27	813.41	861.45
	Symmetry	b _{1g}	b _{2u}	b _{2g}	b _{1u}	a _u	b _{1g}	b _{3g}	b _{3u}	b _{2u}	a _g
	ω (cm ⁻¹)	990.76	1039.73	1063.99	1076.10	1101.30	1140.84	1164.48	1209.38	1234.73	1253.86
	Symmetry	b _{3u}	a _g	b _{2u}	a _g	b _{3g}	b _{1u}	a _g	b _{3u}	b _{2g}	b _{1u}
	ω (cm ⁻¹)	1625.08	1640.74	2540.75	2556.10	2605.82	2610.86	3570.03	3571.94	3657.79	3658.72
5	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	177.49	215.76	319.32	382.11	455.29	610.62	629.22	664.31	704.99	825.96
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	835.30	872.83	893.19	909.68	947.52	973.62	1000.70	1054.75	1085.07	1114.87
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1136.56	1217.32	1254.01	1302.44	1352.70	1441.35	1510.42	1603.66	2470.98	2536.84
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	2657.13	2690.35	3490.15	3598.09	3652.70	3662.56	2657.13	2690.35	3490.15	3598.09
6	Symmetry	a'	a''	a'	a'	a''	a'	a''	a'	a'	a''
	ω (cm ⁻¹)	143.61	281.13	319.56	413.65	481.33	599.99	615.37	695.06	771.85	787.03
	Symmetry	a'	a'	a''	a''	a'	a'	a''	a'	a''	a''

	ω (cm ⁻¹)	795.35	814.59	841.21	887.56	907.58	966.42	983.28	1054.77	1057.51	1124.76
	Symmetry	a''	a''	a''	a'	a'	a''	a'	a'	a'	a'
	ω (cm ⁻¹)	1149.57	1197.47	1231.15	1238.35	1277.96	1491.05	1526.71	1583.35	2380.50	2551.31
	Symmetry	a''	a'	a'	a'	a'	a''				
	ω (cm ⁻¹)	2697.03	2701.67	3395.94	3601.85	3653.26	3654.11				
7	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	90.55	212.34	277.72	376.04	396.27	551.67	613.08	696.00	708.49	750.01
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	790.74	831.39	853.11	876.95	907.63	915.90	986.28	993.17	1034.45	1081.02
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1101.84	1163.70	1208.89	1227.84	1232.17	1252.25	1257.56	1265.31	1313.94	1538.63
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1611.76	1626.15	2481.06	2511.36	2521.88	2585.17	2659.42	3487.04	3499.87	3557.97
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	3579.21	3616.42								
8a	Symmetry	a''	a''	a'	a''	a'	a''	a'	a''	a'	a'
	ω (cm ⁻¹)	68.55	179.00	203.06	216.54	325.05	626.23	640.24	655.74	680.53	799.76
	Symmetry	a''	a'	a'	a''	a''	a'	a'	a''	a'	a'
	ω (cm ⁻¹)	826.56	854.01	1014.68	1077.15	1111.43	1137.83	1188.54	1203.40	1217.98	1226.84
	Symmetry	a''	a'	a'	a'	a'	a''	a'	a'	a''	a'

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[illegible]

	ω (cm ⁻¹)	1628.58	1637.68	2162.93	2586.56	2660.77	2672.98	3589.36	3595.14	3688.57	3698.20
11	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	42.38	83.62	142.24	200.85	262.55	303.56	377.70	530.81	570.94	609.78
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	668.76	703.99	723.78	746.24	795.17	847.56	880.77	925.83	959.88	993.85
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1023.16	1061.82	1073.47	1092.57	1100.15	1146.87	1152.27	1164.09	1182.59	1218.83
	Symmetry	a	a	a	a	a	a	a	a	a	a
	ω (cm ⁻¹)	1242.67	1258.02	1607.37	1630.49	1631.45	1855.57	2048.37	2464.75	2508.39	2627.41
	Symmetry	a	a	a	a	a	a	a	a		
	ω (cm ⁻¹)	2698.68	2725.00	3498.35	3585.76	3589.95	3596.93	3688.15	3689.02		
12^b	Symmetry	a _u	b _g	a _g	a _u	a _g	b _u	a _u	b _g	a _u	b _g
	ω (cm ⁻¹)	90.88	135.29	146.31	186.97	202.66	241.28	296.93	327.82	681.67	684.02
	Symmetry	a _g	b _u	a _g	b _u	b _g	b _u	a _u	a _g	a _g	b _u
	ω (cm ⁻¹)	718.24	728.49	742.23	748.72	1082.96	1089.90	1094.45	1107.01	1196.52	1206.98
	Symmetry	b _g	a _u	a _g	b _u	b _u	a _g	b _g	a _u	b _u	a _g
	ω (cm ⁻¹)	1229.31	1233.21	1255.86	1256.27	1387.98	1401.55	1665.18	1667.68	1668.87	1676.15
	Symmetry	a _g	b _u	b _g	a _u	b _u	a _g	a _g	b _u	a _g	b _u
	ω (cm ⁻¹)	2446.14	2454.53	2487.96	2497.48	2553.87	2556.78	3383.90	3399.45	3549.08	3549.53
	Symmetry	b _g	a _u								

	ω (cm ⁻¹)	3610.89	3610.90								
13	Symmetry	a''	a'	a''	a''	a'	a'	a''	a'	a''	a''
	ω (cm ⁻¹)	79.40	146.18	186.86	319.20	356.87	389.47	516.15	518.34	627.26	704.83
	Symmetry	a'	a'	a''	a''	a'	a'	a''	a'	a'	a'
	ω (cm ⁻¹)	720.90	816.99	831.65	864.12	868.94	949.39	1005.10	1095.67	1119.10	1173.82
	Symmetry	a'	a'	a'	a'	a'	a'	a'	a'	a'	a'
	ω (cm ⁻¹)	1379.31	1510.91	1616.88	1713.88	2184.51	2491.00	2811.16	3542.32	3618.99	3715.95
14	Symmetry	a''	a'	a''	a''	a'	a'	a''	a''	a'	a''
	ω (cm ⁻¹)	75.05	133.14	161.66	198.24	304.89	390.63	417.02	442.84	483.64	573.13
	Symmetry	a''	a''	a'	a'	a''	a''	a''	a'	a'	a'
	ω (cm ⁻¹)	727.94	843.43	852.61	903.46	918.67	953.80	1043.79	1077.17	1111.55	1125.65
	Symmetry	a'	a'	a'	a'	a'	a'	a'	a'	a'	a'
	ω (cm ⁻¹)	1172.91	1196.93	1230.93	1313.64	1361.51	1486.41	1507.63	1643.40	2623.38	2681.80
	Symmetry	a'	a'	a'	a'	a'	a'				
	ω (cm ⁻¹)	2702.39	2715.61	3593.90	3603.20	3645.47	3760.52				

^a B₃N₃H₆ (structure **3**) frequencies already described in Table 3 of the article.

^b Frequencies for the BH₃NH₃ dimer calculated with MP2/aug-cc-pVTZ.

Table S3. Enthalpies (kcal/mol) as a function of method, Entropies (cal/mol·K) and Free Energies (kcal/mol) of Reactions 20-52.

Reaction	$\Delta H(0\text{ K})^a$	$\Delta H(0\text{ K})^b$	$\Delta H(298\text{ K})^a$	$\Delta H(298\text{ K})^b$	$\Delta H(298\text{ K})^c$	$\Delta H(298\text{ K})$	$\Delta S(298\text{ K})^d$	$\Delta G(298\text{ K})$
	CCSD(T)	G3MP2	CCSD(T)	G3MP2	DFT	G3B3	MP2	CCSD(T)
20	-28.1	-31.5	-26.4	-29.7	-23.7	-28.2	15.12	-30.9
21	-57.9	-64.0	-55.9	-61.7	-47.6	-58.1	1.25	-56.2
22	-23.9	-27.5	-18.7	-22.2	-27.4	-20.5	82.81	-43.3
23	-21.0	-22.0	-20.5	-21.4	-16.1	-20.7	-8.98	-17.8
24	-44.7	-47.2	-43.6	-45.8	-34.0		-22.03	-37.1
25	-32.7	-34.7	-33.8	-35.7	-32.0		-9.48	-31.0
26	-134.7	-134.2	-135.9	-135.7	-149.0		-12.62	-132.1
27	-24.7	-26.6	-24.2	-26.0	-22.3		15.75	-28.9
28	-13.2	-16.8	-12.2	-15.9	-13.6		23.28	-19.2
29	0.8	-0.9	5.6	3.8	-5.1		67.06	-14.4
30	-9.2	-7.9	-9.7	-8.8	-6.5		-3.32	-8.7
31	-7.2	-9.5	-5.9	-8.3	-7.6		24.10	-13.1
32	-14.6	-13.7	-16.4	-15.3	-7.8		-44.68	-3.1
33	-61.5	-64.8	-59.5	-62.6	-51.1		-5.64	-57.8
34	-37.6	-37.3	-40.8	-40.1	-23.7		-88.45	-14.4

35	-36.8	-38.2	-35.2	-36.3	-28.8		-21.39	-28.9
36	-32.0	-34.4	-31.5	-33.6	-20.5		-29.73	-22.7
37	7.4	4.2	10.5	7.0	0.2		68.78	-10.0
38	24.4	20.5	28.6	24.2	10.2		111.73	-4.7
39	-6.8	-8.9	-5.0	-7.2	-8.0	-6.2	29.90	-13.9
40	-29.5	-30.4	-27.9	-28.7	-30.6		24.09	-35.1
41	-45.2	-45.9	-43.6	-41.3	-46.6		24.25	-50.9
42	-33.3	-35.6	-30.0	-32.1	-35.2		52.54	-45.7
43	-3.9	-5.2	-2.1	-3.4	-4.6		28.45	-10.6
44	11.8	10.3	13.6	9.2	11.5		28.29	5.1
45	5.6	2.9	9.3	6.5	3.2		58.72	-8.2
46	21.3	18.4	25.0	19.1	19.3		58.56	7.5
47	9.4	8.1	11.4	9.9	7.8		30.27	2.4
48	-14.1	-17.7	-12.1	-15.9	-11.7		46.04	-25.9
49	-7.0	-8.2	-6.2	-7.6	-4.2		21.94	-12.8
50	-14.0	-13.8	-14.3	-13.8	-11.9		-30.92	-5.1
51	-11.8	-11.6	-12.3	-12.0	-11.4		-3.33	-11.3
52	-23.6	-23.2	-24.4	-23.8	-22.0		-10.81	-21.2

53 -4.8 -3.8 -3.7 -2.7 -8.3 8.3 -6.2

^a $\Delta H_{f,0K}(\text{BH}_3\text{NH}_3) = -9.1$ kcal/mol and $\Delta H_{f,298K}(\text{BH}_3\text{NH}_3) = -13.5$ kcal/mol, from Dixon, D. A.; Gutowski, M. *J. Phys. Chem. A* **2005**, *109*, 5129. We used for this level $\Delta H_{f,0K}(\text{H}_2) = 0.03$ kcal/mol and $\Delta H_{f,298K}(\text{H}_2) = 0.08$ kcal/mol.

^b At the G3MP2 level: $\Delta H_{f,0K}(\text{H}_2) = -1.2$ kcal/mol and $\Delta H_{f,298K}(\text{H}_2) = -1.1$ kcal/mol.

^c B3LYP/6-311+G**.

^d The entropy of reaction was calculated from MP2/cc-pVTZ values, where $S(\text{BH}_3\text{NH}_3) = 57.15$ cal/mol·K and $S(\text{H}_2) = 31.10$ cal/mol·K.

Table S4: MP2/cc-pVTZ optimized Cartesian coordinates for B_xN_xH_y.

Molecule	Atom	Cartesian coordinates		
		x	y	z
2a	N	0.663748	1.215054	0.380125
	N	0.663856	-1.215033	-0.380089
	N	-1.528475	-0.000095	-0.000063
	B	-0.683142	-1.277651	0.450661
	B	1.621726	0.000089	-0.000062
	B	-0.683285	1.277659	-0.450564
	H	0.465942	1.207691	1.376279
	H	1.173265	-2.076818	-0.214308
	H	-2.148141	0.243153	0.765350
	H	1.173072	2.076906	0.214432
	H	0.466025	-1.207815	-1.376239
	H	-2.147865	-0.243492	-0.765652
	H	-1.295606	-2.286302	0.203235
	H	2.276911	0.322067	-0.958412
	H	-0.407720	1.158403	-1.618915
	H	-0.407553	-1.158144	1.618982
	H	2.277129	-0.321799	0.958169
	H	-1.295858	2.286185	-0.202900
2b	N	0.000000	1.473187	-0.200681
	N	-1.275818	-0.736594	-0.200681
	N	1.275818	-0.736594	-0.200681
	B	0.000000	-1.568612	0.250841
	B	-1.358458	0.784306	0.250841
	B	1.358458	0.784306	0.250841
	H	0.000000	1.646783	-1.202240
	H	-1.426156	-0.823392	-1.202240
	H	1.426156	-0.823392	-1.202240

	H	0.000000	2.401630	0.212256
	H	-2.079872	-1.200815	0.212256
	H	2.079872	-1.200815	0.212256
	H	0.000000	-1.642521	1.449197
	H	-1.422464	0.821260	1.449197
	H	1.422464	0.821260	1.449197
	H	0.000000	-2.640085	-0.308646
	H	-2.286381	1.320043	-0.308646
	H	2.286381	1.320043	-0.308646
3	B	0.000043	0.000000	1.452370
	H	0.000069	0.000000	2.643371
	B	1.257766	0.000000	-0.726222
	H	2.289182	0.000000	-1.321762
	B	-1.257807	0.000000	-0.726145
	H	-2.289263	0.000000	-1.321617
	N	-1.219414	0.000000	0.704080
	H	-2.090502	0.000000	1.207024
	N	-0.000039	0.000000	-1.408085
	H	-0.000087	0.000000	-2.413942
	N	1.219457	0.000000	0.704005
	H	2.090565	0.000000	1.206912
4	N	1.155888	0.000000	0.000000
	B	0.000000	1.115158	0.000000
	N	-1.155888	0.000000	0.000000
	B	0.000000	-1.115158	0.000000
	H	1.748605	0.000000	0.817298
	H	0.000000	1.753893	1.015275
	H	-1.748605	0.000000	0.817298
	H	0.000000	-1.753893	1.015275
	H	1.748605	0.000000	-0.817298
	H	0.000000	1.753893	-1.015275

	H	-1.748605	0.000000	-0.817298
	H	0.000000	-1.753893	-1.015275
5	B	1.092583	-0.926605	0.398534
	H	1.167520	-0.681220	1.583734
	N	-0.298288	-1.386973	-0.057848
	N	1.261333	0.533566	-0.337451
	B	-1.397781	-0.542678	-0.138095
	B	0.136627	1.455001	0.106016
	N	-1.135371	0.895918	0.109363
	H	2.179126	0.925842	-0.162524
	H	0.381117	2.580843	0.398358
	H	-1.917186	1.497408	0.313128
	H	-2.509110	-0.895832	-0.387896
	H	-0.434061	-2.368093	-0.235310
	H	1.198254	0.347691	-1.336711
	H	1.983476	-1.632804	-0.003496
6	B	-0.230309	-0.711742	1.285833
	H	-0.633136	-1.471966	2.104277
	N	-0.230309	0.650002	1.252525
	N	0.432794	-1.309029	0.000000
	B	0.321763	1.424903	0.000000
	B	-0.230309	-0.711742	-1.285833
	N	-0.230309	0.650002	-1.252525
	H	1.384337	-0.923981	0.000000
	H	-0.633136	-1.471966	-2.104277
	H	-0.613414	1.174066	-2.022740
	H	-0.040520	2.572519	0.000000
	H	-0.613414	1.174066	2.022740
	H	1.541703	1.322600	0.000000
	H	0.496633	-2.319260	0.000000
7	N	0.487524	1.377732	0.045574

	N	0.857621	-1.097703	-0.284976
	N	-1.489736	-0.132894	-0.109518
	B	-0.557323	-1.359096	0.352770
	B	1.575772	0.271610	0.130177
	B	-0.872409	1.284958	-0.036262
	H	1.468522	-1.852950	0.011105
	H	-2.328065	-0.158329	0.465326
	H	0.854032	2.318396	0.081014
	H	0.822621	-1.174755	-1.297681
	H	-1.837775	-0.288226	-1.053824
	H	-1.045460	-2.380001	-0.067423
	H	2.465262	0.494144	-0.660300
	H	-0.467070	-1.311948	1.549056
	H	1.982436	0.133998	1.258961
	H	-1.632565	2.202370	-0.077221
8a	B	1.818583	-1.177014	0.000000
	N	0.218047	-0.753237	0.000000
	H	2.284401	-0.704516	1.008949
	H	2.284401	-0.704516	-1.008949
	H	1.825416	-2.389233	0.000000
	H	0.173626	-1.214725	-0.814272
	H	0.173626	-1.214725	0.814272
	B	0.000000	0.772257	0.000000
	N	1.636620	1.069756	0.000000
	H	0.385196	1.276830	1.016226
	H	0.385196	1.276830	-1.016226
	H	2.105595	0.702974	0.821891
	H	2.105595	0.702974	-0.821891
	H	1.769074	2.076258	0.000000
8b	B	-1.431537	-0.781188	0.079417
	N	-0.810969	0.705666	-0.121949

	H	-1.012592	-1.193942	1.147830
	H	-1.017111	-1.456399	-0.844304
	H	-2.633743	-0.698601	0.070452
	H	-1.061976	1.023106	-1.051527
	H	-1.300760	1.328289	0.510892
	B	0.731417	0.863349	0.140693
	N	1.364500	-0.609783	-0.062277
	H	1.267370	1.598471	-0.647373
	H	0.927799	1.145503	1.292200
	H	1.341536	-0.923613	-1.026262
	H	0.792832	-1.268136	0.470854
	H	2.322526	-0.636668	0.266273
9a	B	-3.470817	0.177307	0.011746
	N	-1.966219	-0.489372	-0.014513
	H	-3.550963	0.873615	-0.973114
	H	-3.546280	0.803095	1.043316
	H	-4.241228	-0.762473	-0.019252
	H	-1.945565	-1.121514	0.779479
	H	-1.951691	-1.073273	-0.844751
	B	-0.796030	0.535349	0.010152
	N	0.624761	-0.308922	-0.001240
	H	-0.788642	1.193064	-0.992455
	H	-0.793274	1.150549	1.039540
	H	0.603859	-0.918769	-0.813904
	H	0.616595	-0.907595	0.819906
	B	1.846575	0.651879	-0.020722
	N	3.230521	-0.250873	0.012109
	H	1.906494	1.253960	-1.052841
	H	1.896094	1.310712	0.976515
	H	4.013540	0.396251	-0.003910
	H	3.333268	-0.863226	-0.791255

	H	3.325712	-0.812899	0.852361
9b	B	-1.564971	1.256715	-0.428586
	N	-1.809062	-0.228121	0.148456
	H	-0.764784	1.175892	-1.350931
	H	-1.114592	1.923363	0.482993
	H	-2.615148	1.696774	-0.825833
	H	-2.449223	-0.140638	0.932287
	H	-2.333402	-0.757610	-0.542626
	B	-0.574467	-1.077581	0.653846
	N	0.523060	-1.047237	-0.516989
	H	-0.132677	-0.552196	1.649068
	H	-0.901889	-2.221196	0.854237
	H	0.097510	-0.636320	-1.345773
	H	0.751178	-2.003256	-0.767926
	B	1.892243	-0.305064	-0.250986
	N	1.500442	1.112126	0.388679
	H	2.538254	-0.910054	0.560523
	H	2.469570	-0.088772	-1.284881
	H	2.311187	1.717432	0.447877
	H	1.115530	0.984831	1.320849
	H	0.763388	1.584021	-0.142254
10	N	1.615973	-0.060680	-0.201003
	H	1.552805	-0.466988	-1.121957
	B	0.388225	0.088035	0.563692
	H	0.449197	0.350919	1.723232
	H	-0.578122	1.073623	-1.120433
	H	-2.275941	-0.864514	0.593743
	H	-1.201671	-1.331041	-1.106746
	H	-0.328253	-1.182661	0.668588
	N	-0.786647	0.744202	-0.190302
	B	-1.287850	-0.753710	-0.064735

	H	2.394995	-0.466676	0.290307
	H	-1.320160	1.431064	0.317620
11	B	-2.103027	1.002988	-0.230584
	N	-2.215922	-0.559672	-0.217387
	H	-1.733368	1.427112	-1.278262
	H	-2.938970	1.561009	0.400844
	H	-2.980007	-0.956831	0.306126
	H	-2.109662	-1.019152	-1.108307
	B	-0.922986	-0.232756	0.587051
	N	0.390219	-0.506607	-0.109919
	H	-1.037066	1.094421	0.558593
	H	-0.992332	-0.500274	1.740174
	H	0.391023	-0.314079	-1.107752
	H	0.691744	-1.470895	-0.009044
	B	1.702323	0.401871	0.478971
	N	2.875190	-0.012334	-0.363672
	H	1.323259	1.541220	0.309561
	H	1.755749	0.071380	1.642280
	H	3.276012	0.717927	-0.929918
	H	3.625667	-0.462058	0.135361
12^a	B	-0.813492	1.658774	0.000000
	N	0.813492	1.593086	0.000000
	H	-1.164976	1.084992	1.009953
	H	-1.164976	1.084992	-1.009953
	H	-1.124308	2.821836	0.000000
	H	1.196818	2.052314	-0.819123
	H	1.144031	0.624425	0.000000
	H	1.196818	2.052314	0.819123
	H	1.164976	-1.084992	-1.009953
	B	0.813492	-1.658774	0.000000
	N	-0.813492	-1.593086	0.000000

	H	1.124308	-2.821836	0.000000
	H	1.164976	-1.084992	1.009953
	H	-1.196818	-2.052314	0.819123
	H	-1.196818	-2.052314	-0.819123
	H	-1.144031	-0.624425	0.000000
13	B	-1.189948	-2.028968	0.000000
	N	-2.067821	-0.967573	0.000000
	B	-0.839228	-0.245606	0.000000
	N	0.000000	0.795152	0.000000
	B	1.586265	0.613767	0.000000
	N	2.485970	1.607621	0.000000
	H	-1.204906	-3.203612	0.000000
	H	-3.058738	-0.812381	0.000000
	H	-0.039703	-1.449746	0.000000
	H	-0.338608	1.746971	0.000000
	H	1.810597	-0.578648	0.000000
	H	2.118868	2.555053	0.000000
14	B	1.048273	-3.086107	0.000000
	N	1.057640	-1.672897	0.000000
	B	-0.111256	-0.821155	0.000000
	N	0.000000	0.596013	0.000000
	B	-1.109715	1.518656	0.000000
	N	-0.915990	2.910629	0.000000
	H	0.001406	-3.650101	0.000000
	H	1.963473	-1.225520	0.000000
	H	-1.184610	-1.328820	0.000000
	H	0.930269	0.991671	0.000000
	H	-2.217014	1.085112	0.000000
	H	-0.018216	3.360218	0.000000
	H	2.083184	-3.677475	0.000000
	H	-1.686558	3.551731	0.000000

^a Optimization for the BH₃NH₃ dimer calculated with MP2/aug-cc-pVTZ.