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Supplementary material

The following tables list the geometries of various $B^+(H_2)_n$ and $BH_2^+(H_2)_{n-1}$, n = 2-4, stationary points optimized at the MP2/aug-cc-pVTZ level of theory. The results are presented in terms of the Cartesian coordinates of all atoms in units of Angstroms.

Table 1. Optimized geometries for $B^+(H_2)_2$ and $BH_2^+(H_2)$.

	X	Y	Z
Electrostatic complex			
B	0.000000	0.780464	0.000000
H	-1.435161	-0.997298	0.375097
H	-1.435161	-0.997298	-0.375097
H	1.718646	-0.707698	0.000000
H	1.151677	-1.200027	0.000000
TS_{21}			
B	0.000000	0.000000	0.769286
H	0.000000	1.735684	-0.708325
H	0.000000	1.181829	-1.214889
H	0.000000	-1.735684	-0.708325
H	0.000000	-1.181829	-1.214889
TS_{22}			
B	0.000000	0.000000	0.526381
H	0.000000	1.153311	-0.288495
H	0.000000	0.690264	-1.027458
H	0.000000	-1.153311	-0.288495
H	0.000000	-0.690264	-1.027458

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Table 1. Continued

	X	Y	Z
Covalent molecular ion			
B	0.000000	0.000000	0.217922
H	0.000000	0.405126	-1.152004
H	0.000000	-0.405125	-1.152004
H	0.000000	-1.106415	0.607198
H	0.000000	1.106415	0.607198
TS_{23}			
B	0.000000	0.000000	0.000000
H	0.000000	1.205575	0.000000
H	1.205575	0.000000	0.000000
H	-1.205575	0.000000	0.000000
H	0.000000	-1.205575	0.000000

Table 2. Optimized geometries for $B^+(H_2)_3$ and $BH_2^+(H_2)_2$.

	X	Y	Z
Electrostatic complex			
B	0.000000	0.000000	0.840750
H	0.000000	1.827405	-0.487182
H	1.582579	-0.913702	-0.487182
H	-1.582579	-0.913702	-0.487182
H	-0.443843	1.397797	-0.914068
H	1.432449	-0.314520	-0.914068
H	-0.988607	-1.083277	-0.914068

Table 2. Continued.

	X	Y	Z
TS_{31}			
B	0.000000	0.000000	0.682700
H	0.000000	1.466663	-0.215814
H	1.270167	-0.733331	-0.215814
H	-1.270167	-0.733331	-0.215814
H	0.000000	1.145286	-0.922019
H	0.991846	-0.572643	-0.922019
H	-0.991846	-0.572643	-0.922019
TS_{32}			
B	0.000000	0.000000	0.000000
H	0.000000	1.102668	0.534677
H	-0.954938	-0.551334	0.534677
H	0.954938	-0.551334	0.534677
H	0.000000	1.102668	-0.534677
H	0.954938	-0.551334	-0.534677
H	-0.954938	-0.551334	-0.534677
Covalent molecular ion			
B	0.000000	0.000000	0.203853
H	-1.006383	-0.409809	-0.638395
H	-1.006383	0.409809	-0.638395
H	0.000000	-1.037977	0.767157
H	0.000000	1.037977	0.767157
H	1.006383	0.409809	-0.638395
H	1.006383	-0.409809	-0.638395

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Table 3. Optimized geometries for $B^+(H_2)_4$ and $BH_2^+(H_2)_3$.

	X	Y	Z
Electrostatic complex			
B	0.000000	0.744607	0.000000
H	0.224410	-0.206875	2.278375
H	-0.282187	0.326483	2.403154
H	-0.282187	0.326483	-2.403154
H	0.224410	-0.206875	-2.278375
H	1.706140	-0.732817	0.000000
H	1.148226	-1.234993	0.000000
H	-1.369406	-0.997220	0.375670
H	-1.369406	-0.997220	-0.375670
TS_{41}			
B	0.000000	0.682777	0.000000
H	0.521325	-0.918770	0.966413
H	-0.021490	-0.445111	1.260218
H	0.521325	-0.918770	-0.966413
H	-0.021490	-0.445111	-1.260218
H	1.741517	0.876880	0.000000
H	1.932827	0.128312	0.000000
H	-2.461099	-0.496074	0.000000
H	-2.212915	-1.195241	0.000000

Table 3. Continued.

	X	Y	Z
Covalent molecular ion$_1$			
B	0.000000	0.636751	0.000000
H	-0.052828	-0.312163	0.994760
H	-0.760946	0.099276	1.008864
H	-0.052828	-0.312163	-0.994769
H	-0.760946	0.099276	-1.008864
H	-0.633592	1.633257	0.000000
H	1.180558	0.623231	0.000000
H	0.185862	-2.615838	0.000000
H	0.894722	-2.398633	0.000000
TS_{42}			
B	0.000000	0.699987	0.000000
H	-0.359054	1.138842	1.036073
H	-0.359054	1.138842	-1.036073
H	1.311502	0.697780	0.409869
H	1.311502	0.697780	-0.409869
H	-1.076936	-2.920296	0.000000
H	-0.355336	-3.085539	0.000000
H	-0.236312	-0.383672	0.409469
H	-0.236312	-0.583672	-0.409469

Table 3. Continued.

	X	Y	Z
Covalent molecular ion$_2$			
B	0.421985	0.161031	0.086632
H	0.246913	1.120424	-0.579343
H	0.243601	0.147088	1.253890
H	1.647939	-0.070725	-0.497661
H	1.647122	-0.453390	0.225461
H	-2.627623	0.358627	-0.173358
H	-2.740742	-0.262730	0.212439
H	-0.263338	-0.629970	-0.799236
H	-0.263596	-1.014480	-0.075350

The following tables list the harmonic frequencies (cm^{-1}) at the various $B^+(H_2)_n$ and $BH_2^+(H_2)_{n-1}$, n = 1-4, stationary points calculated at the MP2/aug-cc-pVTZ level of theory. Results are presented for per-hydrogenated and per-deuterated species (all with the ^{11}B isotope) with the group theoretical symmetry of the associated normal mode indicated in parenthesis.

Table 4. Harmonic frequencies for $B^+(H_2)$ and BH_2^+ and their deuterated analogs.

Electrostatic complex (C_{2v})		Transition state (C_s)[a]		Covalent molecular ion ($D_{\infty h}$)	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2	*per*-H_2	*per*-D_2
4306.0697 (a_1)	3046.0401 (a_1)	547.0813*i* (a')	400.8267*i* (a')	3014.2769 (σ_u)	2291.0514 (σ_u)
510.7329 (b_2)	362.1540 (b_2)	2533.8795 (a')	1864.3911 (a')	2728.8903 (σ_g)	1930.3583 (σ_g)
345.0794 (a_1)	262.2817 (a_1)	279.4205 (a')	202.2792 (a')	1008.4622 (π_u)	766.4985 (π_u)

[a] Calculated at MRCISD/aug-cc-pVTZ level of theory.

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Table 5. Harmonic frequencies for $B^+(H_2)_2$ and $BH_2^+(H_2)$ and their deuterated analogs.

Electrostatic complex (C_s)		TS_{21} (C_s)		TS_{22} (C_{2v})	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2	*per*-H_2	*per*-D_2
27.2970 (a'')	19.3689 (a'')	115.2355*i* (a_2)	81.5151*i* (a_2)	1096.0208*i* (a_1)	818.2138*i* (a_1)
145.9557 (a'')	103.2587 (a'')	64.6464 (b_1)	45.9024 (b_1)	814.5294 (a_1)	609.5440 (a_1)
205.4839 (a')	148.8722 (a')	206.5781 (a_1)	149.9534 (a_1)	888.4728 (b_1)	638.2799 (b_1)
324.4422 (a')	243.7475 (a')	323.0795 (b_2)	241.2989 (b_2)	971.3095 (a_2)	687.0835 (a_2)
337.6207 (a')	260.9395 (a')	325.5955 (a_1)	252.1574 (a_1)	1135.6736 (b_2)	816.4004 (b_2)
495.0740 (a'')	350.9979 (a'')	488.9943 (b_2)	349.1917 (b_2)	1472.5448 (a_1)	1043.0009 (a_1)
518.3432 (a')	369.2267 (a')	507.6461 (a_1)	362.2821 (a_1)	1626.1168 (b_2)	1205.0369 (b_2)
4306.0974 (a')	3046.0638 (a')	4309.3925 (b_2)	3048.3896 (b_1)	2433.9122 (a_1)	1733.9787 (a_1)
4317.7769 (a')	3054.3219 (a')	4310.2124 (a_1)	3048.9795 (a_1)	2965.8162 (b_2)	2099.1008 (b_2)

Table 5. Continued.

Covalent molecular ion (C_{2v})		TS_{23} (D_{4h})	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2
846.7310 (a_2)	598.9593 (a_2)	851.3868*i* (e_u)	636.7422*i* (e_u)
944.9014 (b_2)	690.6806 (b_2)	851.3868*i* (e_u)	636.7422*i* (e_u)
979.9734 (b_1)	765.0581 (b_1)	654.4715 (a_{2u})	521.2384 (a_{2u})
987.1683 (a_1)	777.2337 (a_1)	879.0872 (b_{2g})	621.8474 (b_{2g})
1263.4362 (a_1)	894.0096 (a_1)	1215.2679 (b_{2u})	859.6544 (b_{2g})
1655.1404 (b_2)	1178.5776 (b_2)	2388.6740 (a_{1g})	1689.6966 (a_{1g})
2734.2284 (a_1)	1953.5236 (a_1)	2417.4748 (b_{1g})	1710.0697 (b_{1g})
2939.0964 (b_2)	2224.7699 (b_2)	2689.0539 (e_u)	2025.6313 (e_u)
3579.2737 (a_1)	2534.9130 (a_1)	2689.0539 (e_u)	2025.6313 (e_u)

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Table 6. Harmonic frequencies for $B^+(H_2)_3$ and $BH_2^+(H_2)_2$ and their deuterated analogs.

Electrostatic complex (C_3)		TS_{31} (C_{3v})		TS_{32} (D_{3h})	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2	*per*-H_2	*per*-D_2
118.4876 (e)	83.9672 (e)	493.7295*i* (a_1)	374.0419*i* (a_1)	992.9109*i* (e')	724.0733*i* (e')
118.4876 (e)	83.9672 (e)	307.2322 (e)	217.8087 (a_2)	992.9109*i* (e')	724.0733*i* (e')
203.6462 (a)	144.3081 (a)	307.2322 (e)	218.8618 (e)	495.6115 (a_2'')	390.0685 (a_2'')
214.2684 (e)	153.4728 (e)	307.9096 (a_2)	218.8618 (e)	903.5995 (e')	673.9736 (e')
214.2684 (e)	153.4728 (e)	562.4502 (e)	404.0556 (e)	903.5995 (e')	673.9736 (e')
233.6122 (a)	167.7267 (a)	562.4502 (e)	404.0556 (e)	1053.3733 (e")	745.1336 (e")
320.2224 (a)	245.7585 (e)	602.5033 (a_1)	448.9169 (e)	1053.3733 (e")	745.1336 (e")
327.7581 (e)	245.7585 (e)	609.9614 (e)	448.9169 (e)	1252.2645 (a_1'')	885.8250 (a_1'')
327.7581 (e)	255.7071 (a)	609.9614 (e)	454.5451 (a_1)	1556.8479 (a_1')	1101.2808 (a_1')
507.0293 (e)	360.8098 (e)	805.4216 (e)	580.3935 (e)	2352.0996 (a_1')	1663.8247 (a_1')
507.0293 (e)	360.8098 (e)	805.4216 (e)	580.3935 (e)	2497.3731 (e")	1766.5881 (e")
515.7310 (a)	369.8450 (a)	840.2046 (a_1)	605.2230 (a_1)	2497.3731 (e")	1766.5881 (e")
4306.7922 (a)	3046.5696 (a)	3841.0740 (a_1)	2718.2414 (a_1)	2595.9218 (a_2'')	1920.4491 (a_2'')
4307.4111 (e)	3046.9898 (e)	3940.5996 (e)	2787.6978 (e)	2619.5612 (e')	1983.5900 (e')
4307.4111 (e)	3046.9898 (e)	3940.5996 (e)	2787.6978 (e)	2619.5612 (e')	1983.5900 (e')

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Table 6. Continued.

Covalent molecular ion (C_{2v})	
per-H_2	*per*-D_2
521.7912 (b_2)	375.4417 (b_2)
667.5855 (a_2)	472.2357 (a_2)
830.9469 (a_1)	654.8856 (a_1)
910.0196 (b_2)	676.7788 (b_2)
1066.3332 (b_1)	760.7549 (a_2)
1075.4565 (a_2)	793.9833 (b_1)
1085.0568 (a_1)	777.9164 (a_1)
1311.4862 (b_1)	942.1299 (a_1)
1320.5870 (a_1)	1014.0457 (b_1)
1835.3278 (a_2)	1298.2714 (a_2)
1871.6537 (b_2)	1339.7104 (b_2)
2688.0255 (a_1)	1938.1637 (a_1)
2813.8008 (b_2)	2114.9604 (b_2)
3425.5834 (b_1)	2426.5713 (b_1)
3482.8042 (a_1)	2469.5731 (a_1)

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Table 7. Harmonic frequencies for $B^+(H_2)_4$ and $BH_2^+(H_2)_3$ and their deuterated analogs.

Electrostatic complex (C_s)		TS_{31} (C_s)		Covalent molecular ion$_1$ (C_s)	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2	*per*-H_2	*per*-D_2
101.9381 (a")	72.1130 (a")	505.7836*i* (a')	383.0101*i* (a')	54.0675 (a")	38.2585 (a")
122.5266 (a')	90.5556 (a')	137.8126 (a")	99.4276 (a")	128.7968 (a')	91.7678 (a')
142.5013 (a')	102.6923 (a')	147.9161 (a')	112.9000(a')	206.4126 (a")	146.0395 (a")
145.5126 (a')	104.8456 (a")	163.2224 (a")	115.7973 (a")	232.3002 (a')	167.5852 (a')
148.1004 (a")	104.9899 (a')	199.2417 (a')	144.8825 (a')	399.4020 (a')	282.7489 (a')
194.0871 (a")	138.9947 (a")	293.9701 (a')	208.0926 (a')	531.6616 (a')	382.1806 (a')
217.2683 (a")	155.2843 (a")	308.6756 (a")	218.4125 (a")	667.6248 (a")	472.2651 (a")
222.4807 (a")	163.9012 (a")	319.9593 (a")	228.1076 (a")	835.5689 (a')	656.3471 (a')
230.7501 (a')	165.4004 (a')	371.4748 (a')	262.9911 (a')	905.9314 (a')	675.7308 (a')
235.1804 (a")	178.9734 (a")	557.4816 (a")	400.2654 (a")	1063.3118 (a")	757.7141 (a")
297.2481 (a')	210.9872 (a')	563.2536 (a')	409.0210 (a')	1074.7517 (a")	783.0974 (a')
314.1816 (a')	241.0433 (a')	589.6634 (a')	428.6469 (a')	1090.4442 (a')	795.3548 (a")
327.5928 (a')	251.7325 (a')	616.7973 (a')	463.0792 (a')	1318.1142 (a")	947.0120 (a')
444.2641 (a")	314.3468 (a")	638.7726 (a")	468.8119 (a")	1326.3493 (a')	1017.8955 (a")
453.1832 (a')	326.3574 (a')	782.6197 (a')	563.3907 (a')	1838.2349 (a")	1300.3559 (a")
507.9296 (a')	363.2571 (a')	844.0246 (a")	611.0844 (a")	1874.3732 (a')	1341.2722 (a')
522.6463 (a")	371.8634 (a")	862.4143 (a')	619.5938 (a')	2690.6782 (a')	1940.3013 (a')
4301.1530 (a')	3042.5748 (a')	3822.8886 (a')	2705.3961 (a')	2816.32226 (a')	2116.8163 (a')
4310.5121 (a')	3049.1891 (a')	3918.9852 (a")	2772.4224 (a")	3432.9299 (a")	2431.7455 (a")
4373.9554 (a")	3094.0711 (a")	3965.7951 (a')	2805.6014 (a')	3488.6063 (a')	2473.4126 (a')
4383.4626 (a')	3100.7684 (a')	4445.9632 (a')	3144.9829 (a')	4458.4147 (a')	3153.7883 (a')

Table 7. Continued.

TS_{42} (C_s)		Covalent molecular ion_2 (C_1)	
per-H_2	*per*-D_2	*per*-H_2	*per*-D_2
110.2684*i* (a")	77.9855*i* (a")	29.7512	21.0871
29.6879 (a')	21.1189 (a')	61.6043	44.2124
59.4719 (a")	42.0848 (a")	87.8972	63.9396
203.7096 (a')	148.1173 (a')	219.3070	157.3889
385.8556 (a')	273.1031 (a')	358.7653	253.9066
515.4344 (a")	370.9283 (a")	511.7089	367.1924
665.7422 (a")	470.9313 (a")	653.0696	462.0825
840.6484 (a')	661.0649 (a')	829.2765	653.8338
909.0352 (a")	675.8852 (a")	903.8134	673.0457
1066.4879 (a')	762.6565 (a")	1062.6681	758.5688
1078.1448 (a")	784.1156 (a')	1072.3742	778.3988
1095.5526 (a')	794.2819 (a')	1086.7299	791.9991
1316.9177 (a')	954.8203 (a')	1304.8327	943.4279
1368.6834 (a')	1041.7720 (a')	1337.2427	1018.8906
1830.4776 (a")	1295.3855 (a")	1834.0810	1298.0917
1871.2092 (a")	1339.3351 (a")	1875.9628	1342.1300
2687.6533 (a')	1938.5243 (a')	2689.5979	1939.3845
2811.7796 (a")	2112.8988 (a")	2815.0633	2115.9232
3428.6752 (a')	2428.8466 (a')	3432.9845	2431.8585
3488.3298 (a')	2473.5051 (a')	3492.6331	2476.4148
4474.4735 (a')	3165.1474 (a')	4477.4241	3167.2345