Supporting Information for

A Safe and Efficient Synthetic Method of the Alkali Metal Octahydrotriborate, Unravelling a General Mechanism of Constructing the Delta B3 Unit of Polyhedral Boranes

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1. Experimental Section

1.1. General Remarks. All manipulations were carried out on aSchlenk line or in a glovebox filled with high-purity nitrogen. The ^{11}B NMR spectra were obtained at 193 MHz and externally referenced to $BF_3 \cdot OEt_2$ in C_6D_6 (δ = 0.00 ppm). The ^1H NMR and $^1H\{^{11}B\}$ NMR spectra were obtained at 600 MHz.

Chemicals of $LiBH_4$, $NaBH_4$, KBH_4 were purchased from Sigma-Aldrich, and the $RbBH_4$ and $CsBH_4$ were received from United Boron (Zhengzhou) Energy Materials S&T LLC. $DMS \cdot BH_3$ was purchased from Sinopharm Chemical Reagent Co., Ltd and used as received. 1,4-dioxane, THF, dimethoxyethane (DME), diethyl ether (Et_2O), and toluene were dried over sodium/benzophenone and freshly distilled prior touse. Dichloromethane (CH_2Cl_2) was dried over calcium hydride.

1.2. Computational Details. The M06-2X calculations were performed using the Gaussian 09 program. Basis set 6-311++G(d, p) was employed for all atoms involved in the model reaction. The solvent effect was considered by using the SMD model in dioxane solvent for all kinds of calculations. After the structural optimizations for all the stationary points, frequency calculations at the same level of theory were carried out to identify all of the stationary points as minima (zero imaginary frequency) or transition state (only one frequency), and to provide corrections for free energies.

1.3. Synthesis of unsolvated KB_3H_8. Potassium borohydride (0.54 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS \cdot BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 90 °C under stirring for 48 h (Fig. S1, S2). After reaction, the precipitate was separated by filtration and dried under dynamic vacuum. Then THF (40 mL) was injected into the flask, and stirred 20 mins to extract the KB_3H_8 product. Removal of THF from filtrate resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under dynamic vacuum to produce a free-flowing unsolvated KB_3H_8 white powder. (NMR yield of about 94%, isolated yield of 0.71 g, 89% (Fig. S3). ^{11}B NMR (193 MHZ, CD_3CN): δ -30.0 (nonet, J = 33 Hz) ppm. ^1H NMR (600 MHZ, CD_3CN): δ 0.14 (decet, J =33 Hz, 8H of $B_3H_8^-$) ppm.)

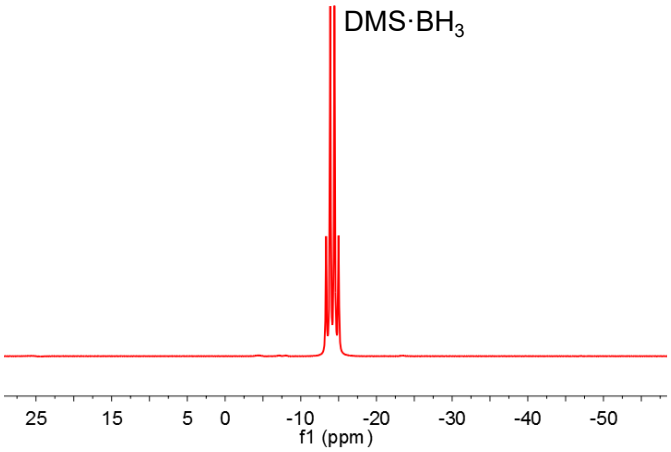

Fig. S1 The ^{11}B NMR spectrum of the reaction mixtures of KBH_4 and $DMS{\cdot}BH_3$ reacted for 48 hours at 90°C

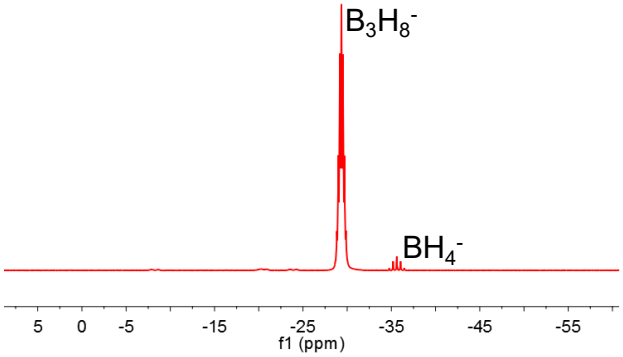

Fig. S2 The ^{11}B NMR spectrum of the precipitate, from the reaction of KBH_4 and $DMS{\cdot}BH_3$ at 90 °C for 48 hours, in DMSO

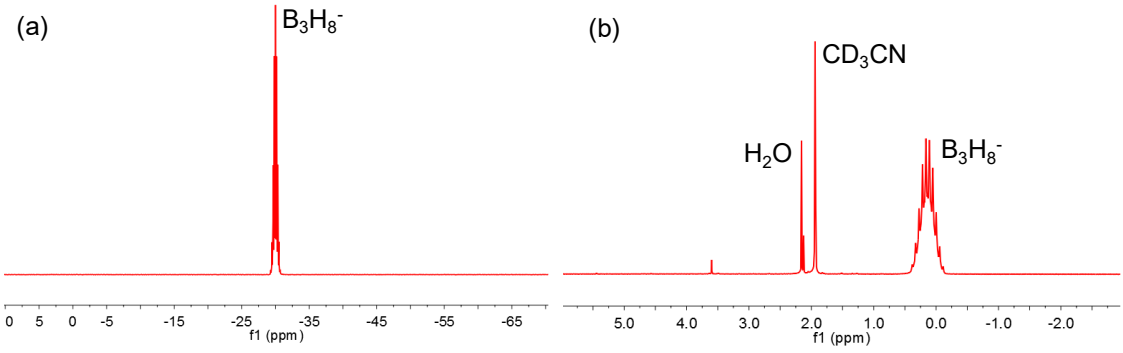

Fig. S3 The ^{11}B NMR (a) and ^{1}H NMR (b) spectra of the unsolvated KB_3H_8 in CD_3CN

1.4. Synthesis of unsolvated RbB_3H_8. Rubidium borohydride (1.0 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 90 °C under stirring for 48 h. After reaction, the precipitate was separated by filtration and dried under dynamic vacuum. Then THF (40 mL) was injected into the flask, and stirred 20 mins to extract the RbB_3H_8 product. Removal of THF from filtrate resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under dynamic vacuum to produce a free-flowing unsolvated RbB_3H_8 white powder.(NMR yield of about 92%, isolated yield of 1.01 g, 80% (Fig. S4). ^{11}B NMR (193 MHz, CD_3CN): δ -30.6 (nonet, J = 33 Hz) ppm. ^{1}H NMR (600 MHz, CD_3CN): δ 0.14 (decet, J = 33 Hz, 8H of $B_3H_8^-$) ppm.)

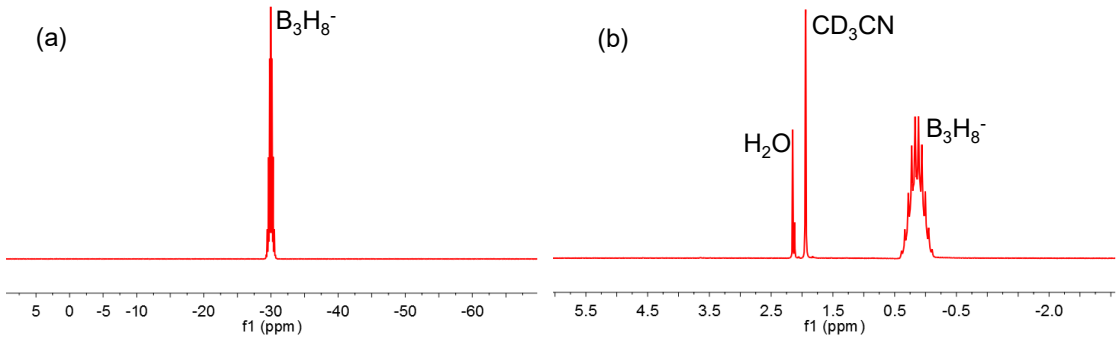

Fig. S4 The ^{11}B NMR (a) and ^{1}H NMR (b) spectra of the unsolvated RbB_3H_8 in CD_3CN

1.5. Synthesis of unsolvated CsB_3H_8. Cesium borohydride (1.48 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 90 °C under stirring for 48 h. After reaction, the precipitate was separated by filtration and dried under dynamic vacuum. Then THF (40 mL) was injected into the flask, and stirred 20 mins to extract the CsB_3H_8 product. Removal of THF from filtrate resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under

dynamic vacuum to produce a free-flowing unsolvated CsB_3H_8 white powder. (NMR yield of about 92%, isolated yield of 1.44g, 83% (Fig. S5). ^{11}B NMR (193 MHz, CD_3CN): δ -30.5 (nonet, J = 33 Hz) ppm. ^{1}H NMR (600 MHz, CD_3CN): δ 0.15 (decet, J = 33 Hz, 8H of $B_3H_8^-$) ppm.)

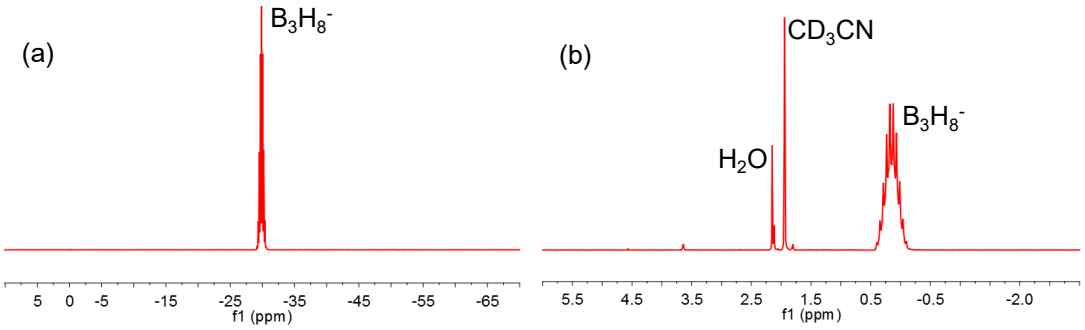

Fig. S5 The ^{11}B NMR (a) and ^{1}H NMR (b) spectra of the unsolvated CsB_3H_8 in CD_3CN

1.6. Synthesis of unsolvated $Na(C_4H_8O_2)B_3H_8$. Sodium borohydride (0.38 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 90 °C under stirring for 48 h. After reaction, the precipitate was separated by filtration and dried under dynamic vacuum. Then THF (40 mL) was injected into the flask. Water (1.0 mL) was injected into the solution to destroy the residue $NaBH_4$. After filtration, THF was removed from the filtrate under dynamic vacuum resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under dynamic vacuum to produce $Na(C_4H_8O_2)B_3H_8$ white powder. (NMR yield of about 97%, isolated yield of 1.24 g, 82% (Fig. S6). ^{11}B NMR (193 MHz, CD_3CN): δ -29.9 (nonet, J = 33 Hz) ppm. ^{1}H NMR (600 MHz, CD_3CN): δ 0.14 (decet, J = 33 Hz, 8H of $B_3H_8^-$), 3.60 (s, 8H of $C_4H_8O_2$) ppm.)

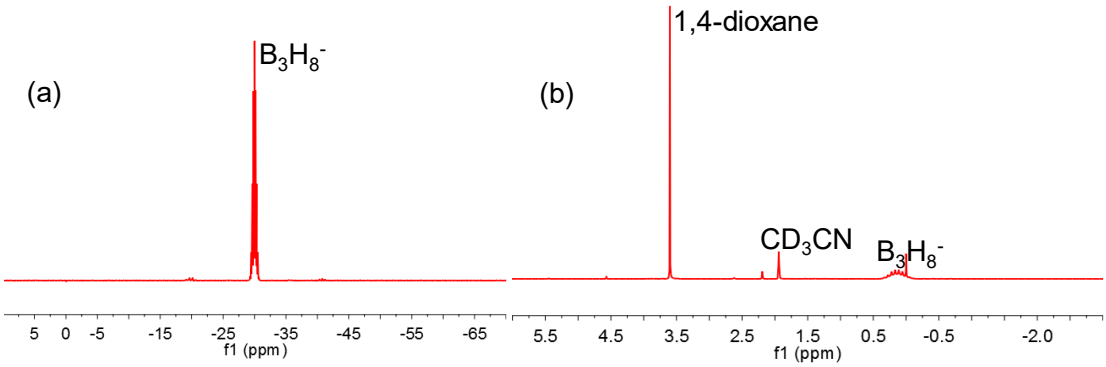

Fig. S6 The ^{11}B NMR (a) and ^{1}H NMR (b) spectra of $Na(C_4H_8O_2)B_3H_8$ in CD_3CN

1.7. Reaction of $LiBH_4$ with $DMS{\cdot}BH_3$ at 76 °C. Lithium borohydride (0.22 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 76°C under stirring for 48 h. After reaction, the solvent was removed under dynamic vacuum. Then THF (40 mL) was injected into the flask. Water (2.0 mL) was injected into the solution to destroy the residue $LiBH_4$. After filtration, THF was removed from the filtrate under dynamic vacuum resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under dynamic vacuum to produce white powder. The white power was dissolved in DMSO to test by ^{11}B NMR (Fig. S7).

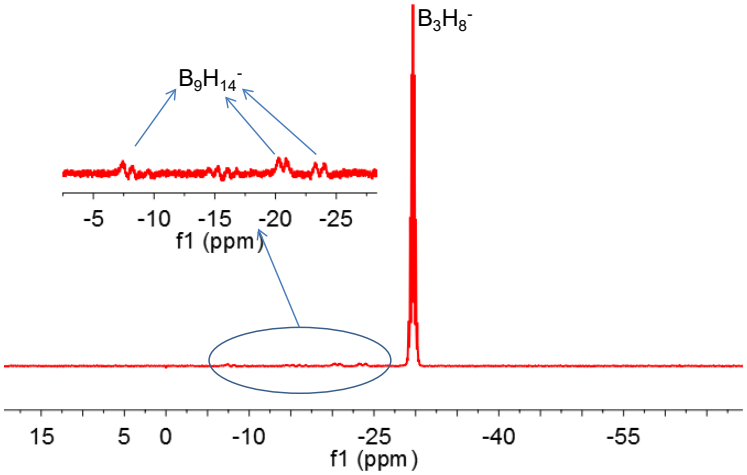

Fig. S7 The ^{11}B NMR spectrum of the white solid abtained from the reaction $LiBH_4$ with $DMS{\cdot}BH_3$ at 76 °C

1.8. Reaction of $LiBH_4$ with $DMS{\cdot}BH_3$ at 66 °C. Lithium borohydride (0.22 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 66°C under stirring for 48 h. After reaction, the solvent was removed under dynamic vacuum. Then THF (40 mL) was injected into the flask. Water (2.0 mL) was injected into the solution to destroy the residue $LiBH_4$. After filtration, THF was removed from the filtrate under dynamic vacuum resulted in a sticky solid, into which CH_2Cl_2 (20 mL) was added to pruduce white precipitate. The precipitate was filtered, washed with CH_2Cl_2 (2 × 20 mL), and then dried under dynamic vacuum to produce $Li(C_4H_8O_2)B_3H_8$ white powder. (NMR yield of about 57%, isolated yield of 0.69 g, 51% (Fig. S8). ^{11}B NMR (193 MHz, CD_3CN): δ -29.98 (nonet, J = 33 Hz) ppm. ^{1}H NMR (600 MHz, CD_3CN): δ 0.14 (decet, J = 33 Hz, 8H of $B_3H_8^-$), 3.60 (s, 8H of $C_4H_8O_2$) ppm.)

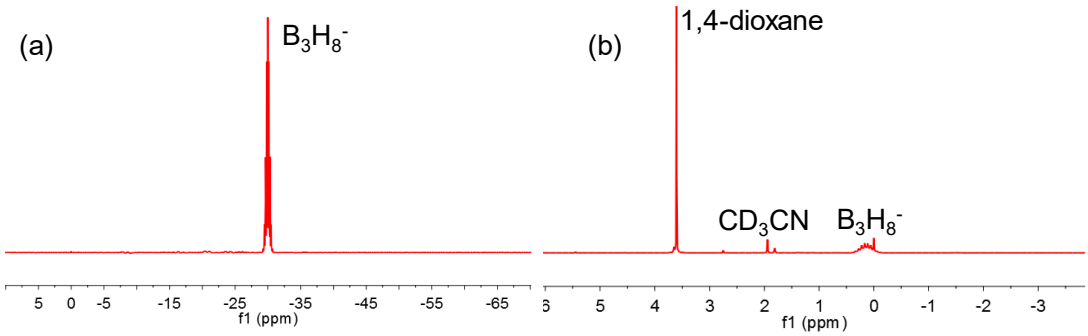

Fig. S8 The ^{11}B NMR (a) and ^{1}H NMR (b) spectra of $Li(C_4H_8O_2)B_3H_8$ in CD_3CN

1.9. The capture of the B_2H_6 intermediate formed in the reaction of $DMS{\cdot}BH_3$ with KBH_4. Potassium borohydride (0.54 g, 10 mmol) was added to a 50 mL flask, and then 8 mL 1,4-dioxane and 10 M $DMS{\cdot}BH_3$ (2 mL, 20 mmol) was condensed into the flask. The reaction mixture was heated at 90 °C under stirring for 20 mins and the forming gases were condensed by ice-water in condensor and then trapped by Et_2O. The trapped Et_2O solution was examined by ^{11}B NMR (Fig. 3).

1.10. Influencing factors on the reaction of KBH_4 and $DMS{\cdot}BH_3$. Similar procedures were peformed for synthesis of KB_3H_8 by KBH_4 with different concentrations of $DMS{\cdot}BH_3$ solutions at different temperature in different solvents (Table S1).

Table S1 The yield of KB_3H_8 in different reaction conditions

c(DMS·BH_3) (M)	Solvent	Reaction conditions	Yield based on NMR integration (%)
2.0	1,4-dioxane	66 °C，48 h	25
2.0	1,4-dioxnae	75 °C，48 h	38
2.0	1,4-dioxane	85 °C，48 h	79
2.0	1,4-dioxane	90 °C，48 h	94
2.0	1,4-dioxane	reflux，24 h	--[a]
0.5	1,4-dioxane	90 °C，48 h	63
4.0	1,4-dioxane	90 °C，48 h	85
2.0 (20% excess)	1,4-dioxane	90 °C，48 h	97
2.0	toulene	90 °C，48 h	--
2.0	THF	reflux，48 h	--

NOTE: The by-product SMe_2 gas produced in the reaction is passed through to the aqueous solution of NaClO for harmless treatment.

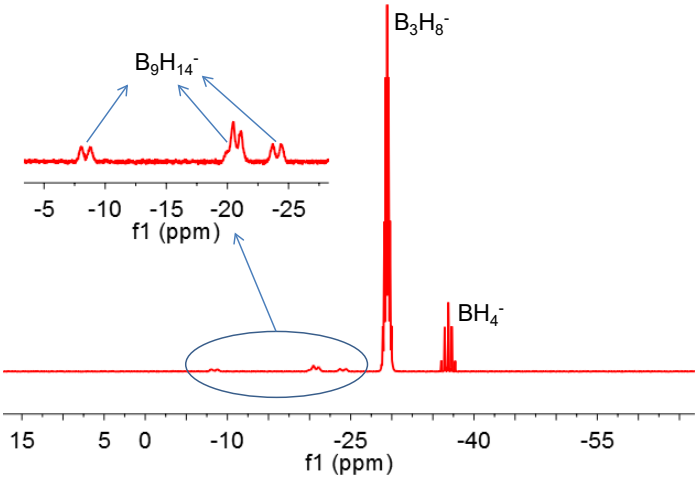

Fig. S9 The ^{11}B NMR spectrum of the reaction precipitate of KBH_4 and DMS·BH_3 reacted at reflux for 24 hours in DMSO[a]

2. Mechanisms

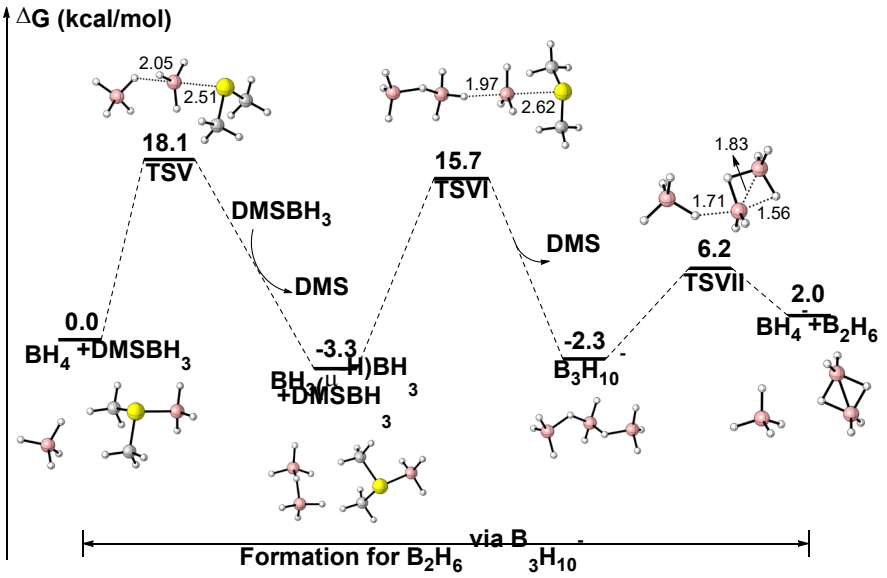

Fig. S10 Energy profile for the formation of $B_3H_{10}^-$ and then divided to BH_4^- and B_2H_6 in 1,4-dioxane

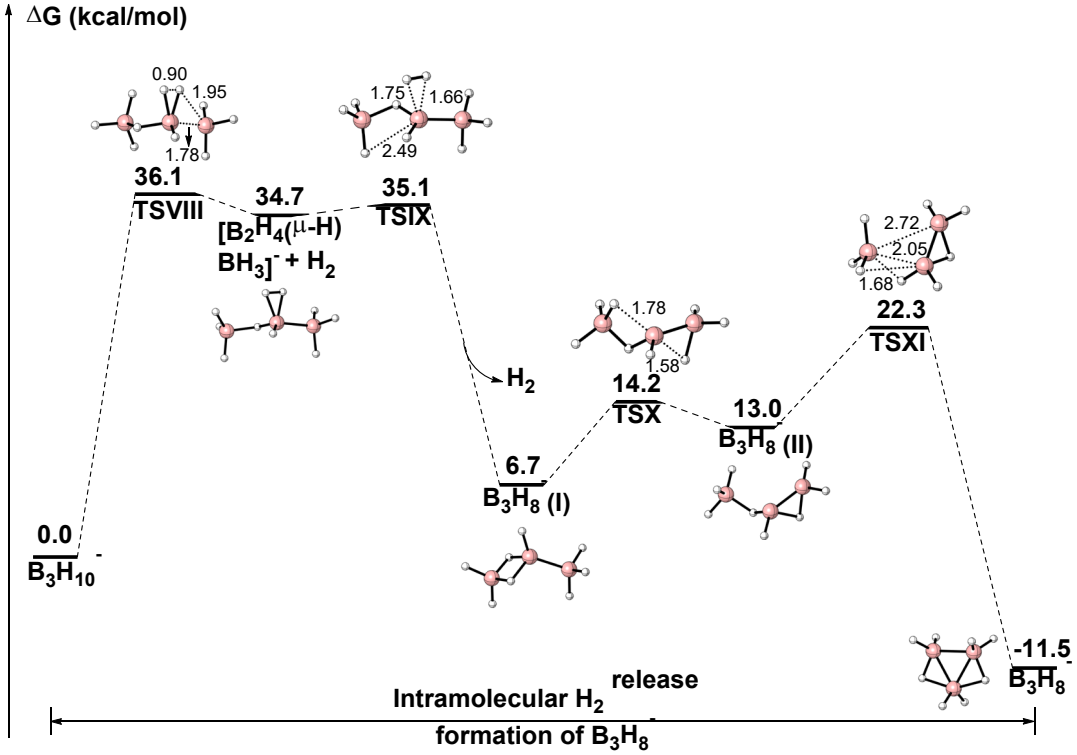

Fig. S11 Energy profile for the transformation from $B_3H_{10}^-$ to $B_3H_8^-$ via intramolecular H_2 release in 1,4-dioxane

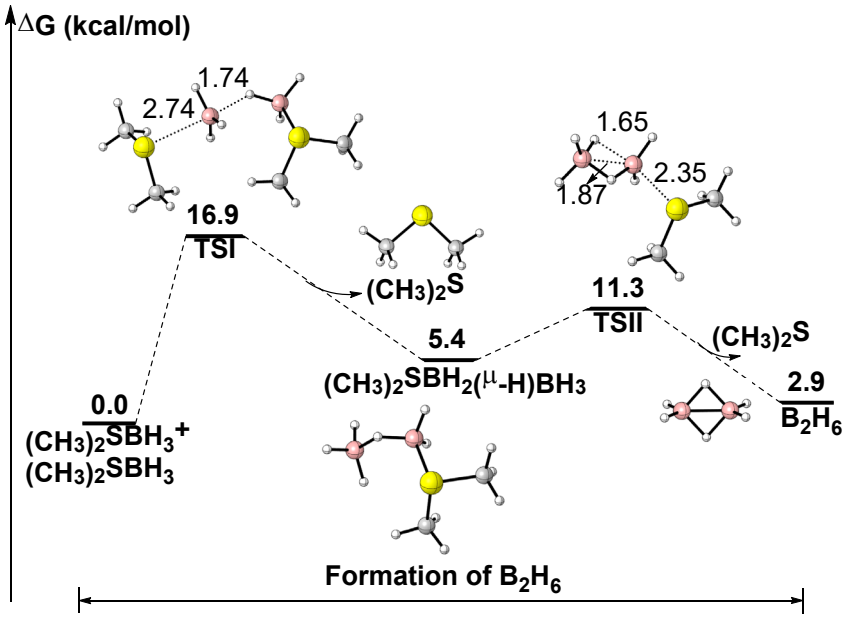

Fig. S12 Energy profile for the transformation from $(CH_3)_2S{\cdot}BH_3$ to B_2H_6 in THF

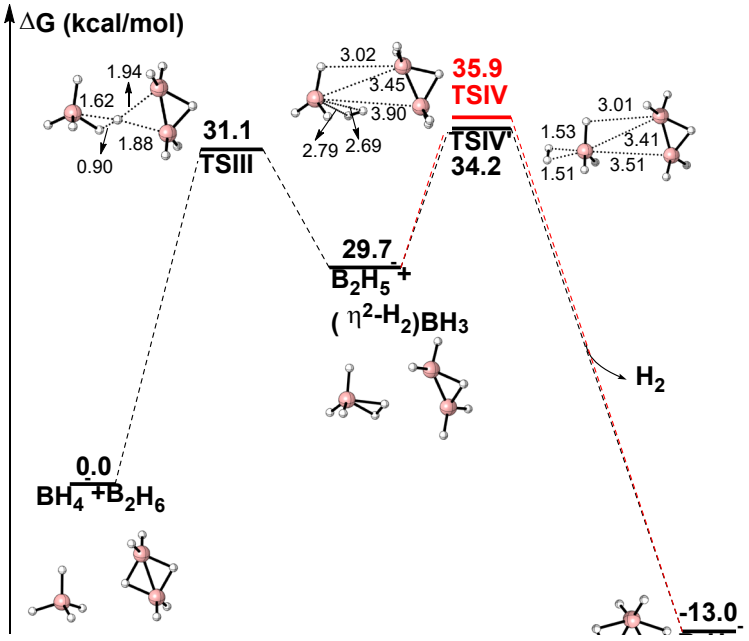

Fig. S13 Energy profile for the transformation from BH_4^- and B_2H_6 to $B_3H_8^-$ via intermolecular H_2 release in THF

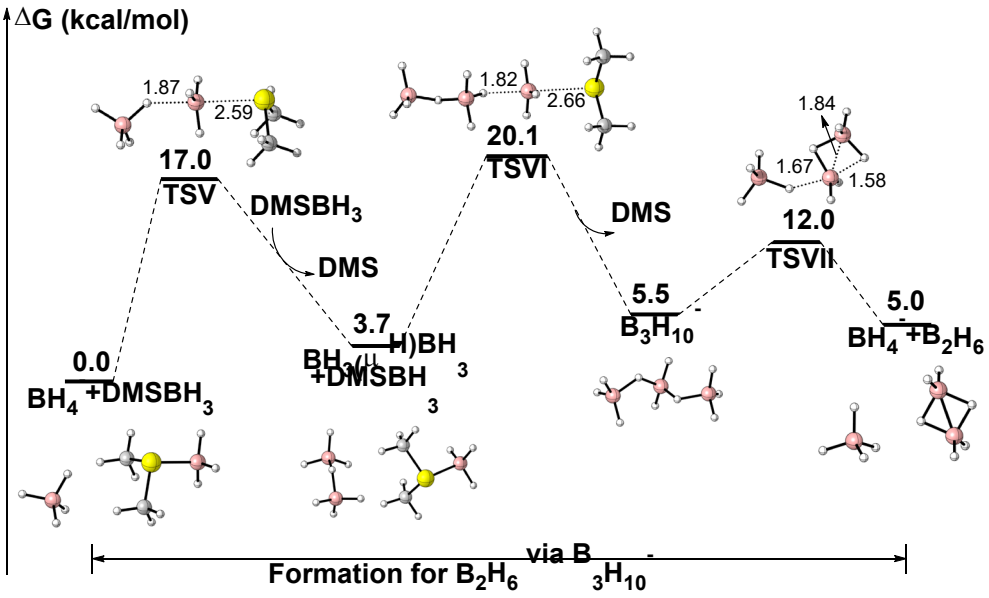

Fig. S14 Energy profile for the formation of $B_3H_{10}^-$ and then divided to BH_4^- and B_2H_6 in THF

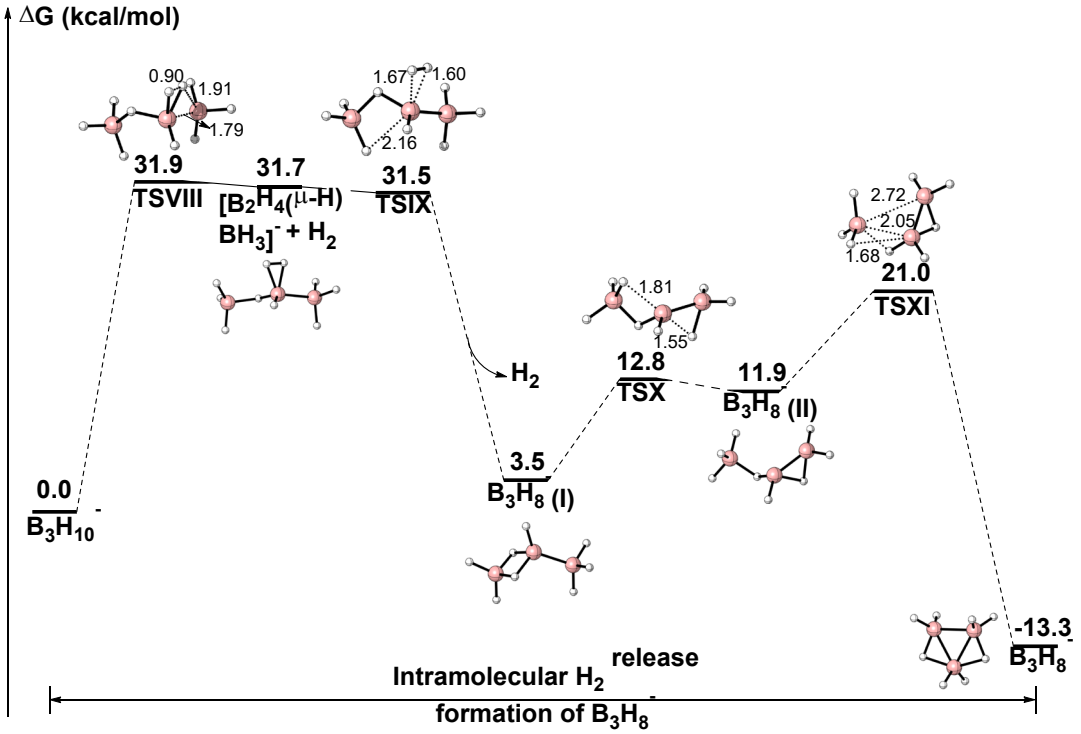

Fig. S15 Energy profile for the transformation from $B_3H_{10}^-$ to $B_3H_8^-$ via intramolecular H_2 release in THF

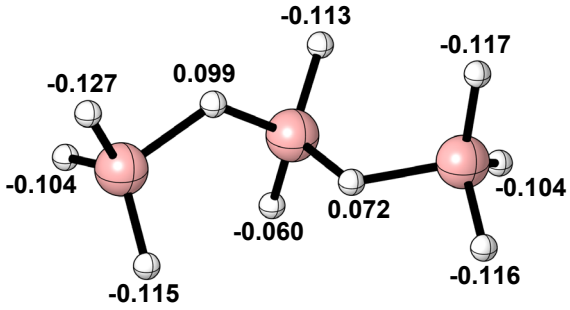

Fig. S16 Mulliken charge analysis for $B_3H_{10}^-$ in 1,4-dioxane.

3. Cartesian coordinates and Vibrational frequencies of all the computed systems

3.1. Solvent: 1,4-dioxane.

$(CH_3)_2S{\cdot}BH_3$ + $(CH_3)_2S{\cdot}BH_3$

Zero-point correction = 0.217746
Thermal correction to Energy = 0.233312
Thermal correction to Enthalpy = 0.234257
Thermal correction to Gibbs Free Energy = 0.174477
Sum of electronic and zero-point Energies = -1009.024889
Sum of electronic and thermal Energies = -1009.009323
Sum of electronic and thermal Enthalpies = -1009.008378
Sum of electronic and thermal Free Energies = -1009.068158
Cartesian coordinates

S	-1.898499	0.060501	-0.198325
C	-3.551714	0.587244	-0.697514
H	-4.243041	0.466075	0.136891
H	-3.489877	1.641040	-0.968543
H	-3.877002	0.007427	-1.561370
C	-2.274227	-1.595754	0.409513
H	-2.583544	-2.227131	-0.423237
H	-1.357501	-1.990249	0.845279
H	-3.054271	-1.532481	1.169337
B	-1.624900	1.098008	1.453247
H	-1.474741	2.224453	1.047203
H	-2.629991	0.922880	2.096376
H	-0.631629	0.615268	1.934562
S	2.653722	-0.103410	-0.568327
C	3.319157	0.216030	1.078533
H	2.495888	0.293610	1.789619
H	3.954029	-0.629661	1.342202

H	3.912831	1.129785	1.065790
C	1.532918	1.304805	-0.716428
H	2.113411	2.225754	-0.777358
H	0.964921	1.170900	-1.636691
H	0.860853	1.327258	0.142280
B	1.431175	-1.607461	-0.224497
H	2.176131	-2.529058	-0.008846
H	0.791720	-1.244356	0.730836
H	0.800058	-1.711645	-1.246260

Vibrational frequencies

29.7891	54.9280	63.9298
82.3308	87.3940	99.9359
114.3233	170.1345	178.5932
199.2026	210.1937	220.3489
229.4337	237.3768	253.9819
263.3499	296.2838	306.4643
496.5079	502.0828	722.0340
722.9590	762.1152	762.7927
811.4589	812.9341	825.5034
836.0940	942.7708	958.4776
1001.6910	1006.4505	1026.5187
1030.0271	1066.3014	1077.8660
1113.7023	1118.8354	1174.9632
1177.8686	1182.4321	1189.9948
1358.5504	1364.5627	1384.4620
1393.9690	1455.0530	1457.6757
1459.7175	1460.6325	1467.4442
1469.8800	1470.4625	1481.5174
2492.8851	2502.0695	2551.5067
2560.8321	2566.1094	2573.3636
3065.8895	3068.2827	3072.2536
3074.7931	3166.2387	3167.5896
3171.3790	3173.3896	3174.4070
3180.2010	3184.0474	3189.8994

TSI

Zero-point correction = 0.216778
Thermal correction to Energy = 0.231854
Thermal correction to Enthalpy = 0.232798
Thermal correction to Gibbs Free Energy = 0.172860
Sum of electronic and zero-point Energies = -1008.998593
Sum of electronic and thermal Energies = -1008.983517
Sum of electronic and thermal Enthalpies = -1008.982572

Sum of electronic and thermal Free Energies = -1009.042511

Cartesian coordinates

S	2.628533	0.005608	-0.490327
C	4.292019	0.173908	0.194334
H	4.245352	0.144778	1.283663
H	4.878481	-0.669000	-0.170633
H	4.736331	1.107014	-0.152409
C	1.822837	1.382348	0.357852
H	2.349129	2.304938	0.108416
H	0.797566	1.436144	-0.002580
H	1.833759	1.201967	1.433207
B	2.020861	-1.602386	0.465672
H	2.831492	-2.427867	0.138115
H	2.007816	-1.303783	1.629539
H	0.929504	-1.874866	-0.002666
S	-3.088941	0.080069	-0.634185
C	-2.766562	1.560906	0.353018
H	-2.109983	1.322256	1.192116
H	-2.274750	2.290005	-0.292093
H	-3.699028	1.992694	0.721522
C	-3.780409	-0.969600	0.666462
H	-4.697895	-0.536927	1.069383
H	-4.010772	-1.937687	0.220329
H	-3.048687	-1.116416	1.464885
B	-0.602834	-1.027155	-0.298055
H	-0.162544	-0.438217	-1.239505
H	-0.648259	-0.498760	0.771634
H	-1.088432	-2.104774	-0.448823

Vibrational frequencies

-303.7202	7.9624	50.6373
58.4103	78.3694	96.4130
119.8758	169.0183	190.4359
206.8845	215.8095	225.1656
237.6807	249.8648	257.2042
262.5386	283.1542	289.9659
308.1426	507.6256	711.6402
719.9678	723.6710	756.4706
775.2826	793.5005	816.6181
847.6789	942.9998	952.6281
974.1685	991.7954	1006.8417
1020.6083	1047.2841	1069.9495
1075.7417	1108.5514	1144.8733
1170.2209	1173.0098	1194.0191

1354.7435	1361.4590	1380.3874
1389.0096	1454.1848	1462.7318
1464.0280	1471.9161	1474.8124
1476.9763	1481.7194	1490.2776
2407.4737	2546.7792	2580.2369
2603.8932	2680.3066	2702.2587
3052.9472	3056.4863	3065.3054
3070.0490	3141.2415	3147.3745
3152.8631	3155.8558	3165.3327
3167.4375	3173.0111	3190.5949

$(CH_3)_2S$

Zero-point correction = 0.076098
Thermal correction to Energy = 0.081057
Thermal correction to Enthalpy = 0.082001
Thermal correction to Gibbs Free Energy = 0.048840
Sum of electronic and zero-point Energies = -477.906394
Sum of electronic and thermal Energies = -477.901435
Sum of electronic and thermal Enthalpies = -477.900491
Sum of electronic and thermal Free Energies = -477.933652
Cartesian coordinates

S	0.000002	0.663616	-0.000067
C	1.375005	-0.514830	0.000168
H	1.355388	-1.141236	-0.893311
H	2.300422	0.062263	0.000134
H	1.355297	-1.140989	0.893818
C	-1.375007	-0.514828	-0.000064
H	-1.355326	-1.141138	0.893479
H	-2.300422	0.062268	-0.000026
H	-1.355371	-1.141083	-0.893648

Vibrational frequencies

129.9196	173.6567	270.8676
720.8453	769.8630	944.2806
953.7349	989.2807	1072.5360
1364.3459	1388.8889	1461.7484
1468.6425	1469.1283	1480.9351
3062.4025	3065.2164	3147.6068
3153.5322	3157.2381	3158.3766

$(CH_3)_2BH_2(\mu\text{-}H)BH_3$

Zero-point correction = 0.141371
Thermal correction to Energy = 0.150388

Thermal correction to Enthalpy = 0.151332
Thermal correction to Gibbs Free Energy = 0.108491
Sum of electronic and zero-point Energies = -531.093332
Sum of electronic and thermal Energies = -531.084315
Sum of electronic and thermal Enthalpies = -531.083370
Sum of electronic and thermal Free Energies = -531.126212
Cartesian coordinates

S	0.534186	-0.002135	-0.554417
C	1.941187	-0.736816	0.307982
H	1.749743	-0.744509	1.381156
H	2.050542	-1.757002	-0.058106
H	2.839430	-0.165982	0.074802
C	0.468509	1.601335	0.275841
H	1.426108	2.102056	0.132037
H	-0.323400	2.184778	-0.189692
H	0.253486	1.458601	1.334989
B	-0.904986	-1.060728	0.262496
H	-0.657853	-2.180883	-0.083690
H	-0.896046	-0.839175	1.430076
H	-1.889203	-0.805740	-0.481063
B	-2.801612	0.053352	0.049412
H	-3.292412	0.173348	-1.043781
H	-2.294907	1.050021	0.479015
H	-3.437654	-0.591586	0.832451

Vibrational frequencies

57.6319	104.3746	156.6676
195.2879	238.2262	253.1808
273.3920	303.2282	318.6318
494.9267	576.0991	661.5428
718.3511	769.4166	801.8739
886.0937	959.8687	975.4918
1007.3090	1034.7309	1058.4840
1082.9306	1111.1350	1163.2709
1181.0901	1191.9548	1364.6285
1393.8396	1461.9150	1468.7193
1472.7231	1483.2751	1654.6571
2254.2705	2531.7760	2591.1052
2598.4484	2624.3518	2683.9949
3076.8121	3079.5844	3178.5404
3181.2633	3187.1017	3192.5885

TSII

Zero-point correction = 0.140729

Thermal correction to Energy = 0.149375
Thermal correction to Enthalpy = 0.150319
Thermal correction to Gibbs Free Energy = 0.108058
Sum of electronic and zero-point Energies = -531.087188
Sum of electronic and thermal Energies = -531.078542
Sum of electronic and thermal Enthalpies = -531.077598
Sum of electronic and thermal Free Energies = -531.119859
Cartesian coordinates

S	0.674951	0.028706	-0.611661
C	1.731437	-1.087925	0.334171
H	1.395514	-1.122502	1.372005
H	1.643965	-2.079843	-0.108849
H	2.768757	-0.758208	0.278747
C	0.906313	1.545302	0.341888
H	1.925002	1.914155	0.223653
H	0.208589	2.288846	-0.044746
H	0.685960	1.355787	1.393531
B	-1.304662	-0.696679	0.311445
H	-1.244068	-1.784173	-0.161430
H	-0.945717	-0.441102	1.416057
H	-1.779925	0.264703	-0.438264
B	-3.000249	0.101973	-0.009773
H	-3.581398	-0.172438	-1.016136
H	-3.228250	1.139852	0.537396
H	-2.949595	-0.835106	0.769891

Vibrational frequencies

-381.2251	51.7181	124.9646
179.9229	232.6957	234.1896
257.4345	278.5989	302.5361
376.5940	418.0390	720.0315
772.3459	790.9506	851.5594
935.6529	947.8273	981.0179
1006.3695	1023.0932	1049.1098
1075.7072	1117.5451	1153.4363
1165.6315	1214.0133	1358.6956
1387.2829	1463.9503	1470.5646
1478.8182	1484.5550	1893.6551
2070.7174	2471.7976	2586.1840
2636.0734	2649.1683	2734.1038
3068.2730	3072.3782	3162.5638
3167.5374	3177.3132	3178.2049

B_2H_6

Zero-point correction = 0.063297
Thermal correction to Energy = 0.066893
Thermal correction to Enthalpy = 0.067837
Thermal correction to Gibbs Free Energy = 0.040175
Sum of electronic and zero-point Energies = -53.190495
Sum of electronic and thermal Energies = -53.186899
Sum of electronic and thermal Enthalpies = -53.185955
Sum of electronic and thermal Free Energies = -53.213616
Cartesian coordinates

B	-0.874206	0.000054	-0.000004
H	-1.450932	1.035967	0.000105
H	-1.450852	-1.035932	-0.000095
B	0.874195	0.000056	0.000001
H	1.450915	-1.035887	-0.000135
H	0.000009	-0.000179	-0.980067
H	0.000028	-0.000509	0.980141
H	1.450886	1.035995	0.000067

Vibrational frequencies

339.6962	822.3794	858.7116
893.8501	923.0744	954.2852
994.1610	1052.0965	1184.4206
1200.8964	1698.2131	1876.1596
2025.1031	2177.3636	2644.1087
2662.0912	2732.4862	2745.1698

B_2H_6 + DMS

Zero-point correction = 0.141197
Thermal correction to Energy = 0.151006
Thermal correction to Enthalpy = 0.151950
Thermal correction to Gibbs Free Energy = 0.106093
Sum of electronic and zero-point Energies = -531.099530
Sum of electronic and thermal Energies = -531.089721
Sum of electronic and thermal Enthalpies = -531.088777
Sum of electronic and thermal Free Energies = -531.134634
Cartesian coordinates

B	-2.529183	0.674351	0.521045
H	-2.939900	1.721893	0.145986
H	-2.250302	0.488669	1.660461
B	-2.315847	-0.631943	-0.621021
H	-1.905872	-1.669766	-0.220302
H	-3.347223	-0.264872	0.122936
H	-1.511892	0.334213	-0.231070
H	-2.595921	-0.461578	-1.759651

S	1.216896	-0.185480	-0.617899
C	0.950949	-1.194180	0.862983
H	0.020187	-0.916326	1.361814
H	0.886314	-2.236121	0.548081
H	1.785039	-1.088506	1.558811
C	1.211780	1.443315	0.175094
H	2.035341	1.532083	0.885601
H	1.337369	2.194632	-0.605318
H	0.265301	1.626504	0.690455

Vibrational frequencies

55.7420	65.6047	102.5826
118.3465	146.9369	167.5364
186.4418	224.3892	276.3940
377.2749	726.4552	779.6233
822.3402	863.0774	883.4045
925.3533	926.5863	963.0506
969.2289	992.5181	1002.2251
1059.3928	1066.7070	1180.3001
1198.9484	1355.9225	1383.9140
1458.3683	1467.6713	1476.8312
1486.7759	1687.7276	1861.9288
2034.4978	2178.9067	2648.3446
2672.7486	2738.7624	2761.1686
3047.3293	3053.0879	3127.9810
3134.6778	3156.0759	3164.9668

BH_4^- + B_2H_6

Zero-point correction = 0.100114
Thermal correction to Energy = 0.107605
Thermal correction to Enthalpy = 0.108550
Thermal correction to Gibbs Free Energy = 0.069238
Sum of electronic and zero-point Energies = -80.452952
Sum of electronic and thermal Energies = -80.445461
Sum of electronic and thermal Enthalpies = -80.444517
Sum of electronic and thermal Free Energies = -80.483828
Cartesian coordinates

B	-1.264622	0.874800	-0.000254
H	-1.269175	1.453761	1.035758
H	-1.256720	1.453783	-1.036167
B	-1.308969	-0.862461	-0.000230
H	-1.327561	-1.441860	-1.035869
H	-0.303275	-0.019121	0.005496
H	-2.276594	0.029719	-0.006184

H	-1.339985	-1.441330	1.035456
B	2.296996	-0.011812	0.000427
H	1.867898	-0.581664	1.000946
H	1.869465	-0.577364	-1.003195
H	1.896040	1.151921	0.002568
H	3.522887	-0.030480	0.001471

Vibrational frequencies

27.9383	69.7967	181.2808
182.0792	249.0170	250.9637
375.0659	835.7208	846.6799
864.8433	931.1921	962.7164
979.9143	1049.8177	1098.7136
1099.4178	1140.0173	1188.0877
1206.7641	1235.7456	1240.5400
1675.2478	1868.4775	2046.1537
2178.3733	2328.7635	2363.3530
2364.9701	2366.3696	2632.6233
2653.9540	2718.6970	2731.5331

TSIII

Zero-point correction = 0.095190
Thermal correction to Energy = 0.102082
Thermal correction to Enthalpy = 0.103026
Thermal correction to Gibbs Free Energy = 0.065986
Sum of electronic and zero-point Energies = -80.410631
Sum of electronic and thermal Energies = -80.403739
Sum of electronic and thermal Enthalpies = -80.402795
Sum of electronic and thermal Free Energies = -80.439835
Cartesian coordinates

B	-2.080526	-0.015142	0.048494
H	-3.013822	-0.496207	-0.550817
H	-1.204848	-0.750346	-0.606243
H	-2.013073	-0.320879	1.208264
B	1.325246	-0.764886	0.019403
H	2.249210	0.206062	0.060326
H	1.390703	-1.378305	1.053470
H	1.504370	-1.394519	-0.993421
H	-1.883833	1.145233	-0.193719
B	1.056789	0.849282	-0.007211
H	-0.518473	-0.309973	-0.249535
H	1.046429	1.469688	-1.039773
H	0.935788	1.482978	1.008015

Vibrational frequencies

-539.9741	57.1641	148.4668
168.5293	186.0243	254.0511
515.6843	586.7655	828.3547
843.6356	886.3191	907.6382
917.9713	969.7300	998.7431
1037.3522	1047.4033	1116.0489
1171.7279	1193.1864	1207.5762
1211.3055	1470.2649	1832.1339
1952.9581	2412.7778	2501.8713
2519.5269	2549.7754	2550.8758
2570.0092	2573.4211	2596.2888

$B_2H_5^-$ + (η^2-H_2)BH_3

Zero-point correction = 0.096977
Thermal correction to Energy = 0.104915
Thermal correction to Enthalpy = 0.105859
Thermal correction to Gibbs Free Energy = 0.065964
Sum of electronic and zero-point Energies = -80.410567
Sum of electronic and thermal Energies = -80.402629
Sum of electronic and thermal Enthalpies = -80.401685
Sum of electronic and thermal Free Energies = -80.441580
Cartesian coordinates

B	-2.415583	-0.003103	-0.071842
H	-2.852440	0.350804	0.984616
H	-2.104186	0.889500	-0.810430
H	-2.939412	-0.935160	-0.611172
B	1.303378	0.831096	-0.016361
H	2.161621	0.125886	0.772576
H	1.975701	1.609712	-0.649903
H	0.493064	1.339392	0.727125
H	-1.367729	-0.724353	0.427954
B	1.563066	-0.769250	-0.060677
H	-1.018172	-0.139334	-0.015863
H	0.954362	-1.546021	0.644123
H	2.442887	-1.264137	-0.724622

Vibrational frequencies

41.2058	79.7546	130.4665
170.5267	192.6345	258.6266
316.1401	517.2804	812.9924
842.1503	867.3850	884.2475
899.2136	975.0658	1035.5638
1051.0354	1112.6055	1168.2882

1200.7029	1206.1421	1208.8945
1278.3465	1380.2462	1764.8120
1864.3167	2464.7454	2496.6612
2511.3164	2532.3866	2548.1187
2621.5823	2638.3785	3496.0700

TSIV

Zero-point correction = 0.092696
Thermal correction to Energy = 0.100872
Thermal correction to Enthalpy = 0.101816
Thermal correction to Gibbs Free Energy = 0.061785
Sum of electronic and zero-point Energies = -80.397725
Sum of electronic and thermal Energies = -80.389549
Sum of electronic and thermal Enthalpies = -80.388605
Sum of electronic and thermal Free Energies = -80.428636
Cartesian coordinates

B	2.222241	0.100659	-0.378154
H	3.157386	-0.124326	0.325846
H	1.506287	-0.831206	1.932773
H	1.809628	-0.749764	-1.096321
B	-1.362871	-0.727354	-0.269404
H	-2.329397	0.099855	0.225547
H	-1.715043	-1.044304	-1.382971
H	-1.251390	-1.641500	0.518218
H	1.783341	1.201782	-0.437219
B	-1.166752	0.820151	0.169281
H	0.845477	-0.757477	1.594388
H	-0.904544	1.142672	1.306919
H	-1.364832	1.736988	-0.595796

Vibrational frequencies

-174.6815	50.6819	90.4421
115.9542	142.1707	189.8770
346.6982	366.9844	463.5818
508.5870	640.0530	800.7006
831.8881	854.6063	879.1018
889.9434	972.4630	1050.4313
1127.0912	1156.8923	1190.9479
1198.4905	1206.4437	1352.0073
1821.3637	2459.6811	2491.1036
2497.7188	2513.6709	2619.0795
2725.0486	2754.9751	4380.1410

TSIV'

Zero-point correction = 0.094895
Thermal correction to Energy = 0.102303
Thermal correction to Enthalpy = 0.103247
Thermal correction to Gibbs Free Energy = 0.064897
Sum of electronic and zero-point Energies = -80.398078
Sum of electronic and thermal Energies = -80.390670
Sum of electronic and thermal Enthalpies = -80.389726
Sum of electronic and thermal Free Energies = -80.428076
Cartesian coordinates

B	1.960585	-0.046589	0.040220
H	1.658115	1.107019	0.047202
H	1.856027	-0.636541	-1.001897
H	1.895380	-0.693795	1.044495
B	-1.338100	0.821253	-0.004578
H	-2.468298	0.072449	-0.223637
H	-1.561239	1.491407	0.980126
H	-1.129386	1.445564	-1.022005
H	3.452706	0.280447	0.305234
B	-1.441001	-0.794949	0.011510
H	3.427296	-0.088627	-0.380732
H	-1.298081	-1.459883	-0.992498
H	-1.739942	-1.416617	1.007954

Vibrational frequencies

-147.8064	58.3562	96.1265
150.7640	170.2758	224.5350
398.9879	529.7250	550.4395
789.0794	827.2559	872.3942
901.3300	903.4423	974.2619
1002.6798	1046.5777	1157.5967
1163.4842	1166.6592	1176.6039
1206.2585	1338.4893	1411.4130
1815.1443	2450.2625	2480.7155
2488.0892	2501.9815	2560.1852
2642.5798	2697.3281	3900.9572

H_2

Zero-point correction =0.010163 (Hartree/Particle)
Thermal correction to Energy =0.012523
Thermal correction to Enthalpy = 0.013467
Thermal correction to Gibbs Free Energy =-0.001320
Sum of electronic and zero-point Energies =-1.158372
Sum of electronic and thermal Energies =-1.156011
Sum of electronic and thermal Enthalpies =-1.155067

Sum of electronic and thermal Free Energies =-1.169854
Cartesian coordinates

H	0.00000000	0.00000000	0.37037600
H	0.00000000	0.00000000	-0.37037600

Vibrational frequencies
4460.8708

$B_3H_8^-$

Zero-point correction = 0.083120
Thermal correction to Energy = 0.087968
Thermal correction to Enthalpy = 0.088913
Thermal correction to Gibbs Free Energy = 0.057491
Sum of electronic and zero-point Energies = -79.313443
Sum of electronic and thermal Energies = -79.308595
Sum of electronic and thermal Enthalpies = -79.307651
Sum of electronic and thermal Free Energies = -79.339072
Cartesian coordinates

B	0.911475	-0.538304	0.000007
H	1.312036	-1.027877	1.023825
H	1.312721	-1.028177	-1.023434
H	1.423177	0.612652	0.000330
B	-0.912136	-0.537606	-0.000098
H	0.001193	1.637764	-1.017620
H	-1.313152	-1.028527	-1.023051
H	-1.312604	-1.025186	1.024702
B	0.000646	0.997687	-0.000150
H	-1.423138	0.613698	-0.001562
H	-0.000158	1.636766	1.018014

Vibrational frequencies

165.5061	413.0538	538.1598
539.2852	702.6503	708.8468
795.5798	798.2173	823.2480
876.1470	982.7581	1022.2826
1070.5729	1153.2564	1160.6709
1163.3862	1193.5773	1272.3051
1423.2711	2218.2379	2256.0870
2496.8698	2503.6453	2536.2649
2544.9631	2552.8580	2573.8324

BH_4^- + DMS·BH_3

Zero-point correction = 0.145446
Thermal correction to Energy = 0.155916

Thermal correction to Enthalpy = 0.156860
Thermal correction to Gibbs Free Energy = 0.110983
Sum of electronic and zero-point Energies = -531.780166
Sum of electronic and thermal Energies = -531.769696
Sum of electronic and thermal Enthalpies = -531.768752
Sum of electronic and thermal Free Energies = -531.814629
Cartesian coordinates

B	2.543966	-0.100499	-0.138175
H	2.973096	-1.128213	0.326971
H	3.064572	0.887714	0.319853
H	2.451420	-0.100281	-1.343179
S	0.696657	-0.005769	0.519090
C	-0.127056	-1.331515	-0.385050
H	-1.201808	-1.264491	-0.211769
H	0.107079	-1.238513	-1.446065
H	0.264266	-2.273388	0.000060
C	0.048149	1.426541	-0.364333
H	0.269528	1.321934	-1.427123
H	-1.025453	1.487922	-0.191715
H	0.552539	2.306378	0.034878
B	-3.430411	0.003864	0.091814
H	-4.474185	0.616003	0.277596
H	-2.628820	0.262415	0.989707
H	-3.648438	-1.204892	0.082682
H	-2.944638	0.332733	-0.989234

Vibrational frequencies

68.2339	113.4201	138.7195
144.1977	171.5966	209.2355
234.0038	244.9656	253.9316
268.1111	286.7615	329.7988
518.3496	720.6231	760.7719
807.2701	822.7873	951.7914
1016.4346	1037.9040	1075.0433
1094.2086	1106.1390	1111.6850
1121.2240	1173.5967	1177.3630
1235.4422	1237.9116	1355.1086
1384.8527	1456.2531	1466.5408
1476.6463	1484.7030	2340.4998
2342.2970	2349.1048	2367.1639
2480.3817	2533.6113	2542.6500
3063.1439	3066.7790	3162.9999
3168.6000	3182.7418	3187.7695

TSV

Zero-point correction = 0.143219
Thermal correction to Energy = 0.154097
Thermal correction to Enthalpy = 0.155041
Thermal correction to Gibbs Free Energy = 0.107027
Sum of electronic and zero-point Energies = -531.749518
Sum of electronic and thermal Energies = -531.738640
Sum of electronic and thermal Enthalpies = -531.737696
Sum of electronic and thermal Free Energies = -531.785710
Cartesian coordinates

B	1.221884	-0.080768	0.586114
H	1.231572	-1.185842	1.040618
H	1.342129	0.860815	1.309450
H	1.181346	0.073465	-0.596281
S	-1.284867	-0.001304	0.590258
C	-1.482467	-1.349699	-0.595655
H	-2.469821	-1.321555	-1.059231
H	-0.699703	-1.290293	-1.354471
H	-1.369038	-2.285973	-0.048833
C	-1.443942	1.398618	-0.541242
H	-0.700867	1.315136	-1.336270
H	-2.450527	1.455572	-0.958583
H	-1.239645	2.304266	0.030856
B	4.134668	0.024921	-0.292417
H	5.227843	-0.202008	0.215951
H	4.043745	1.209872	-0.590541
H	3.974659	-0.677152	-1.284544
H	3.261878	-0.249727	0.540646

Vibrational frequencies

-360.4862	51.6089	74.2089
103.7708	127.3259	147.8130
162.3973	175.3202	204.5370
228.8060	254.9828	289.3144
292.7091	722.3022	753.2036
775.4403	795.0659	939.7400
978.6940	1002.7849	1009.5598
1071.5474	1088.4097	1095.0072
1116.7266	1149.9738	1159.3204
1210.9086	1228.1007	1360.1697
1386.5629	1459.5887	1465.2505
1476.3569	1484.6296	2270.0758
2345.6769	2378.6798	2382.4595
2564.2828	2664.8924	2686.1235

3053.6491	3059.2980	3144.0994
3151.5339	3159.8184	3163.2934

DMS·BH_3

Zero-point correction = 0.107978
Thermal correction to Energy = 0.114999
Thermal correction to Enthalpy = 0.115944
Thermal correction to Gibbs Free Energy = 0.078048
Sum of electronic and zero-point Energies = -504.509704
Sum of electronic and thermal Energies = -504.502683
Sum of electronic and thermal Enthalpies = -504.501738
Sum of electronic and thermal Free Energies = -504.539634
Cartesian coordinates

S	0.018092	0.000506	-0.544460
C	-0.819648	1.372227	0.275282
H	-0.698073	1.278054	1.354938
H	-0.344749	2.291725	-0.066204
H	-1.873614	1.380499	-0.002112
C	-0.794026	-1.386627	0.275025
H	-1.850837	-1.404660	0.009323
H	-0.312871	-2.298346	-0.078121
H	-0.661600	-1.298423	1.353899
B	1.795231	0.015459	0.310510
H	2.295170	1.028767	-0.105303
H	1.553968	0.015752	1.492635
H	2.309027	-0.992357	-0.102081

Vibrational frequencies

95.7667	185.4369	186.3346
228.2337	243.9873	283.1960
486.7816	711.7305	750.9414
809.5419	830.8052	945.0275
1003.6213	1023.8354	1070.3906
1117.0301	1170.8901	1173.5013
1357.8563	1385.5886	1454.1581
1459.3071	1466.1144	1472.2281
2498.5432	2560.7758	2573.9040
3070.9349	3073.4169	3171.4545
3172.8803	3180.2766	3182.2290

BH_3(μ-H)BH_3 + DMS·BH_3

Zero-point correction = 0.178233
Thermal correction to Energy = 0.191127

Thermal correction to Enthalpy = 0.192071
Thermal correction to Gibbs Free Energy = 0.140179
Sum of electronic and zero-point Energies = -558.387745
Sum of electronic and thermal Energies = -558.374851
Sum of electronic and thermal Enthalpies = -558.373907
Sum of electronic and thermal Free Energies = -558.425799
Cartesian coordinates

B	2.961163	-0.234924	0.323461
H	3.458125	-1.017559	-0.448840
H	2.686283	-0.704632	1.401669
H	3.539024	0.823592	0.375137
S	1.234804	0.211052	-0.498367
C	0.442067	1.218030	0.772718
H	-0.591503	1.411874	0.486995
H	0.494251	0.694632	1.727708
H	1.001255	2.152384	0.829408
C	0.303139	-1.325583	-0.328507
H	0.302436	-1.637271	0.715984
H	-0.712696	-1.172047	-0.686693
H	0.811200	-2.071322	-0.940479
B	-2.900603	0.798209	-0.827634
H	-2.956428	1.633185	0.034265
H	-1.840789	0.775678	-1.417492
H	-3.857000	0.790259	-1.566248
B	-2.986670	-0.793799	0.863708
H	-2.042826	-0.342776	1.459670
H	-2.863880	-1.978184	0.624265
H	-4.062532	-0.498727	1.315566
H	-2.962471	-0.438028	-0.399992

Vibrational frequencies

46.0507	83.0082	96.3730
103.2253	138.2876	160.3637
180.4002	197.1999	216.4816
236.1592	247.3476	259.1086
265.2530	292.8322	299.7914
514.3518	660.9136	720.5202
764.2854	815.9091	824.0980
825.0236	883.1109	952.4655
1003.9795	1005.7857	1027.6298
1069.4790	1071.6756	1117.5162
1130.9658	1177.8427	1180.8229
1181.0682	1182.2728	1189.1500
1210.2920	1352.0579	1380.3045

1455.0477	1462.7444	1468.4146
1476.5120	1534.1038	2218.9957
2463.1807	2472.1359	2486.5447
2505.9603	2536.4998	2543.8160
2547.8099	2570.8281	2574.2197
3067.2411	3073.6429	3168.4296
3170.6486	3181.9990	3192.8998

TSVI

Zero-point correction = 0.176309
Thermal correction to Energy = 0.189539
Thermal correction to Enthalpy = 0.190484
Thermal correction to Gibbs Free Energy = 0.136107
Sum of electronic and zero-point Energies = -558.355325
Sum of electronic and thermal Energies = -558.342095
Sum of electronic and thermal Enthalpies = -558.341150
Sum of electronic and thermal Free Energies = -558.395527
Cartesian coordinates

B	0.431803	-0.166721	-0.637541
H	0.506063	0.927530	-1.104799
H	0.447591	-1.123221	-1.349629
H	0.357602	-0.305111	0.544804
S	-2.180375	0.004020	-0.587214
C	-2.130962	1.432240	0.519087
H	-3.084559	1.560773	1.033828
H	-1.319636	1.318092	1.240275
H	-1.933474	2.313421	-0.092113
C	-2.437444	-1.296509	0.641783
H	-1.646651	-1.259433	1.393458
H	-3.415847	-1.201318	1.115812
H	-2.380844	-2.253841	0.122760
B	3.136105	0.023894	0.311172
H	2.924392	1.145085	0.694199
H	2.400499	-0.308596	-0.613084
H	3.197669	-0.818575	1.163489
B	5.412797	-0.025050	0.026592
H	5.931758	0.630536	-0.851918
H	5.677885	-1.201211	-0.032147
H	5.535778	0.462017	1.118444
H	4.194678	0.074531	-0.454291

Vibrational frequencies

-336.0714	31.1314	58.0132

79.2067	82.8108	94.8804
135.7534	146.3690	170.7934
192.8063	216.7169	218.4847
228.3522	280.8575	296.0391
304.2454	654.8202	716.2735
748.0944	768.8150	795.9792
835.6973	880.7068	941.6624
977.6169	1003.7971	1010.4764
1018.9628	1071.6302	1090.5220
1128.1145	1158.9739	1163.9654
1167.4557	1176.8510	1190.3762
1198.3428	1359.2340	1387.8126
1463.5150	1471.7356	1476.6688
1484.6130	1569.7336	2193.7822
2350.9037	2473.6096	2518.6439
2532.1794	2572.5625	2585.6004
2588.2374	2694.9928	2696.4978
3056.5002	3060.3257	3145.9811
3151.5783	3159.0766	3161.1626

$B_3H_{10}^-$

Zero-point correction = 0.100877
Thermal correction to Energy = 0.107949
Thermal correction to Enthalpy = 0.108893
Thermal correction to Gibbs Free Energy = 0.071816
Sum of electronic and zero-point Energies = -80.461533
Sum of electronic and thermal Energies = -80.454462
Sum of electronic and thermal Enthalpies = -80.453517
Sum of electronic and thermal Free Energies = -80.490595
Cartesian coordinates

B	-1.999059	-0.328655	-0.005211
H	-2.168436	-0.540404	-1.176870
H	-2.204522	-1.281452	0.709578
H	-2.469120	0.696660	0.408092
B	-0.017235	0.687595	0.003226
H	-0.375431	1.429862	-0.859549
H	-0.688642	-0.386061	0.201905
H	0.230991	1.153038	1.068709
B	2.010289	-0.326316	0.008615
H	2.378717	-0.982171	-0.938451
H	1.733708	-0.980255	0.976447
H	2.676308	0.654054	0.214860
H	0.916449	0.073611	-0.637869

Vibrational frequencies

84.0585	89.5769	199.7582
249.1660	270.8760	319.1510
516.4511	644.2260	772.6824
814.6184	903.1266	963.2127
1023.0316	1036.1624	1106.7772
1109.8883	1170.0165	1179.2299
1183.9846	1194.9296	1203.6651
1602.7749	1658.8760	2152.8442
2258.9802	2499.2879	2503.9085
2553.5696	2556.2833	2586.1943
2591.1966	2602.7351	2678.8606

TSVII

Zero-point correction = 0.098994
Thermal correction to Energy = 0.105660
Thermal correction to Enthalpy = 0.106604
Thermal correction to Gibbs Free Energy = 0.069666
Sum of electronic and zero-point Energies = -80.447707
Sum of electronic and thermal Energies = -80.441041
Sum of electronic and thermal Enthalpies = -80.440096
Sum of electronic and thermal Free Energies = -80.477034
Cartesian coordinates

B	-2.063770	-0.262728	-0.000254
H	-1.913798	-0.938546	-1.002334
H	-1.911114	-0.920188	1.013394
H	-3.122714	0.339136	-0.004193
B	1.701698	-0.552929	-0.000043
H	2.063924	0.628342	0.005304
H	1.978059	-1.086033	1.031959
H	1.987739	-1.079452	-1.032818
H	-1.168807	0.614697	-0.010513
B	0.522329	0.842387	0.000402
H	0.415610	-0.482383	-0.006329
H	0.439228	1.400167	-1.043468
H	0.430592	1.390610	1.048478

Vibrational frequencies

-428.5970	37.4719	120.7041
144.3261	322.6114	410.4389
441.0680	528.3307	813.1218
843.9350	941.0980	955.1283
982.6280	1078.8632	1079.9591
1118.1616	1133.6719	1143.3499

1174.8565	1193.3229	1215.0582
1301.9875	1817.5202	2139.3876
2202.5288	2394.8874	2415.5673
2441.8366	2445.7580	2580.4119
2646.1197	2647.5044	2741.5654

BH_4^- + B_2H_6

Zero-point correction = 0.100114
Thermal correction to Energy = 0.107605
Thermal correction to Enthalpy = 0.108550
Thermal correction to Gibbs Free Energy = 0.069238
Sum of electronic and zero-point Energies = -80.452952
Sum of electronic and thermal Energies = -80.445461
Sum of electronic and thermal Enthalpies = -80.444517
Sum of electronic and thermal Free Energies = -80.483828
Cartesian coordinates

B	-1.264622	0.874800	-0.000254
H	-1.269175	1.453761	1.035758
H	-1.256720	1.453783	-1.036167
B	-1.308969	-0.862461	-0.000230
H	-1.327561	-1.441860	-1.035869
H	-0.303275	-0.019121	0.005496
H	-2.276594	0.029719	-0.006184
H	-1.339985	-1.441330	1.035456
B	2.296996	-0.011812	0.000427
H	1.867898	-0.581664	1.000946
H	1.869465	-0.577364	-1.003195
H	1.896040	1.151921	0.002568
H	3.522887	-0.030480	0.001471

Vibrational frequencies

27.9383	69.7967	181.2808
182.0792	249.0170	250.9637
375.0659	835.7208	846.6799
864.8433	931.1921	962.7164
979.9143	1049.8177	1098.7136
1099.4178	1140.0173	1188.0877
1206.7641	1235.7456	1240.5400
1675.2478	1868.4775	2046.1537
2178.3733	2328.7635	2363.3530
2364.9701	2366.3696	2632.6233
2653.9540	2718.6970	2731.5331

TSVIII

Zero-point correction = 0.097292
Thermal correction to Energy = 0.103791
Thermal correction to Enthalpy = 0.104735
Thermal correction to Gibbs Free Energy = 0.069422
Sum of electronic and zero-point Energies = -80.405208
Sum of electronic and thermal Energies = -80.398709
Sum of electronic and thermal Enthalpies = -80.397765
Sum of electronic and thermal Free Energies = -80.433078
Cartesian coordinates

B	-0.248980	0.779853	-0.177486
H	1.397609	-1.283166	-0.727061
H	-0.588761	1.650501	-0.920281
H	-0.073656	1.582139	0.877752
B	1.652264	-0.376408	0.012704
H	2.704585	0.174923	-0.219444
H	0.996304	0.727576	-0.389216
H	1.461752	-0.577397	1.179985
B	-1.440633	-0.534176	-0.005919
H	-0.557758	0.840383	1.054922
H	-2.545640	-0.028318	0.142230
H	-1.398551	-1.136268	-1.064039
H	-1.209137	-1.296713	0.918656

Vibrational frequencies

-554.2799	105.6057	180.5064
212.0587	282.2164	316.3935
495.1987	651.5126	676.1198
788.0313	805.3937	863.0646
933.6084	985.3080	1018.0080
1089.0522	1113.0083	1168.2373
1176.8962	1184.8808	1188.2681
1252.0699	1635.8473	2214.2705
2285.2068	2357.5219	2403.5289
2425.5718	2484.6631	2563.1724
2589.5119	2605.0517	2656.4846

$[B_2H_4(\mu\text{-}H)BH_3]^- + H_2$

Zero-point correction = 0.098480
Thermal correction to Energy = 0.105331
Thermal correction to Enthalpy = 0.106276
Thermal correction to Gibbs Free Energy = 0.070415
Sum of electronic and zero-point Energies = -80.407247
Sum of electronic and thermal Energies = -80.400395
Sum of electronic and thermal Enthalpies = -80.399451

Sum of electronic and thermal Free Energies = -80.435311
Cartesian coordinates

B	0.202649	0.431646	0.200794
H	-2.164042	-1.096220	-0.861482
H	-0.031064	1.058415	1.182527
H	-0.193876	1.452817	-0.638025
B	-1.902254	-0.265084	-0.023466
H	-2.084666	-0.631077	1.105606
H	-0.579963	-0.450184	-0.259460
H	-2.332237	0.826182	-0.284153
B	1.780928	-0.319480	-0.023049
H	0.547246	1.116547	-0.877528
H	2.669524	0.491083	0.213669
H	1.825689	-1.224187	0.795543
H	1.936776	-0.778789	-1.148092

Vibrational frequencies

114.9375	185.7191	204.0525
266.7186	300.9342	357.1029
521.4821	651.9470	709.4120
769.9879	825.9542	845.4349
884.1508	1025.1070	1058.7532
1083.4217	1114.7736	1174.6881
1178.5407	1183.5140	1186.2908
1219.6015	1581.5441	2062.2588
2209.5723	2350.8950	2367.8560
2394.9382	2503.5138	2556.0993
2581.8533	2674.6892	3081.8441

TSIX

Zero-point correction = 0.095891
Thermal correction to Energy = 0.102621
Thermal correction to Enthalpy = 0.103566
Thermal correction to Gibbs Free Energy = 0.068011
Sum of electronic and zero-point Energies = -80.406747
Sum of electronic and thermal Energies = -80.400017
Sum of electronic and thermal Enthalpies = -80.399072
Sum of electronic and thermal Free Energies = -80.434627
Cartesian coordinates

B	-0.223280	0.354025	-0.280959
H	2.192928	-0.891384	1.051597
H	0.133850	0.873681	-1.289208
H	0.118405	1.910730	0.450289
B	1.857880	-0.299285	0.053452

H	1.765721	-1.000274	-0.919306
H	0.635695	-0.110906	0.550908
H	2.420267	0.750060	-0.114231
B	-1.733067	-0.349244	0.067679
H	-0.532638	1.624183	0.744177
H	-2.655189	0.305443	-0.401380
H	-1.665775	-1.421159	-0.530194
H	-1.920930	-0.567850	1.256485

Vibrational frequencies

-469.0900	115.1111	216.4443
239.4389	295.6292	300.5662
354.6624	587.6636	627.4039
662.0718	735.4231	762.1756
847.5326	979.7426	999.9265
1034.7246	1079.9458	1099.6692
1153.7894	1163.7845	1170.8544
1184.8429	1194.7606	1681.0856
2142.4486	2348.5915	2384.8301
2390.7741	2501.3350	2554.9644
2581.4032	2685.1693	4014.5981

$B_3H_8^-$(I)

Zero-point correction = 0.082064
Thermal correction to Energy = 0.087421
Thermal correction to Enthalpy = 0.088365
Thermal correction to Gibbs Free Energy = 0.055706
Sum of electronic and zero-point Energies = -79.283768
Sum of electronic and thermal Energies = -79.278412
Sum of electronic and thermal Enthalpies = -79.277468
Sum of electronic and thermal Free Energies = -79.310127
Cartesian coordinates

B	1.558226	-0.218183	-0.000054
H	2.188834	0.149922	0.989902
H	2.189176	0.149025	-0.990133
B	0.038397	0.546833	-0.000083
H	-0.803733	0.066097	-0.969834
B	-1.569096	-0.261804	-0.000001
H	-1.658102	-1.453293	-0.000287
H	-2.567126	0.397871	0.000277
H	-0.803322	0.065465	0.969752
H	1.472760	-1.443138	0.000738
H	-0.156119	1.733821	0.000270

Vibrational frequencies

166.7366	195.1495	336.2038
473.4417	594.7861	707.9866
797.0421	847.8346	859.5741
943.6669	944.7575	1048.1913
1052.4624	1106.8074	1159.2426
1162.1523	1185.5388	1633.7797
1687.8449	2115.4930	2215.9530
2324.3408	2332.0494	2343.7580
2553.3745	2586.5200	2647.3317

TSX

Zero-point correction = 0.080265
Thermal correction to Energy = 0.085225
Thermal correction to Enthalpy = 0.086170
Thermal correction to Gibbs Free Energy = 0.054361
Sum of electronic and zero-point Energies = -79.272268
Sum of electronic and thermal Energies = -79.267308
Sum of electronic and thermal Enthalpies = -79.266364
Sum of electronic and thermal Free Energies = -79.298172
Cartesian coordinates

B	-0.172912	-0.529464	-0.041349
H	0.692123	0.025232	0.831478
H	-0.034538	-1.718997	-0.036970
B	-1.571495	0.282896	-0.068334
H	-1.616251	1.478218	0.098780
H	-2.582966	-0.260213	-0.443975
H	-1.265746	-0.269502	1.072917
H	2.533250	-0.397642	0.404669
B	1.609539	0.233759	-0.040536
H	1.723269	1.428593	-0.073958
H	1.225197	-0.221640	-1.101846

Vibrational frequencies

-501.6197	195.7485	377.8858
447.8666	460.2991	512.6480
715.6272	798.5181	882.8767
937.7774	964.7945	1026.0610
1088.2989	1105.4691	1135.7048
1164.0915	1184.0883	1215.4776
1778.5562	1931.9804	2109.4123
2473.6892	2483.7740	2522.1228
2534.6978	2581.4530	2603.2705

$B_3H_8^-$(II)

Zero-point correction = 0.081271
Thermal correction to Energy = 0.086818
Thermal correction to Enthalpy = 0.087762
Thermal correction to Gibbs Free Energy = 0.054670
Sum of electronic and zero-point Energies = -79.273421
Sum of electronic and thermal Energies = -79.267874
Sum of electronic and thermal Enthalpies = -79.266930
Sum of electronic and thermal Free Energies = -79.300021
Cartesian coordinates

B	-0.285181	-0.611686	-0.001464
H	0.705836	-0.216867	0.731496
H	-0.204777	-1.792257	-0.172572
B	-1.554626	0.357886	-0.098616
H	-1.501119	1.516579	0.221721
H	-2.635671	-0.075810	-0.409294
H	-1.167065	-0.383332	1.010817
H	2.553595	-0.256733	0.577825
B	1.655050	0.242526	-0.062311
H	1.566117	1.437820	0.041463
H	1.606870	-0.173029	-1.189497

Vibrational frequencies

144.4406	239.6032	291.3045
423.1175	449.7434	706.4478
779.6560	798.8013	861.4335
915.5735	983.8874	1042.8796
1064.6643	1102.8819	1180.2460
1199.1951	1206.3242	1288.2621
1720.9070	1829.7765	2120.3602
2486.9472	2522.8701	2544.8056
2572.1098	2577.9305	2619.6241

TSXI

Zero-point correction = 0.080673
Thermal correction to Energy = 0.085669
Thermal correction to Enthalpy = 0.086613
Thermal correction to Gibbs Free Energy = 0.054641
Sum of electronic and zero-point Energies = -79.259249
Sum of electronic and thermal Energies = -79.254253
Sum of electronic and thermal Enthalpies = -79.253309
Sum of electronic and thermal Free Energies = -79.285281
Cartesian coordinates

B	0.296011	0.796327	0.040367
H	-0.629925	0.854152	0.825734

H	0.484260	1.805952	-0.574055
B	1.272337	-0.498073	-0.056961
H	1.113929	-1.480772	0.613387
H	2.264093	-0.465605	-0.737254
H	1.280732	0.561779	0.863415
H	-2.080619	-0.362519	0.938693
B	-1.437828	-0.297971	-0.083942
H	-1.180131	-1.380580	-0.535740
H	-1.904942	0.466180	-0.891499

Vibrational frequencies

-573.0641	175.8419	344.1600
390.2481	452.3914	633.8264
814.8191	821.7620	882.6058
917.8581	946.6616	984.7795
1058.7962	1103.8674	1146.9382
1190.6576	1208.4458	1231.6120
1332.1936	1993.6655	2471.7752
2497.8214	2526.4748	2543.3995
2558.5777	2585.3225	2596.7989

3.2. Solvent: THF.

$(CH_3)_2S\cdot BH_3$ + $(CH_3)_2S\cdot BH_3$

Zero-point correction = 0.217416
Thermal correction to Energy = 0.232973
Thermal correction to Enthalpy = 0.233917
Thermal correction to Gibbs Free Energy = 0.173771
Sum of electronic and zero-point Energies = -1009.029542
Sum of electronic and thermal Energies = -1009.013985
Sum of electronic and thermal Enthalpies = -1009.013041
Sum of electronic and thermal Free Energies = -1009.073187
Cartesian coordinates

S	1.918575	-0.065383	-0.197245
C	3.567818	-0.606527	-0.695701
H	4.260736	-0.476031	0.135823
H	3.498789	-1.660566	-0.960906
H	3.887316	-0.030544	-1.564535
C	2.303558	1.597202	0.391367
H	2.620007	2.211747	-0.451307
H	1.389503	2.003944	0.822398
H	3.085952	1.536625	1.148986
B	1.638640	-1.068589	1.465413
H	1.488993	-2.206294	1.092325

H	2.637555	-0.885155	2.116363
H	0.642410	-0.582653	1.939282
S	-2.675626	0.105525	-0.562140
C	-3.329833	-0.211522	1.090941
H	-2.498879	-0.295451	1.792104
H	-3.962466	0.634131	1.358833
H	-3.922734	-1.125701	1.075676
C	-1.564025	-1.307961	-0.724306
H	-2.154092	-2.223599	-0.759925
H	-1.016769	-1.187701	-1.658914
H	-0.875933	-1.322723	0.121913
B	-1.446566	1.599959	-0.237707
H	-2.181098	2.529567	-0.012660
H	-0.785950	1.247362	0.708020
H	-0.826005	1.706759	-1.265660

Vibrational frequencies

19.8857	54.2736	60.5741
75.9533	82.7250	99.6459
132.7975	178.2963	185.7513
196.4215	213.1132	224.4554
232.0837	238.2650	252.0029
257.8595	294.4650	298.7655
515.8542	517.5552	720.8408
722.0407	759.2548	760.5834
808.8838	812.3483	818.5573
829.0883	944.3420	957.9595
1002.3186	1007.7987	1026.6160
1028.1035	1063.1556	1073.9831
1107.9016	1114.4490	1173.3969
1175.6214	1178.7221	1188.9870
1355.2625	1359.1993	1378.2861
1386.4693	1446.7299	1449.4107
1452.2086	1454.0901	1457.8094
1461.0688	1463.4344	1467.8631
2488.8118	2494.9665	2544.2061
2548.1104	2552.8491	2561.3908
3067.3025	3068.7370	3071.7684
3073.8704	3169.7290	3171.0097
3173.2190	3175.3802	3176.7784
3182.8203	3187.1481	3188.9691

TSI

Zero-point correction = 0.216186

Thermal correction to Energy = 0.231404
Thermal correction to Enthalpy = 0.232348
Thermal correction to Gibbs Free Energy = 0.172519
Sum of electronic and zero-point Energies = -1009.002495
Sum of electronic and thermal Energies = -1008.987277
Sum of electronic and thermal Enthalpies = -1008.986333
Sum of electronic and thermal Free Energies = -1009.046162
Cartesian coordinates

S	2.627410	0.008809	-0.485024
C	4.294565	0.157557	0.194969
H	4.248188	0.120632	1.283597
H	4.875264	-0.682635	-0.183861
H	4.734809	1.094359	-0.144587
C	1.830041	1.386284	0.371067
H	2.362974	2.302539	0.117690
H	0.803084	1.447243	0.015073
H	1.850704	1.204174	1.445609
B	2.004352	-1.596574	0.448165
H	2.799913	-2.436301	0.117243
H	1.983276	-1.323528	1.617788
H	0.908840	-1.860394	-0.023993
S	-3.090305	0.070207	-0.631842
C	-2.738900	1.566829	0.322727
H	-2.083902	1.329946	1.163198
H	-2.235547	2.271740	-0.340028
H	-3.663421	2.018618	0.684697
C	-3.794583	-0.945699	0.690134
H	-4.704926	-0.490729	1.082506
H	-4.036679	-1.919580	0.263954
H	-3.064070	-1.078605	1.490446
B	-0.604259	-1.039221	-0.301019
H	-0.175060	-0.438380	-1.239522
H	-0.656786	-0.515823	0.769716
H	-1.087552	-2.118376	-0.458784

Vibrational frequencies

-322.8782	21.7675	35.7648
49.2174	70.6128	98.0695
123.6560	167.0979	185.3317
188.9149	208.6765	214.0199
228.5148	241.9635	251.2376
258.6488	277.8772	285.0454
307.4073	526.2098	710.3255
717.4756	720.3919	757.5070

769.6594	801.3594	817.1625
857.4475	934.6498	953.8915
969.7013	991.9145	1000.4355
1020.0975	1040.4846	1066.4665
1068.4527	1102.7670	1144.4864
1161.2919	1167.7420	1197.2544
1350.9170	1352.1501	1375.3105
1375.7712	1443.9688	1449.8104
1454.7381	1458.7989	1461.2287
1465.3238	1470.7979	1477.0735
2384.3865	2537.9362	2579.0943
2594.6923	2680.3615	2692.6969
3053.9559	3057.9880	3068.2580
3074.1730	3145.7072	3151.7199
3154.8792	3157.1393	3171.1070
3175.9348	3179.3086	3188.5302

$(CH_3)_2S$

Zero-point correction = 0.076173
Thermal correction to Energy = 0.081046
Thermal correction to Enthalpy = 0.081990
Thermal correction to Gibbs Free Energy = 0.049115
Sum of electronic and zero-point Energies = -477.907129
Sum of electronic and thermal Energies = -477.902256
Sum of electronic and thermal Enthalpies = -477.901312
Sum of electronic and thermal Free Energies = -477.934187
Cartesian coordinates

S	0.000002	0.663616	-0.000067
C	1.375005	-0.514830	0.000168
H	1.355387	-1.141236	-0.893311
H	2.300422	0.062263	0.000134
H	1.355296	-1.140989	0.893818
C	-1.375007	-0.514827	-0.000064
H	-1.355327	-1.141137	0.893479
H	-2.300422	0.062269	-0.000026
H	-1.355372	-1.141082	-0.893648

Vibrational frequencies

160.6987	191.4375	272.9580
720.2820	770.3654	945.3411
959.7087	991.7952	1070.5156
1362.4267	1385.3094	1456.6870
1462.1332	1463.9013	1472.5420
3062.7049	3066.0241	3149.2290

3155.4779	3157.5714	3159.0236

$(CH_3)_2BH_2(\mu\text{-}H)BH_3$

Zero-point correction = 0.141088
Thermal correction to Energy = 0.150151
Thermal correction to Enthalpy = 0.151095
Thermal correction to Gibbs Free Energy = 0.108078
Sum of electronic and zero-point Energies = -531.097375
Sum of electronic and thermal Energies = -531.088312
Sum of electronic and thermal Enthalpies = -531.087368
Sum of electronic and thermal Free Energies = -531.130385
Cartesian coordinates

S	0.535915	-0.003545	-0.551475
C	1.941300	-0.752822	0.303202
H	1.755027	-0.751559	1.377014
H	2.038982	-1.773454	-0.064202
H	2.838124	-0.184406	0.060234
C	0.486687	1.602522	0.276034
H	1.445362	2.094983	0.114426
H	-0.309237	2.187753	-0.180374
H	0.292931	1.459114	1.338954
B	-0.907834	-1.035931	0.267633
H	-0.688794	-2.165277	-0.064936
H	-0.912461	-0.805387	1.433356
H	-1.889401	-0.775045	-0.488124
B	-2.813989	0.047669	0.044628
H	-3.322616	0.165039	-1.041712
H	-2.339357	1.058739	0.476683
H	-3.442010	-0.610674	0.825550

Vibrational frequencies

51.4727	109.1965	152.3098
193.4013	232.2240	250.5289
260.8532	296.1059	323.2418
498.2444	579.0088	668.2377
715.0912	766.3256	798.8293
888.3333	959.8861	976.5808
1006.3841	1031.3574	1052.5283
1079.3017	1108.4108	1162.9719
1177.8581	1194.1396	1358.7755
1385.4211	1451.6116	1457.1739
1461.0910	1469.2732	1670.2879
2232.3547	2524.9338	2584.9681
2595.0582	2615.8579	2683.6264

3077.2565	3080.1930	3182.3306
3184.8493	3191.1747	3191.4115

TSII

Zero-point correction = 0.140598
Thermal correction to Energy = 0.149220
Thermal correction to Enthalpy = 0.150164
Thermal correction to Gibbs Free Energy = 0.108045
Sum of electronic and zero-point Energies = -531.088492
Sum of electronic and thermal Energies = -531.079870
Sum of electronic and thermal Enthalpies = -531.078926
Sum of electronic and thermal Free Energies = -531.121045
Cartesian coordinates

S	0.684293	0.034312	-0.614917
C	1.707619	-1.117022	0.327349
H	1.357054	-1.157960	1.359991
H	1.608033	-2.099954	-0.132776
H	2.750313	-0.802649	0.290778
C	0.945295	1.538365	0.351981
H	1.973090	1.882482	0.239905
H	0.265547	2.299648	-0.031758
H	0.719712	1.342179	1.401197
B	-1.348164	-0.681391	0.332568
H	-1.266838	-1.766311	-0.142127
H	-0.963469	-0.409942	1.423711
H	-1.785099	0.295767	-0.438658
B	-3.000399	0.119030	-0.027013
H	-3.587149	-0.189178	-1.020084
H	-3.264157	1.149946	0.516016
H	-2.930396	-0.809271	0.768714

Vibrational frequencies

-381.5994	62.9639	123.4338
178.3287	219.0977	232.6561
240.6038	281.5020	319.8917
386.9023	438.6160	718.9208
771.5563	796.0211	848.6284
938.5212	948.6567	981.3167
1005.7657	1019.0421	1038.0051
1071.5994	1112.2372	1147.8581
1174.1670	1237.5041	1354.9576
1380.6043	1452.7641	1460.1706
1467.6190	1472.3502	1841.5973
2110.7593	2451.4180	2584.6661

2638.3529	2648.0375	2736.9152
3066.9299	3070.3399	3163.4289
3167.2585	3172.7955	3180.4760

B_2H_6

Zero-point correction = 0.063142
Thermal correction to Energy = 0.066750
Thermal correction to Enthalpy = 0.067694
Thermal correction to Gibbs Free Energy = 0.040013
Sum of electronic and zero-point Energies = -53.189578
Sum of electronic and thermal Energies = -53.185970
Sum of electronic and thermal Enthalpies = -53.185026
Sum of electronic and thermal Free Energies = -53.212707
Cartesian coordinates

B	-0.874206	0.000054	-0.000004
H	-1.450932	1.035967	0.000105
H	-1.450852	-1.035932	-0.000095
B	0.874195	0.000056	0.000001
H	1.450915	-1.035888	-0.000135
H	0.000009	-0.000179	-0.980067
H	0.000028	-0.000509	0.980141
H	1.450886	1.035994	0.000067

Vibrational frequencies

334.8457	818.8099	856.3643
890.0867	916.4785	954.3785
987.2047	1050.2024	1174.2816
1195.0240	1678.7295	1872.2070
2037.1136	2184.8761	2639.3777
2659.9181	2727.8909	2738.4438

B_2H_6 + DMS

Zero-point correction = 0.141099
Thermal correction to Energy = 0.150853
Thermal correction to Enthalpy = 0.151797
Thermal correction to Gibbs Free Energy = 0.106187
Sum of electronic and zero-point Energies = -531.099401
Sum of electronic and thermal Energies = -531.089647
Sum of electronic and thermal Enthalpies = -531.088703
Sum of electronic and thermal Free Energies = -531.134313
Cartesian coordinates

B	-2.529425	0.671091	0.521863
H	-2.942290	1.719018	0.150008

H	-2.250458	0.482259	1.660365
B	-2.312237	-0.628268	-0.622780
H	-1.898861	-1.666778	-0.226999
H	-3.346032	-0.269266	0.120469
H	-1.509462	0.336351	-0.230253
H	-2.590180	-0.453807	-1.761856
S	1.216765	-0.184120	-0.616641
C	0.948639	-1.197954	0.860371
H	0.018709	-0.916046	1.358386
H	0.881648	-2.239137	0.543361
H	1.783292	-1.092165	1.555061
C	1.211003	1.444860	0.176894
H	2.033888	1.528104	0.888278
H	1.338036	2.197373	-0.602093
H	0.263931	1.624465	0.692524

Vibrational frequencies

62.6083	63.3477	103.8353
124.1524	158.5065	180.6552
186.9408	218.0319	277.6592
378.0612	725.5716	779.3101
823.7690	861.4724	880.9932
922.3295	928.6682	965.4857
970.8924	987.5118	1004.1964
1058.0137	1064.1373	1174.4403
1197.5648	1352.4780	1379.9768
1451.9987	1457.8410	1470.4046
1479.0964	1669.4462	1860.6487
2038.8431	2180.1950	2645.7322
2669.7152	2735.1709	2753.6307
3047.1962	3054.5905	3130.3231
3137.5499	3155.8303	3166.3217

$BH_4^- + B_2H_6$

Zero-point correction = 0.099961
Thermal correction to Energy = 0.107428
Thermal correction to Enthalpy = 0.108372
Thermal correction to Gibbs Free Energy = 0.069895
Sum of electronic and zero-point Energies = -80.482605
Sum of electronic and thermal Energies = -80.475139
Sum of electronic and thermal Enthalpies = -80.474194
Sum of electronic and thermal Free Energies = -80.512672
Cartesian coordinates

B	1.264622	0.874800	0.001899

H	1.313431	1.453372	-1.034182
H	1.211465	1.454172	1.037433
B	1.308971	-0.862461	0.001667
H	1.283311	-1.444472	1.036449
H	0.303410	-0.019137	-0.042536
H	2.276444	0.029737	0.051326
H	1.384241	-1.438719	-1.033571
B	-2.296996	-0.011812	-0.003641
H	-1.868759	-0.587039	-1.001603
H	-1.868624	-0.571986	1.002543
H	-1.895012	1.151918	-0.011956
H	-3.522893	-0.030479	-0.003530

Vibrational frequencies

65.9230	106.4329	146.7946
176.9297	217.6932	240.9004
370.9980	833.6029	857.4716
883.7996	922.6462	966.5270
987.0054	1059.2605	1098.1687
1100.4530	1117.2244	1178.2679
1199.8119	1232.2835	1237.9047
1664.1117	1866.7132	2053.1603
2175.2262	2322.6107	2357.2420
2359.9395	2361.7811	2627.5275
2650.1229	2714.1077	2725.2233

TSIII

Zero-point correction = 0.094805
Thermal correction to Energy = 0.101778
Thermal correction to Enthalpy = 0.102722
Thermal correction to Gibbs Free Energy = 0.065147
Sum of electronic and zero-point Energies = -80.433506
Sum of electronic and thermal Energies = -80.426534
Sum of electronic and thermal Enthalpies = -80.425590
Sum of electronic and thermal Free Energies = -80.463164
Cartesian coordinates

B	-2.050092	-0.022803	0.044350
H	-3.016645	-0.505212	-0.494966
H	-1.199980	-0.726839	-0.664381
H	-1.915330	-0.326620	1.199395
B	1.311443	-0.761895	0.017801
H	2.221313	0.216970	0.130427
H	1.316354	-1.386916	1.045309
H	1.562660	-1.374514	-0.987015

H	-1.879648	1.143324	-0.196821
B	1.034452	0.848815	-0.005649
H	-0.490384	-0.311369	-0.292560
H	1.080204	1.481853	-1.027746
H	0.842444	1.468736	1.005846

Vibrational frequencies

-814.7548	36.1835	130.5407
173.7206	179.7024	250.8855
513.8826	584.6539	828.6934
834.5619	900.0778	905.7868
933.7691	969.8858	1013.2301
1033.1261	1044.1483	1114.7838
1170.7804	1192.3480	1206.4256
1212.1128	1466.6485	1817.4015
1972.2518	2296.6528	2504.5091
2511.4661	2548.1783	2555.2717
2560.6323	2575.2627	2577.1315

$B_2H_5^-$ + (η^2-H_2)BH_3

Zero-point correction = 0.097099
Thermal correction to Energy = 0.105042
Thermal correction to Enthalpy = 0.105986
Thermal correction to Gibbs Free Energy = 0.066231
Sum of electronic and zero-point Energies = -80.434404
Sum of electronic and thermal Energies = -80.426462
Sum of electronic and thermal Enthalpies = -80.425517
Sum of electronic and thermal Free Energies = -80.465272
Cartesian coordinates

B	-2.422554	0.001339	-0.086565
H	-2.784579	0.639247	0.857035
H	-1.994490	0.640992	-1.005949
H	-3.078595	-0.946195	-0.407737
B	1.276404	0.831141	-0.008582
H	2.177207	0.162139	0.762466
H	1.902270	1.651605	-0.635668
H	0.447911	1.286550	0.745320
H	-1.486917	-0.785682	0.550071
B	1.610730	-0.751636	-0.069461
H	-1.059293	-0.293977	0.069089
H	1.047775	-1.559189	0.633348
H	2.505809	-1.199708	-0.744934

Vibrational frequencies

54.9905	107.4152	123.2148
135.0902	162.4701	199.4839
443.5258	513.0684	817.2225
839.3796	872.8657	885.0556
897.4329	977.2850	1024.8750
1047.6536	1094.8709	1167.3481
1199.7990	1206.2490	1210.6283
1237.7502	1372.8525	1764.2960
1870.4851	2473.8634	2506.5677
2513.7797	2530.1878	2559.1944
2634.9996	2653.1776	3524.6004

TSIV

Zero-point correction = 0.092095
Thermal correction to Energy = 0.100615
Thermal correction to Enthalpy = 0.101559
Thermal correction to Gibbs Free Energy = 0.061088
Sum of electronic and zero-point Energies = -80.424414
Sum of electronic and thermal Energies = -80.415895
Sum of electronic and thermal Enthalpies = -80.414951
Sum of electronic and thermal Free Energies = -80.455421
Cartesian coordinates

B	2.286570	0.189921	-0.335929
H	3.163747	-0.527975	0.023221
H	1.435382	-1.763608	1.469606
H	1.782898	0.026561	-1.398309
B	-1.547089	-0.549220	-0.440080
H	-2.325913	0.303029	0.277768
H	-1.917011	-0.469405	-1.587814
H	-1.670438	-1.640134	0.065957
H	1.958859	1.108501	0.342694
B	-1.036054	0.738420	0.398498
H	0.814867	-1.456534	1.196228
H	-0.761465	0.674844	1.574423
H	-0.998062	1.849117	-0.076214

Vibrational frequencies

-189.0849	65.9533	109.8566
129.1758	139.2659	151.7465
242.5255	293.0642	370.5857
509.8509	543.6794	788.7950
806.9276	843.7020	881.3012
896.3835	977.8799	1048.1671
1121.0953	1161.9037	1195.1357

1204.4023	1206.7004	1365.5904
1852.3693	2474.1312	2508.4625
2510.5138	2524.4968	2617.1142
2724.3443	2748.1266	4411.8424

TSIV'

Zero-point correction = 0.095584
Thermal correction to Energy = 0.102632
Thermal correction to Enthalpy = 0.103576
Thermal correction to Gibbs Free Energy = 0.066530
Sum of electronic and zero-point Energies = -80.429144
Sum of electronic and thermal Energies = -80.422097
Sum of electronic and thermal Enthalpies = -80.421152
Sum of electronic and thermal Free Energies = -80.458199
Cartesian coordinates

B	1.970760	-0.049623	0.039212
H	1.673072	1.105276	0.034694
H	1.852381	-0.649498	-0.995404
H	1.892912	-0.686462	1.048938
B	-1.325529	0.822578	-0.005762
H	-2.473319	0.096534	-0.205969
H	-1.518229	1.497820	0.981739
H	-1.121865	1.442285	-1.026753
H	3.449256	0.259292	0.302997
B	-1.459674	-0.791012	0.011874
H	3.420499	-0.110053	-0.384927
H	-1.347500	-1.457775	-0.994414
H	-1.754994	-1.407133	1.012475

Vibrational frequencies

-149.2422	115.8973	121.0883
157.3320	208.4799	246.7705
503.7072	526.5672	543.9145
793.3113	835.2263	878.1022
903.3409	929.1150	976.3287
1012.4514	1048.8338	1157.0201
1164.0274	1172.4973	1183.0837
1208.9233	1322.7483	1423.9986
1822.7207	2452.2420	2484.1598
2491.0432	2502.6659	2557.5293
2636.6869	2687.0766	3889.6861

H_2

Zero-point correction = 0.010162
Thermal correction to Energy = 0.012522
Thermal correction to Enthalpy = 0.013466
Thermal correction to Gibbs Free Energy = -0.001320
Sum of electronic and zero-point Energies = -1.157684
Sum of electronic and thermal Energies = -1.155324
Sum of electronic and thermal Enthalpies = -1.154380
Sum of electronic and thermal Free Energies = -1.169166

Cartesian coordinates

H	0.000000	0.000000	0.370376
H	0.000000	0.000000	-0.370376

Vibrational frequencies
4460.5004

$B_3H_8^-$

Zero-point correction = 0.083331
Thermal correction to Energy = 0.088124
Thermal correction to Enthalpy = 0.089069
Thermal correction to Gibbs Free Energy = 0.057786
Sum of electronic and zero-point Energies = -79.338604
Sum of electronic and thermal Energies = -79.333811
Sum of electronic and thermal Enthalpies = -79.332867
Sum of electronic and thermal Free Energies = -79.364150
Cartesian coordinates

B	0.911473	-0.538307	0.000007
H	1.312033	-1.027881	1.023825
H	1.312718	-1.028181	-1.023434
H	1.423179	0.612648	0.000330
B	-0.912138	-0.537603	-0.000098
H	0.001198	1.637764	-1.017620
H	-1.313155	-1.028523	-1.023051
H	-1.312607	-1.025182	1.024702
B	0.000649	0.997687	-0.000150
H	-1.423136	0.613702	-0.001562
H	-0.000153	1.636766	1.018014

Vibrational frequencies

186.9607	422.0440	539.4918
540.6254	700.6161	716.4494
798.3789	806.4464	821.0250
881.6059	991.6920	1029.8899
1069.6160	1153.8506	1168.1755

1168.6364	1201.0340	1274.5156
1424.0542	2224.0403	2255.6507
2495.5174	2502.4464	2537.2050
2543.9076	2550.6956	2573.6945

BH_4^- + DMS·BH_3

Zero-point correction = 0.144509
Thermal correction to Energy = 0.155575
Thermal correction to Enthalpy = 0.156519
Thermal correction to Gibbs Free Energy = 0.107825
Sum of electronic and zero-point Energies = -531.809402
Sum of electronic and thermal Energies = -531.798336
Sum of electronic and thermal Enthalpies = -531.797392
Sum of electronic and thermal Free Energies = -531.846086
Cartesian coordinates

B	-2.559950	-0.102528	0.107730
H	-2.970329	-1.141488	-0.346916
H	-3.083181	0.872034	-0.373851
H	-2.490334	-0.082544	1.313125
S	-0.704298	-0.003950	-0.515501
C	0.095910	-1.335613	0.402722
H	1.170295	-1.289709	0.229123
H	-0.135809	-1.228635	1.462675
H	-0.306458	-2.274844	0.023582
C	-0.075427	1.431359	0.379521
H	-0.287585	1.310362	1.442165
H	0.994727	1.520833	0.201247
H	-0.596157	2.306333	-0.008854
B	3.518416	0.001744	-0.103239
H	4.547208	0.642583	-0.272241
H	2.727569	0.238181	-1.011671
H	3.775029	-1.196453	-0.092898
H	3.008558	0.315988	0.966614

Vibrational frequencies

16.8169	83.0406	100.4574
140.3302	171.2096	176.1710
191.6645	214.7613	231.2431
239.8515	252.8824	280.0017
519.4943	718.8802	759.6712
807.1167	816.9630	944.8024
1009.6117	1031.0234	1064.1489
1095.7375	1100.5662	1108.1202
1109.4592	1176.1411	1178.8983

1229.5906	1236.5645	1349.7950
1376.6159	1445.9956	1456.1255
1461.8307	1467.4214	2358.0587
2362.3402	2365.8882	2373.4270
2483.6831	2535.4611	2545.9715
3065.1503	3069.3368	3167.6365
3172.0341	3181.3671	3188.8417

TSV

Zero-point correction = 0.143346
Thermal correction to Energy = 0.154099
Thermal correction to Enthalpy = 0.155043
Thermal correction to Gibbs Free Energy = 0.107606
Sum of electronic and zero-point Energies = -531.783240
Sum of electronic and thermal Energies = -531.772487
Sum of electronic and thermal Enthalpies = -531.771543
Sum of electronic and thermal Free Energies = -531.818980
Cartesian coordinates

B	-1.306645	-0.079633	-0.532109
H	-1.291771	-1.203178	-0.937980
H	-1.415617	0.830107	-1.296760
H	-1.211838	0.130237	0.639339
S	1.278982	-0.001504	-0.598823
C	1.495886	-1.355428	0.580544
H	2.494140	-1.327304	1.018888
H	0.735857	-1.290742	1.361466
H	1.368605	-2.291274	0.036232
C	1.482362	1.396319	0.531363
H	0.756728	1.322293	1.343033
H	2.497174	1.427559	0.929454
H	1.289254	2.307762	-0.035035
B	-4.120229	0.033167	0.286846
H	-5.150576	-0.262854	-0.299713
H	-4.096893	1.226009	0.545584
H	-3.999342	-0.631363	1.304141
H	-3.174554	-0.226203	-0.472602

Vibrational frequencies

-425.8532	64.0081	84.7656
113.3651	134.9739	159.0089
165.7427	181.1061	195.1961
218.5292	269.5859	286.9593
303.4745	720.2618	770.1969
801.9974	811.9867	933.9217

980.8309	982.6174	1008.2395
1064.0058	1084.8624	1091.9669
1117.0769	1156.0129	1162.4027
1211.2724	1227.9938	1354.5852
1378.1979	1451.7425	1457.4939
1465.7374	1475.0081	2219.8741
2381.6693	2400.4918	2406.6327
2560.3777	2662.9798	2672.3238
3054.9165	3058.4448	3146.9805
3152.9215	3158.7432	3160.3064

DMS·BH_3

Zero-point correction = 0.107701
Thermal correction to Energy = 0.114783
Thermal correction to Enthalpy = 0.115727
Thermal correction to Gibbs Free Energy = 0.077623
Sum of electronic and zero-point Energies = -504.513032
Sum of electronic and thermal Energies = -504.505951
Sum of electronic and thermal Enthalpies = -504.505007
Sum of electronic and thermal Free Energies = -504.543111
Cartesian coordinates

S	-0.017002	-0.000253	-0.541551
C	0.810384	-1.380250	0.274512
H	0.693350	-1.282096	1.354123
H	0.330793	-2.296928	-0.068377
H	1.862841	-1.388796	-0.006685
C	0.802475	1.384753	0.274370
H	1.856806	1.393510	0.000265
H	0.324190	2.299364	-0.075596
H	0.678486	1.290959	1.353559
B	-1.794491	-0.004693	0.306759
H	-2.306435	-1.012905	-0.109097
H	-1.565899	-0.009106	1.491186
H	-2.306806	1.006487	-0.101657

Vibrational frequencies

87.8181	173.2941	176.8263
224.0838	243.1282	280.1673
498.7042	710.1589	748.3708
807.2041	824.7004	946.0416
1003.1203	1021.6531	1067.9395
1109.9238	1169.7476	1174.4113
1354.2024	1379.5003	1444.5881
1449.4313	1453.5977	1459.2712

2491.8583	2549.3193	2560.7098
3071.8497	3074.5755	3173.0054
3174.3249	3184.9351	3187.0079

$BH_3(\mu\text{-}H)BH_3$ + DMS·BH_3

Zero-point correction = 0.177999
Thermal correction to Energy = 0.191030
Thermal correction to Enthalpy = 0.191974
Thermal correction to Gibbs Free Energy = 0.139525
Sum of electronic and zero-point Energies = -558.410656
Sum of electronic and thermal Energies = -558.397625
Sum of electronic and thermal Enthalpies = -558.396681
Sum of electronic and thermal Free Energies = -558.449130
Cartesian coordinates

B	-2.990522	0.221695	0.284960
H	-3.468148	1.024354	-0.477940
H	-2.748486	0.664612	1.381796
H	-3.570910	-0.835929	0.295534
S	-1.244122	-0.199622	-0.497347
C	-0.483808	-1.226573	0.778211
H	0.548462	-1.438018	0.502972
H	-0.537434	-0.705794	1.734533
H	-1.056321	-2.153130	0.823032
C	-0.334087	1.343745	-0.270734
H	-0.358336	1.624364	0.782481
H	0.688859	1.210300	-0.617183
H	-0.837118	2.100528	-0.872642
B	2.940723	-0.760893	-0.866743
H	3.007793	-1.626936	-0.038045
H	1.882219	-0.742635	-1.456583
H	3.899640	-0.708064	-1.599078
B	3.074931	0.738738	0.866911
H	2.144358	0.296714	1.489436
H	2.995338	1.936311	0.692994
H	4.158600	0.384159	1.251144
H	2.939156	0.462384	-0.405406

Vibrational frequencies

54.9567	65.3248	83.6962
99.0701	119.2964	143.4101
162.1814	198.1050	232.0049
239.7852	244.7185	247.1360
261.3413	291.7276	304.7508
520.8384	663.9410	719.5553

763.3799	816.1219	820.3972
822.1331	879.9252	952.0285
999.2762	1006.2651	1026.5150
1055.6024	1067.2343	1115.8885
1125.1380	1175.8121	1180.1323
1182.8338	1183.0558	1190.0178
1204.3793	1353.3564	1378.3526
1448.3841	1455.7164	1459.3974
1466.2400	1570.1689	2211.7875
2467.9161	2475.9184	2488.1652
2513.0984	2532.0852	2542.8843
2547.5940	2566.3594	2571.0556
3069.7972	3074.5477	3173.1191
3174.3262	3184.0285	3190.3947

TSVI

Zero-point correction = 0.175589
Thermal correction to Energy = 0.188995
Thermal correction to Enthalpy = 0.189939
Thermal correction to Gibbs Free Energy = 0.135131
Sum of electronic and zero-point Energies = -558.382554
Sum of electronic and thermal Energies = -558.369148
Sum of electronic and thermal Enthalpies = -558.368204
Sum of electronic and thermal Free Energies = -558.423012
Cartesian coordinates

B	0.518295	0.007676	-0.559276
H	0.532968	1.043541	-1.151690
H	0.561511	-1.023363	-1.158741
H	0.402378	0.002209	0.628538
S	-2.140521	-0.014086	-0.603292
C	-2.322284	1.372472	0.544613
H	-3.320314	1.381036	0.984408
H	-1.563803	1.308657	1.326910
H	-2.172199	2.291936	-0.021697
C	-2.320442	-1.378848	0.570189
H	-1.555408	-1.306480	1.345365
H	-3.314705	-1.373316	1.018573
H	-2.181189	-2.309214	0.019205
B	3.133015	0.090507	0.370438
H	3.031538	1.118826	0.983593
H	2.338906	0.023464	-0.565178
H	3.139608	-0.915827	1.021419
B	5.361908	-0.069253	-0.025069

H	5.909839	0.753340	-0.723457
H	5.543625	-1.205566	-0.384624
H	5.537053	0.116481	1.148656
H	4.148801	0.213254	-0.437885

Vibrational frequencies

-369.1173	39.7789	61.7140
68.6545	81.9916	91.9638
122.9235	130.0324	160.6038
170.1758	174.3737	208.4550
232.4926	281.8849	293.5308
313.2036	661.8521	719.8483
768.2642	787.8700	791.1425
826.6116	882.5796	931.0434
975.2040	990.3581	1001.5301
1008.0704	1061.2163	1079.4551
1128.2772	1142.8443	1158.8935
1160.1289	1175.6080	1182.7600
1203.7810	1352.7533	1376.0754
1449.0957	1455.5493	1462.5382
1469.0659	1600.1269	2173.9695
2335.7789	2481.6850	2524.6671
2538.7254	2566.2631	2567.7689
2594.7945	2671.6433	2675.8871
3050.7814	3054.8164	3142.5906
3147.8839	3155.0708	3158.0037

$B_3H_{10}^-$

Zero-point correction = 0.101030
Thermal correction to Energy = 0.108116
Thermal correction to Enthalpy = 0.109061
Thermal correction to Gibbs Free Energy = 0.071929
Sum of electronic and zero-point Energies = -80.483031
Sum of electronic and thermal Energies = -80.475944
Sum of electronic and thermal Enthalpies = -80.475000
Sum of electronic and thermal Free Energies = -80.512131

Cartesian coordinates

B	1.979976	-0.329297	0.004690
H	2.172105	-0.520094	1.175357
H	2.180669	-1.291465	-0.695619
H	2.442296	0.687986	-0.433557
B	0.017303	0.688853	-0.002674
H	0.378973	1.442335	0.847507
H	0.671818	-0.398833	-0.175847

H	-0.222817	1.142152	-1.074740
B	-1.991359	-0.326607	-0.008074
H	-2.371947	-0.962253	0.945419
H	-1.689377	-1.004055	-0.951274
H	-2.667838	0.633921	-0.259172
H	-0.923485	0.105557	0.652217

Vibrational frequencies

77.9657	92.1161	190.1388
250.3605	273.9731	323.3465
514.1956	651.5318	765.1322
807.2866	904.8504	961.0121
1019.3449	1032.4897	1104.9544
1105.0137	1170.7098	1182.2116
1184.6064	1193.6731	1202.0199
1623.7308	1681.4280	2151.1786
2261.6195	2510.2843	2511.1808
2561.7800	2565.2004	2589.5781
2593.5393	2608.9538	2681.4412

TSVII

Zero-point correction = 0.098838
Thermal correction to Energy = 0.105580
Thermal correction to Enthalpy = 0.106524
Thermal correction to Gibbs Free Energy = 0.069282
Sum of electronic and zero-point Energies = -80.472187
Sum of electronic and thermal Energies = -80.465445
Sum of electronic and thermal Enthalpies = -80.464501
Sum of electronic and thermal Free Energies = -80.501742
Cartesian coordinates

B	-2.049922	-0.268177	-0.000151
H	-1.879169	-0.959919	-0.986118
H	-1.916125	-0.904090	1.028145
H	-3.105942	0.335739	-0.036269
B	1.703448	-0.545472	-0.000068
H	2.067442	0.631560	0.004446
H	1.977448	-1.082791	1.030681
H	1.982027	-1.076629	-1.032830
H	-1.156489	0.612438	-0.007980
B	0.499872	0.840877	0.000245
H	0.417205	-0.483797	-0.002536
H	0.426476	1.397907	-1.044737
H	0.420138	1.393441	1.047073

Vibrational frequencies

-477.5982	35.6391	94.5557
142.7098	319.1180	411.9709
439.7591	510.3780	813.5164
846.3966	939.9822	945.5790
982.5501	1075.7821	1080.3008
1113.4761	1128.3328	1143.5327
1174.0915	1192.8956	1220.0030
1284.8449	1818.0915	2137.9602
2193.6640	2414.1905	2418.4624
2445.7197	2450.2460	2580.4408
2644.3737	2646.6030	2739.6994

BH_4^- + B_2H_6

Zero-point correction = 0.099886
Thermal correction to Energy = 0.107401
Thermal correction to Enthalpy = 0.108345
Thermal correction to Gibbs Free Energy = 0.069647
Sum of electronic and zero-point Energies = -80.482685
Sum of electronic and thermal Energies = -80.475170
Sum of electronic and thermal Enthalpies = -80.474226
Sum of electronic and thermal Free Energies = -80.512924
Cartesian coordinates

B	-1.264630	0.874790	0.001393
H	-1.224932	1.454140	1.037068
H	-1.301989	1.453384	-1.034625
B	-1.308966	-0.862472	0.001209
H	-1.371811	-1.439260	-1.035022
H	-0.303376	-0.019135	-0.031543
H	-2.276483	0.029714	0.038961
H	-1.295721	-1.443952	1.037076
B	2.296998	-0.011794	-0.002788
H	1.867055	-0.576273	1.000299
H	1.870323	-0.582725	-1.003860
H	1.897019	1.151935	-0.006827
H	3.522903	-0.030450	-0.000591

Vibrational frequencies

64.0568	87.8707	146.0692
179.7318	216.6315	236.8580
368.3109	833.5517	856.1440
882.4472	922.5063	965.0916
985.7801	1057.1633	1098.0475
1101.1982	1116.6021	1178.0179
1199.7025	1233.5715	1236.7990

1663.4623	1866.0809	2052.6736
2175.2447	2327.0809	2357.4075
2360.2337	2361.5886	2627.0520
2649.7099	2713.4337	2724.8317

TSVIII

Zero-point correction = 0.097460
Thermal correction to Energy = 0.103908
Thermal correction to Enthalpy = 0.104853
Thermal correction to Gibbs Free Energy = 0.069708
Sum of electronic and zero-point Energies = -80.433621
Sum of electronic and thermal Energies = -80.427173
Sum of electronic and thermal Enthalpies = -80.426229
Sum of electronic and thermal Free Energies = -80.461373
Cartesian coordinates

B	-0.201877	0.750691	-0.156461
H	1.435055	-0.756224	-1.093318
H	-0.256000	1.424524	-1.136579
H	-0.363443	1.778194	0.695150
B	1.640312	-0.368791	0.021530
H	2.690305	0.219874	0.136100
H	0.977020	0.753897	0.322236
H	1.415448	-1.154386	0.899679
B	-1.418621	-0.546409	-0.002921
H	-0.910302	1.083681	0.860027
H	-2.537638	-0.072476	-0.151886
H	-1.183591	-1.324134	-0.910094
H	-1.365922	-1.130398	1.067946

Vibrational frequencies

-497.9241	123.3472	162.5773
230.7190	271.7481	334.0134
495.2875	652.7331	685.6709
792.9598	809.1733	867.4462
939.2910	970.1680	1050.6393
1087.8753	1110.1936	1176.2333
1179.0792	1191.8340	1194.6944
1255.7982	1683.0885	2183.8874
2222.8193	2357.6798	2390.0694
2414.6323	2491.7545	2561.9805
2605.9886	2615.9160	2670.9068

$[B_2H_4(\mu\text{-}H)BH_3]^- + H_2$

Zero-point correction = 0.099148
Thermal correction to Energy = 0.105786
Thermal correction to Enthalpy = 0.106730
Thermal correction to Gibbs Free Energy = 0.071452
Sum of electronic and zero-point Energies = -80.433935
Sum of electronic and thermal Energies = -80.427297
Sum of electronic and thermal Enthalpies = -80.426353
Sum of electronic and thermal Free Energies = -80.461631
Cartesian coordinates

B	0.202756	0.443822	0.191980
H	-2.165528	-1.044176	-0.912982
H	-0.042365	1.010098	1.206768
H	-0.190043	1.516478	-0.575832
B	-1.885706	-0.275037	-0.024255
H	-2.020284	-0.734229	1.076927
H	-0.577944	-0.409438	-0.322763
H	-2.343099	0.822907	-0.181179
B	1.764842	-0.326735	-0.025437
H	0.532544	1.194830	-0.854809
H	2.671285	0.456217	0.232816
H	1.796777	-1.251070	0.773751
H	1.929197	-0.771865	-1.154140

Vibrational frequencies

160.8503	195.5320	219.5708
269.0801	302.1765	419.1984
569.8474	654.7538	706.4156
758.3376	821.2778	824.5094
890.7541	1030.4319	1056.9802
1083.3784	1107.5738	1182.2444
1188.7643	1191.3101	1194.5436
1226.5696	1609.7012	2020.8183
2212.3770	2354.8038	2366.8052
2377.0985	2504.1542	2565.0682
2593.4188	2667.5497	3195.0213

TSIX

Zero-point correction = 0.095801
Thermal correction to Energy = 0.102543
Thermal correction to Enthalpy = 0.103487
Thermal correction to Gibbs Free Energy = 0.067733
Sum of electronic and zero-point Energies = -80.433906
Sum of electronic and thermal Energies = -80.427164
Sum of electronic and thermal Enthalpies = -80.426220

Sum of electronic and thermal Free Energies = -80.461974
Cartesian coordinates

B	-0.182442	0.530136	-0.243187
H	1.854845	-1.096239	0.979942
H	0.070356	1.182341	-1.209683
H	-0.224315	2.017186	0.526344
B	1.723423	-0.346254	0.047944
H	1.297589	-0.878847	-0.942192
H	0.816618	0.426197	0.588798
H	2.633468	0.415864	-0.147435
B	-1.545945	-0.472019	0.030692
H	-0.796241	1.570127	0.803146
H	-2.583165	0.105455	-0.275640
H	-1.419193	-1.451497	-0.694293
H	-1.625146	-0.849900	1.193770

Vibrational frequencies

-485.2655	79.0361	178.2138
252.7080	332.3731	358.8958
413.5799	519.6882	557.6600
664.7156	744.9214	802.3515
833.7785	919.0012	1006.7581
1025.5117	1090.1587	1111.0880
1169.6784	1177.5407	1181.7747
1188.9730	1210.7900	1788.8261
2130.1539	2351.6596	2360.1928
2377.0026	2505.5530	2563.5985
2581.7604	2655.2717	3918.7470

$B_3H_8^-$(I)

Zero-point correction = 0.082660
Thermal correction to Energy = 0.087892
Thermal correction to Enthalpy = 0.088836
Thermal correction to Gibbs Free Energy = 0.056455
Sum of electronic and zero-point Energies = -79.311216
Sum of electronic and thermal Energies = -79.305984
Sum of electronic and thermal Enthalpies = -79.305040
Sum of electronic and thermal Free Energies = -79.337421
Cartesian coordinates

B	1.553072	0.214493	0.000001
H	2.188923	-0.142822	-0.988266
H	2.189371	-0.143096	0.987851
B	0.027579	-0.548132	0.000113
H	-0.799805	-0.078839	0.973524

B	-1.561356	0.266280	-0.000080
H	-1.631428	1.457526	-0.000236
H	-2.562894	-0.381404	-0.000073
H	-0.799648	-0.079021	-0.973490
H	1.473587	1.439094	0.000231
H	-0.154584	-1.734642	0.000287

Vibrational frequencies

180.6593	215.7847	358.8970
493.4024	607.8995	722.6904
815.2763	855.6483	872.4140
943.1245	952.3398	1053.5120
1059.8322	1114.5113	1172.1840
1176.9613	1192.8311	1633.2103
1728.3307	2091.8133	2200.7962
2328.6641	2336.0325	2344.0367
2565.7843	2601.4990	2665.4366

TSX

Zero-point correction = 0.080593
Thermal correction to Energy = 0.085522
Thermal correction to Enthalpy = 0.086467
Thermal correction to Gibbs Free Energy = 0.054713
Sum of electronic and zero-point Energies = -79.296615
Sum of electronic and thermal Energies = -79.291685
Sum of electronic and thermal Enthalpies = -79.290741
Sum of electronic and thermal Free Energies = -79.322495
Cartesian coordinates

B	-0.176591	-0.538071	-0.035401
H	0.693590	-0.004742	0.831370
H	-0.051673	-1.727034	-0.049754
B	-1.563803	0.288494	-0.071083
H	-1.600668	1.480348	0.112859
H	-2.583970	-0.241178	-0.437083
H	-1.243018	-0.279870	1.056932
H	2.534665	-0.369557	0.415895
B	1.603264	0.236564	-0.043978
H	1.685860	1.433501	-0.067676
H	1.250862	-0.226399	-1.110236

Vibrational frequencies

-497.0686	198.8715	377.6529
451.4222	467.3824	525.9009
731.7435	798.7110	881.9825
938.4117	969.4418	1023.4918

1089.8761	1110.3732	1137.0156
1167.4090	1186.7950	1218.4828
1809.5764	1943.9302	2095.2793
2484.6658	2490.3715	2529.5052
2544.8159	2584.3962	2618.5196

$B_3H_8^-$(II)

Zero-point correction = 0.081513
Thermal correction to Energy = 0.087035
Thermal correction to Enthalpy = 0.087979
Thermal correction to Gibbs Free Energy = 0.054993
Sum of electronic and zero-point Energies = -79.297412
Sum of electronic and thermal Energies = -79.291890
Sum of electronic and thermal Enthalpies = -79.290945
Sum of electronic and thermal Free Energies = -79.323932
Cartesian coordinates

B	-0.280067	0.617346	0.001191
H	0.708454	0.233068	-0.736292
H	-0.206751	1.796207	0.174987
B	-1.543660	-0.359216	0.097498
H	-1.482585	-1.515735	-0.224464
H	-2.626117	0.063714	0.408807
H	-1.161546	0.383456	-1.003360
H	2.548749	0.225402	-0.581312
B	1.640834	-0.244280	0.061900
H	1.529717	-1.438256	-0.025856
H	1.604544	0.182895	1.184547

Vibrational frequencies

163.5283	232.9564	298.4432
419.0843	448.0166	703.5911
775.4293	798.2819	859.1721
917.1514	984.4327	1043.8469
1063.6505	1102.5796	1177.7802
1197.1180	1202.4076	1301.6661
1742.8811	1855.8393	2123.9510
2499.5244	2531.8792	2552.0168
2577.0103	2579.8802	2628.0565

TSXI

Zero-point correction = 0.080706
Thermal correction to Energy = 0.085677
Thermal correction to Enthalpy = 0.086621

Thermal correction to Gibbs Free Energy = 0.054719
Sum of electronic and zero-point Energies = -79.283497
Sum of electronic and thermal Energies = -79.278527
Sum of electronic and thermal Enthalpies = -79.277582
Sum of electronic and thermal Free Energies = -79.309485
Cartesian coordinates

B	0.296011	0.796327	0.040367
H	-0.629925	0.854152	0.825734
H	0.484260	1.805952	-0.574055
B	1.272337	-0.498073	-0.056961
H	1.113929	-1.480772	0.613387
H	2.264093	-0.465605	-0.737254
H	1.280732	0.561779	0.863415
H	-2.080619	-0.362519	0.938693
B	-1.437828	-0.297971	-0.083942
H	-1.180131	-1.380580	-0.535740
H	-1.904942	0.466180	-0.891499

Vibrational frequencies

-579.1702	189.5467	341.1059
391.6743	454.2161	638.5973
816.2923	824.8347	882.0981
917.7821	945.9226	983.4509
1061.3714	1105.5053	1142.0123
1191.2502	1209.5231	1231.4671
1326.5134	1996.9454	2471.4640
2500.2929	2526.4755	2542.7422
2556.5310	2584.2448	2593.9773