Supporting Information

Controllable syntheses of B/N anionic aminoborane chain complexes by the reaction of NH_3BH_3 with NaH and the mechanistic study

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1. Experimental Section:

1.1. General Remarks.

All manipulations were carried out on a high-vacuum line or in a glovebox filled with high-purity nitrogen. The ^{11}B NMR and $^{11}B\{^{1}H\}$ NMRspectra were recorded at 128 or 193 MHz spectrometers and externally referenced to $BF_3{\cdot}OEt_2$ in C_6D_6 (δ = 0.00 ppm). The ^{1}H NMR and $^{1}H\{^{11}B\}$ NMR spectra was obtained at 600 MHz spectrometer. IR spectra were measured by a Spectrum 400F.

NH_3BH_3 was used as received. NaH was washed with tetrahydrofuran (THF) and n-hexane and then dried in vacuo. THF, n-hexane and toluene were dried over sodium and freshly distilled prior to use. $NaNH_2BH_3$ was prepared according the literature methods.[S1]

The M06-2X[S2] calculations were performed using the Gaussian 09 program.[S3] 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[S4] model in THF 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.

1.2. Reaction of NaH with 2 equiv. of NH_3BH_3.

NaH (0.24 g, 10 mmol) was added to a flask and then a sulution of NH_3BH_3 in THF (20 mL, 0.62 g, 20 mmol) was injected, and the reaction solution was stirred for 12 hours at 55 °C. Then 20 mL of n-hexane was added into the solution and a white precipitate was formed. After filtration, THF and n-hexane were removed from the filtrate under dynamic vacuum to leave a white powder product $Na[BH_3NH_2BH_3]$ (0.31 g, 46 %). ^{11}B NMR (193 MH_Z, CD_3CN): δ -19.4 (*q*, $J_{B\text{-}H}$ = 90 Hz) ppm (Fig. S1a). $^{11}B\{^{1}H\}$ NMR (193 MH_Z, CD_3CN): δ -19.4 (*s*) ppm (Fig. S1b). ^{1}H NMR (600 MH_Z, CD_3CN): δ 1.64 (*br t*, 2 H of NH_2, $J_{N\text{-}H}$ = 32 Hz), 1.20 (*q*, 6 H of 2 BH_3, $J_{B\text{-}H}$ = 90 Hz) ppm (Fig. S2a). $^{1}H\{^{11}B\}$ NMR (600 MH_Z, CD_3CN): δ 1.64 (*br t*, 2 H of NH_2, $J_{N\text{-}H}$ = 32 Hz), 1.20 (*s*, 6 H of 2 BH_3) ppm (Fig. S2b). IR (cm^{-1}): 3541 (s), 3314 (s), 3278 (s), 2294 (s, br), 1620 (w), 1575 (w), 1396 (w), 1220 (m), 1156 (s), 1052 (w) (Fig. S3).

1.3. Reaction of NaH with 3 equiv. of NH_3BH_3.

NaH (0.24 g, 10 mmol) was added to a flask and then a sulution of NH_3BH_3 in THF (20 mL, 0.93 g, 30 mmol) was injected, and the reaction solution stirred for 5 days at room temperature and formed more precipitate. The white precipitate was filtered and then the solid was washed with toluene (3 × 20 mL), and then was dried under vacuum to yield a free-flowing white powder

$Na[BH_3NH_2BH_2NH_2BH_3]$ (0.69 g, 72%). ^{11}B NMR (193 MH_Z, CD_3CN): δ -8.3 (*t*, J_{B-H} = 100 Hz, BH_2), -21.8 ppm (*q*, J_{B-H} = 91 Hz, BH_3) (Fig. S4a). $^{11}B\{^1H\}$ NMR (193 MH_Z, CD_3CN): δ -8.3 (*s*, BH_2), -21.8 ppm (*s*, BH_3) (Fig. S4b). ^1H NMR (600 MH_Z, CD_3CN): δ 2.04 (*br t*, 4 H of 2 NH_2, J_{N-H} = 33 Hz), 1.87 (*q*, 2 H of BH_2, J_{B-H} = 98 Hz), 1.23 (*q*, 6 H of 2 BH_3, J_{B-H} = 91 Hz) ppm (Fig. S5a). $^1H\{^{11}B\}$ NMR (600 MH_Z, CD_3CN): δ 2.04 (*br t*, 4 H of 2 NH_2, J_{N-H} = 33 Hz), 1.87 (*quint*, 2 H of BH_2, J_{H-H} = 4 Hz), 1.23 (*br, t*, 6 H of 2 BH_3, J_{N-H} = 82 Hz) ppm (Fig. S5b). IR (cm^{-1}): 3302 (s), 3255 (s), 2365 (s), 2283 (s, br), 1575 (m), 1556 (s), 1248 (s, br), 1197 (s), 1174 (s), 1127 (m), 1073 (m), 1053 (m), 997 (m), 867 (w) (Fig. S6).

1.4. Reaction of NaH with 4 equiv. of NH_3BH_3.

NaH (0.12 g, 5 mmol) was added to a flask and then a sulution of NH_3BH_3 in THF (20 mL, 0.62 g, 20 mmol) was injected, and the reaction solution was stirred for 28 hours under reflux condition (65 °C). Then the reaction solution was monitored by ^{11}B NMR (Fig. S7).

1.5. Reaction of $NaNH_2BH_3$ with 1 equiv. of NH_3BH_3.

$NaNH_2BH_3$ (0.53 g, 10 mmol) and NH_3BH_3 (0.31 g, 10 mmol) were placed in a 100 mL flask. About 30 mL of THF was condensed into the flask, and the mixture solution was stirred for 12 hours at 55 °C. Then 30 mL of n-hexane was added into the solution and a white precipitate was formed. After filtration, THF and n-hexane were removed from the filtrate under dynamic vacuum to leave a white powder product $Na[BH_3NH_2BH_3]$ (0.27 g, 41 %). ^{11}B NMR (128 MH_Z, THF): δ -19.9 (*q*, J_{B-H} = 90 Hz) ppm (Fig. S8a). $^{11}B\{^1H\}$ NMR (128 MH_Z, THF): δ -19.9 (*s*) ppm (Fig. S8b).

1.6. Reaction of $NaNH_2BH_3$ with 2 equiv. of NH_3BH_3.

$NaNH_2BH_3$ (0.53 g, 10 mmol) and NH_3BH_3 (0.62 g, 20 mmol) were placed in a 100 mL flask. About 20 mL of THF was condensed into the flask, and the mixture solution was stirred for 5 days at room temperature and formed more precipitate. The white precipitate was filtered and then the solid was washed with toluene (3 × 20 mL), and then was dried under vacuum to yield a free-flowing white powder $Na[BH_3NH_2BH_2NH_2BH_3]$ (0.72 g, 75%). ^{11}B NMR (128 MH_Z, THF): δ -8.5 (*t*, J_{B-H} = 96 Hz, BH_2), -22.3 ppm (*q*, J_{B-H} = 91 Hz, BH_3) (Fig. S9).

1.7. Reaction of $NaNH_2BH_3$ with $NH_2B_2H_5$.

$NaNH_2BH_3$ (0.53 g, 10 mmol) was added to a flask and 5 mL of THF was injected to the flask. Then $NH_2B_2H_5$·THF (1.14 g, 10 mmol) was injected was injected to the solution and stirred for 1 hour at room temperature, and turbidity developed during this time. The precipitate white solid was filtered

and then the solid was washed with toluene (3 × 20 mL), and then was dried under vacuum to yield a free-flowing white powder $Na[BH_3NH_2BH_2NH_2BH_3]$ (0.81 g, 85%). ^{11}B NMR (193 MH_Z, THF): δ -8.5 (*t*, J_{B-H} = 96 Hz, BH_2), -22.3 ppm (*q*, J_{B-H} = 92 Hz, BH_3) (Fig. 10a). $^{11}B\{^1H\}$ NMR (193 MH_Z, THF): δ -8.5 ppm (*s*, BH_2), -22.3 ppm (*s*, BH_3) (Fig. 10b). ^1H NMR (600 MH_Z, CD_3CN): δ 2.05 (*br t*, 4 H of 2 NH_2, J_{N-H} = 33 Hz), 1.87 (*q*, 2 H of BH_2, J_{B-H} = 98 Hz), 1.22 (*q*, 6 H of 2 BH_3, J_{B-H} = 91 Hz) ppm (Fig. S11a). $^1H\{^{11}B\}$ NMR (600 MH_Z, CD_3CN): δ 2.05 (*br t*, 4 H of 2 NH_2, J_{N-H} = 33 Hz), 1.87 (*quint*, 2 H of BH_2, J_{H-H} = 4 Hz), 1.22 (*br, t*, 6 H of 2 BH_3, J_{N-H} = 82 Hz) ppm (Fig. S11b).

1.8. Reaction of $Na[BH_3NH_2BH_3]$ with 1 equiv. of NH_3BH_3.

$Na[BH_3NH_2BH_3]$ (0.34 g, 5 mmol) and NH_3BH_3 (0.16 g, 5 mmol) were placed in a flask. About 20 mL of THF was injected into the flask, and the mixture solution was stirred for 1 days at room temperature. This reaction cannot form new compound, only the starting materials were observed in the ^{11}B NMR (Fig. S12).

1.9. Reaction of $Na[BH_3NH_2BH_2NH_2BH_3]$ with 1 equiv. of NH_3BH_3.

$Na[BH_3NH_2BH_2NH_2BH_3]$ (0.19 g, 2 mmol) and NH_3BH_3 (0.06 g, 2 mmol) were placed in a flask. About 15 mL of THF was injected into the flask, and the reaction solution was stirred for 28 hours at 65 °C. Then the reaction solution was monitored by ^{11}B NMR (Fig. S13).

1.10. The formation of DADB from two NH_3BH_3 molecules.

NH_3BH_3 (0.31 g, 10 mmol) was placed in a 10 mL flask. About 5 mL of THF was condensed into the flask, and the mixture solution was stirred for 10 hours at room temperature. Then the reaction solution was monitored by ^{11}B NMR (Fig. S16).

2. Table:

Table S1 Energetics of the reaction between NH_3BH_3 and THF·NaH to produce different B/N anionic aminoborane chain complexes (kcal/mol at 0 and 298 K) calculated at M06-2X/6-311++G(d, p)/SMD_{THF} level.

	ΔE_{0K} (SMD)	ΔG_{298K} (SMD)
NH_3BH_3+ THF·NaH	0	0
TS1	-6.6	1.7
$NH_2BH_3^-$+NH_3BH_3	13.5	1.0
TS2	32.0	27.7
$[BH_3NH_2BH_3]^-$+NH_3	-1.4	-15.1
$[NH_2BH_3]^-$+$NH_2B_2H_5$	13.5	1.0
TS3	16.7	14.1
$[BH_3NH_2BH_2NH_2BH_3]^-$	-23.7	-22.5
TS4	-3.9	7.8
$[NH_2BH_3]^-$+$BH_3NH_2BH(\mu$-H)BH_2NH_2	11.2	-2.1
TS5	7.2	5.6
$[BH_3(NH_2BH_2)_2NH_2BH_3]^-$	-35.0	-32.9
TS6	7.7	6.0
$[BH(NH_2BH_3)_3]^-$	-38.1	-36.7
NH_3BH_3+NH_3BH_3	0	0
TS7	24.1	22.7
AaDB+NH_3	12.3	2.5

3. Supporting Results:

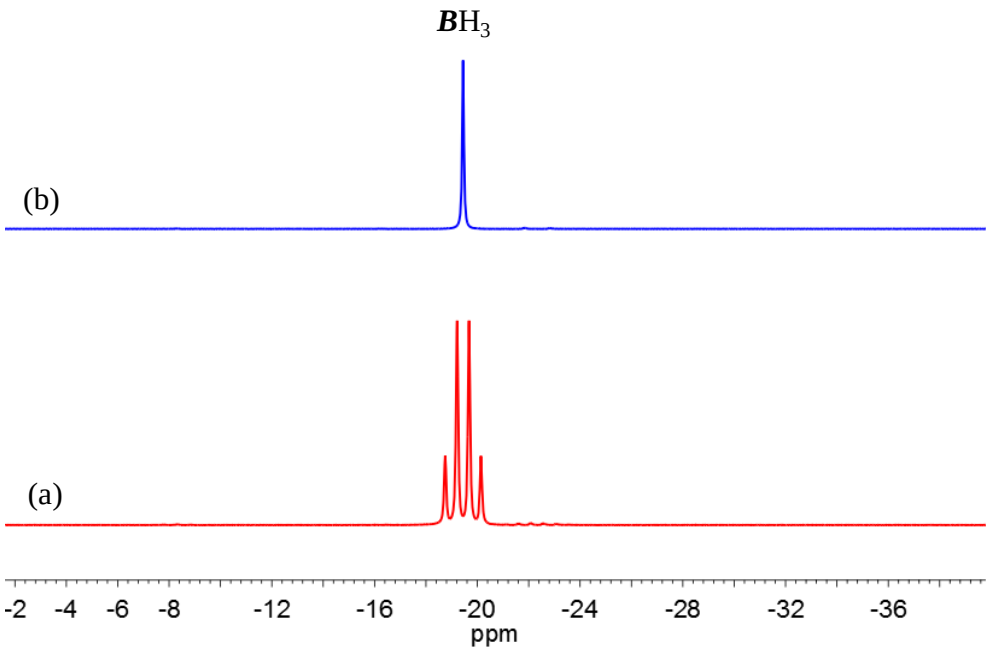

Fig. S1 ^{11}B NMR (a) and ^{11}B{^{1}H} NMR (b) spectra of the Na[$BH_3NH_2BH_3$] in CD_3CN, which was isolated from the reaction of NaH with 2 equiv. of NH_3BH_3.

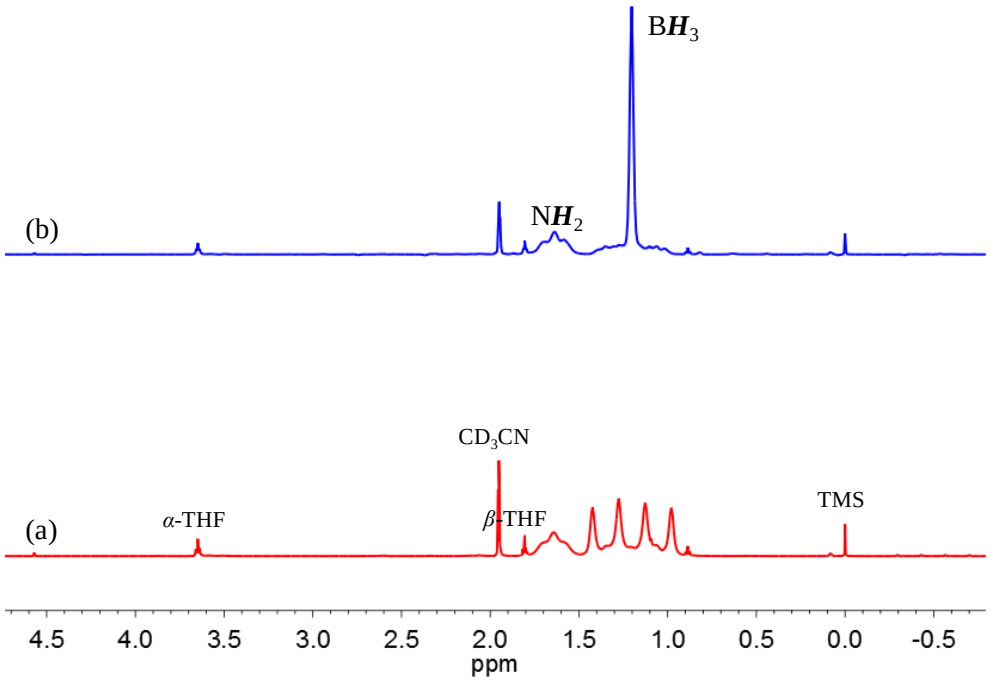

Fig. S2 ^{1}H NMR (a) and ^{1}H{^{11}B} NMR (b) spectra of the Na[$BH_3NH_2BH_3$] in CD_3CN, which was isolated from the reaction of NaH with 2 equiv. of NH_3BH_3.

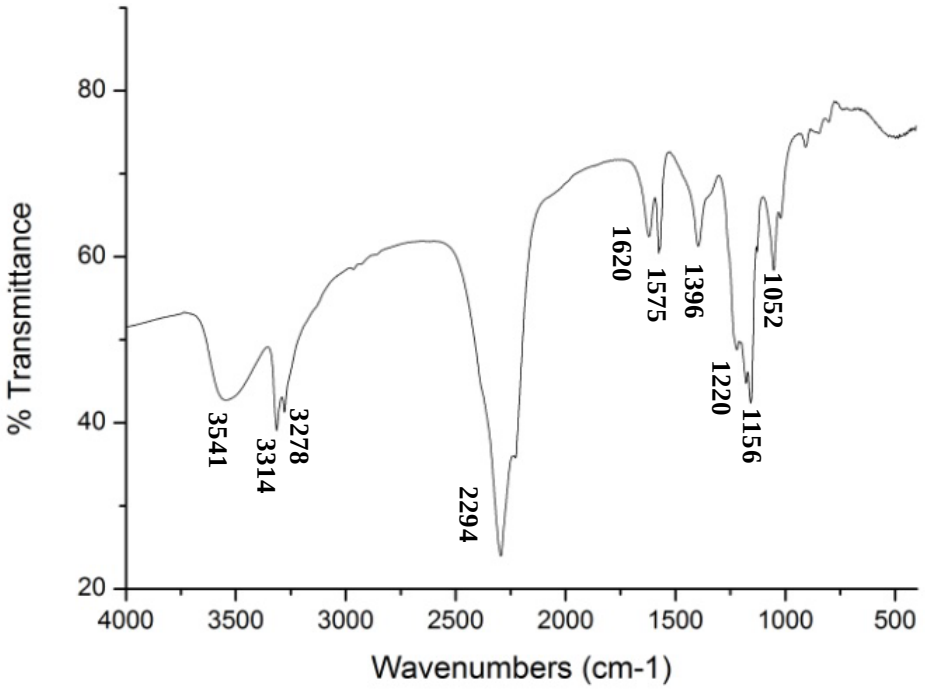

Fig. S3 IR spectrum of the $Na[BH_3NH_2BH_3]$ isolated from the reaction of NaH with 2 equiv. of NH_3BH_3.

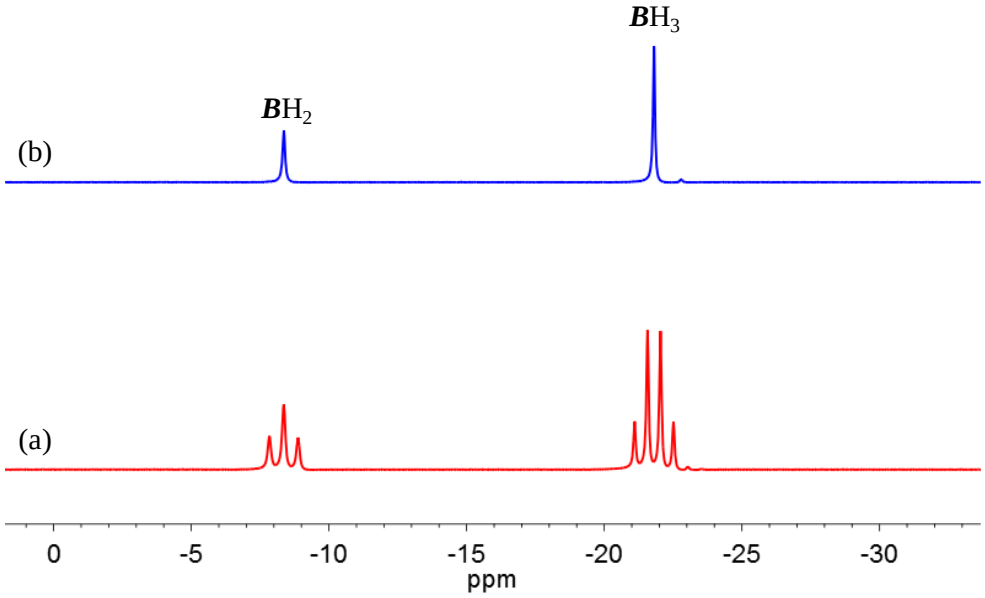

Fig. S4 ^{11}B NMR (a) and $^{11}B\{^1H\}$ NMR (b) spectra of the $Na[BH_3NH_2BH_2NH_2BH_3]$ in CD_3CN, which was isolated from the reaction of NaH with 3 equiv. of NH_3BH_3.

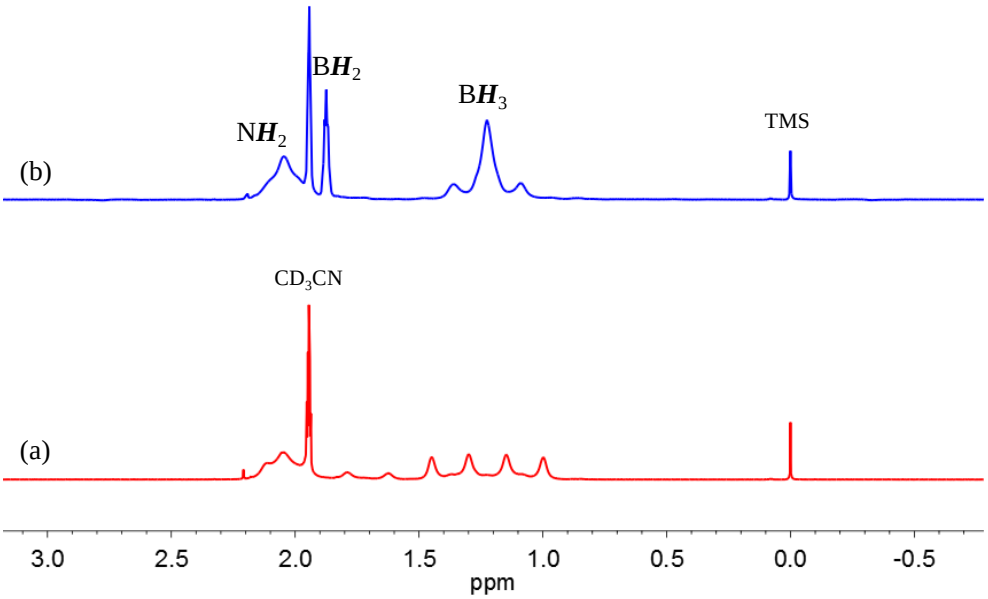

Fig. S5 ^{1}H NMR (a) and $^{1}H\{^{11}B\}$ NMR (b) spectra of the $Na[BH_3NH_2BH_2NH_2BH_3]$ in CD_3CN, which was isolated from the reaction of NaH with 3 equiv. of NH_3BH_3.

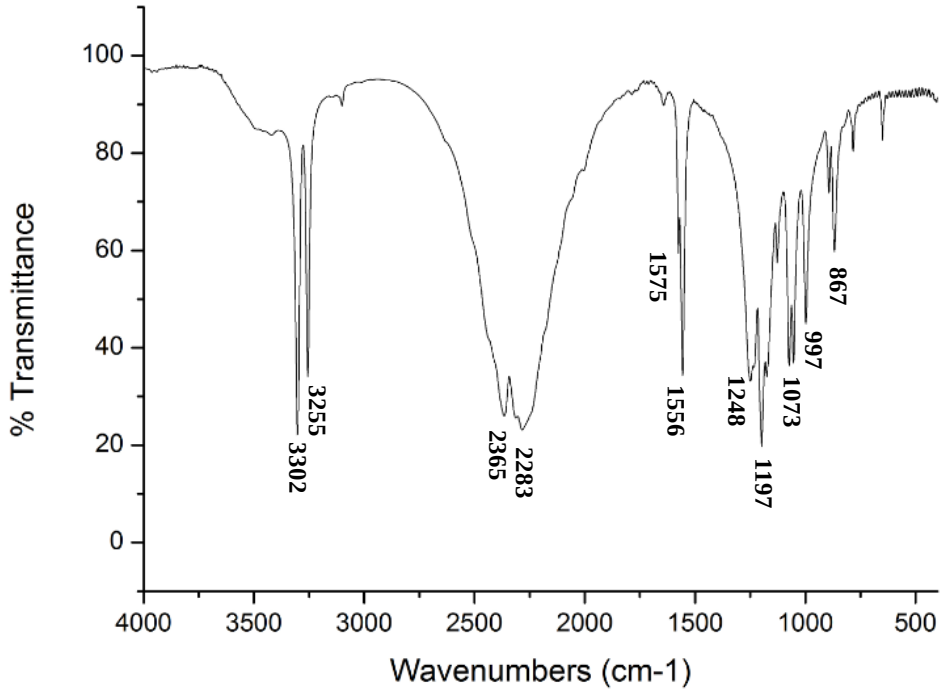

Fig. S6 IR spectrum of the $Na[BH_3NH_2BH_2NH_2BH_3]$ isolated from the reaction of NaH with 3 equiv. of NH_3BH_3.

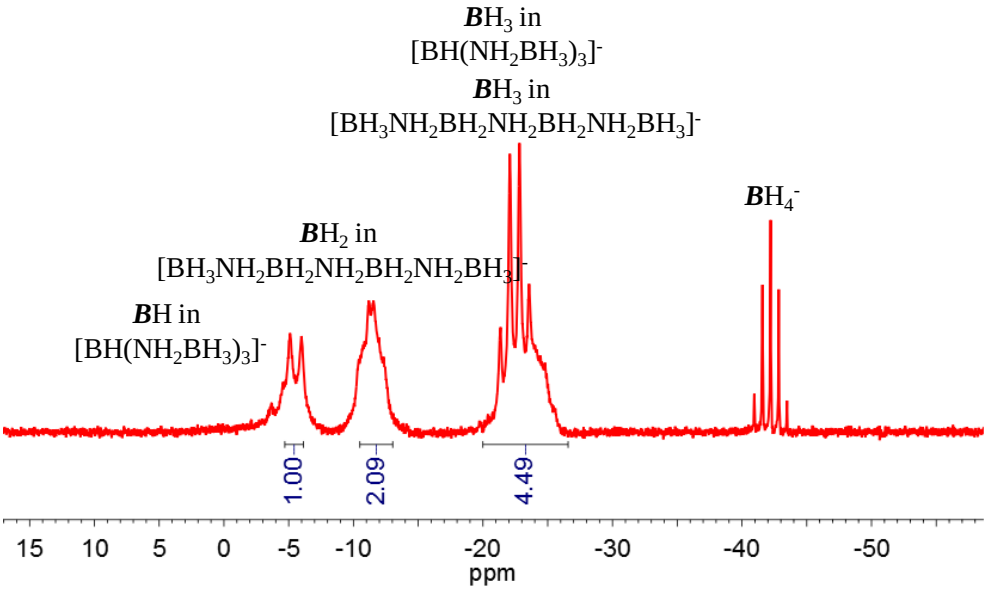

Fig. S7 ^{11}B NMR spectrum of the reaction solution of the NaH with 4 equiv. of NH_3BH_3 in THF.

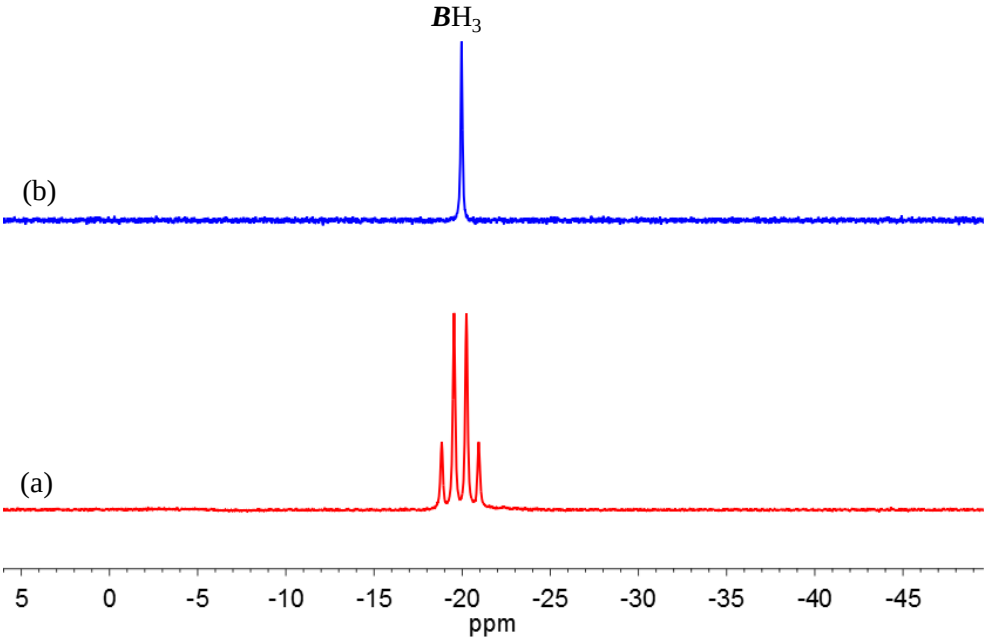

Fig. S8 ^{11}B NMR (a) and ^{11}B{^{1}H} NMR (b) spectra of the $Na[BH_3NH_2BH_3]$ in THF, which was isolated from the reaction of $NaNH_2BH_3$ with 1 equiv. of NH_3BH_3.

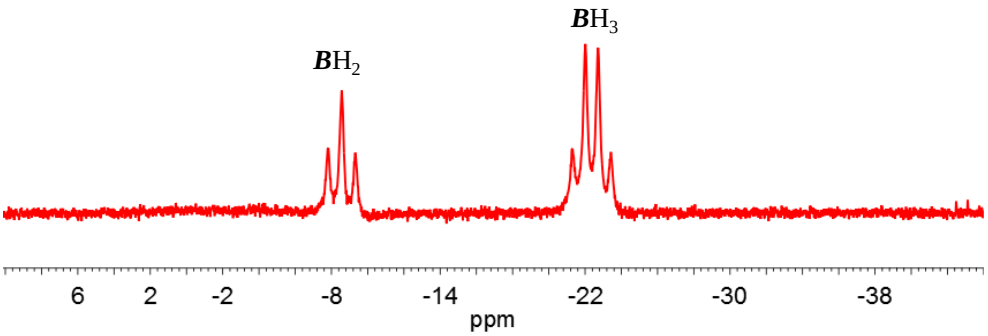

Fig. S9 ^{11}B NMR spectrum of the Na[$BH_3NH_2BH_2NH_2BH_3$] in THF, which was isolated from the reaction of $NaNH_2BH_3$ with 2 equiv. of NH_3BH_3.

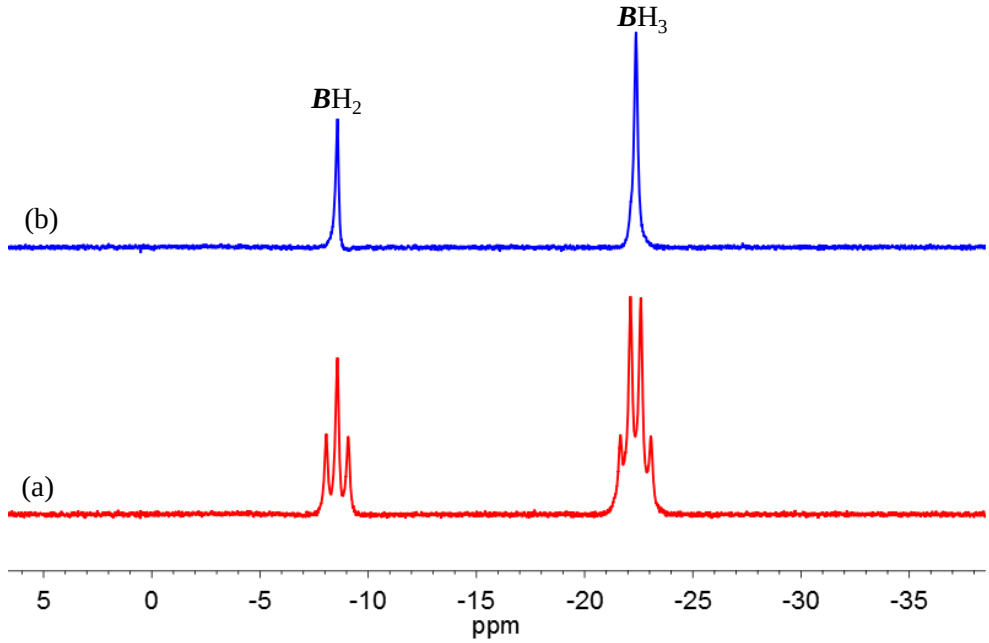

Fig. S10 ^{11}B NMR (a) and ^{11}B{^{1}H} NMR (b) spectra of the Na[$BH_3NH_2BH_2NH_2BH_3$] in THF, which was isolated from the reaction of $NaNH_2BH_3$ with ADB.

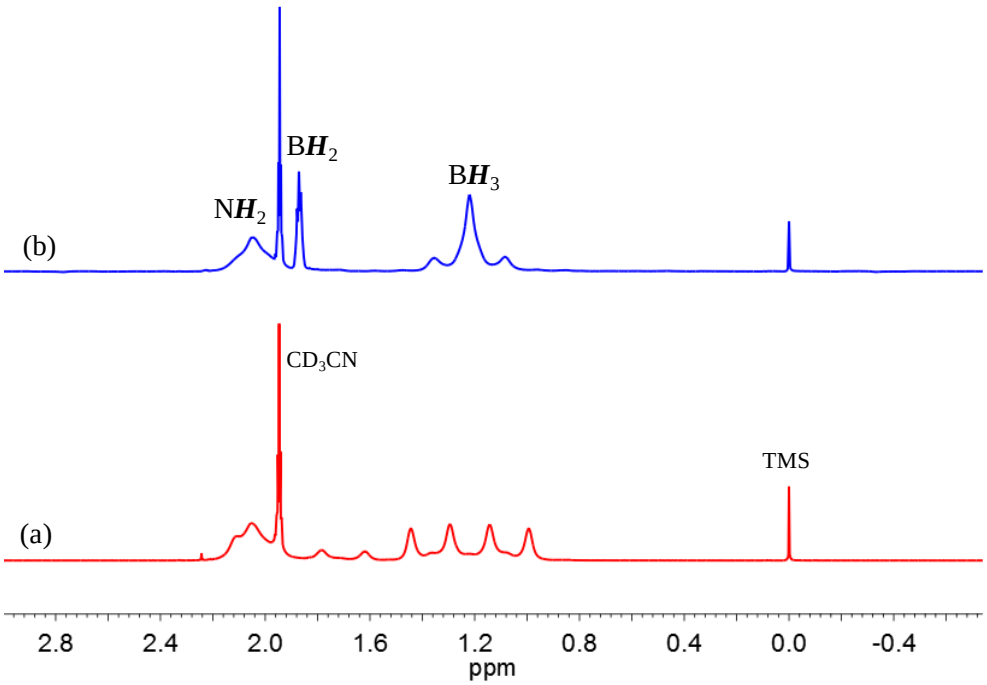

Fig. S11 ^{1}H NMR (a) and $^{1}H\{^{11}B\}$ NMR (b) spectra of the $Na[BH_3NH_2BH_2NH_2BH_3]$ in CD_3CN, which was isolated from the reaction of $NaNH_2BH_3$ with ADB.

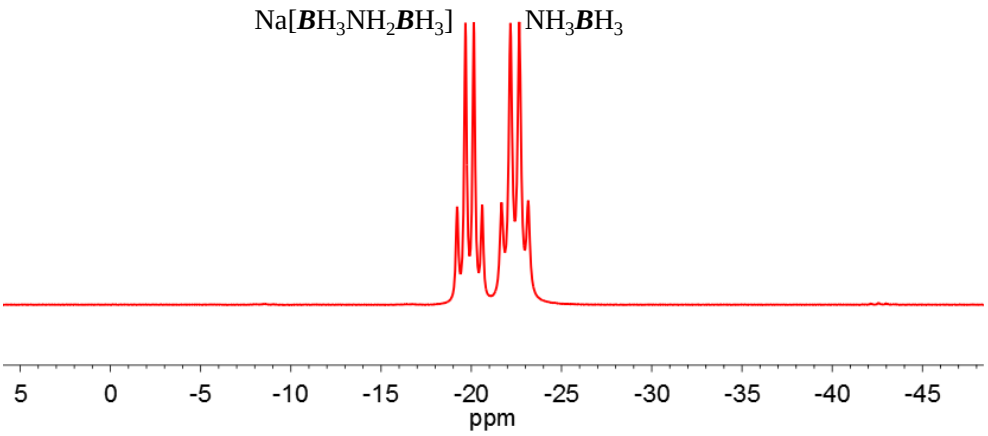

Fig. S12 ^{11}B NMR spectrum of the mixture solution of the reaction of $Na[BH_3NH_2BH_3]$ with NH_3BH_3 in THF.

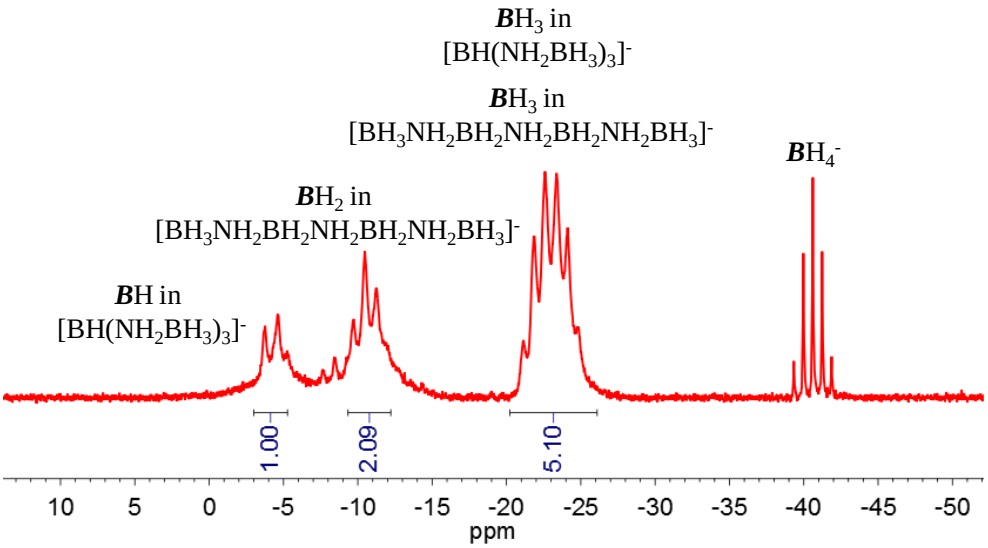

Fig. S13 ^{11}B NMR spectrum of the reaction solution of the $Na[BH_3NH_2BH_2NH_2BH_3]$ with 1 equiv. of NH_3BH_3 in THF.

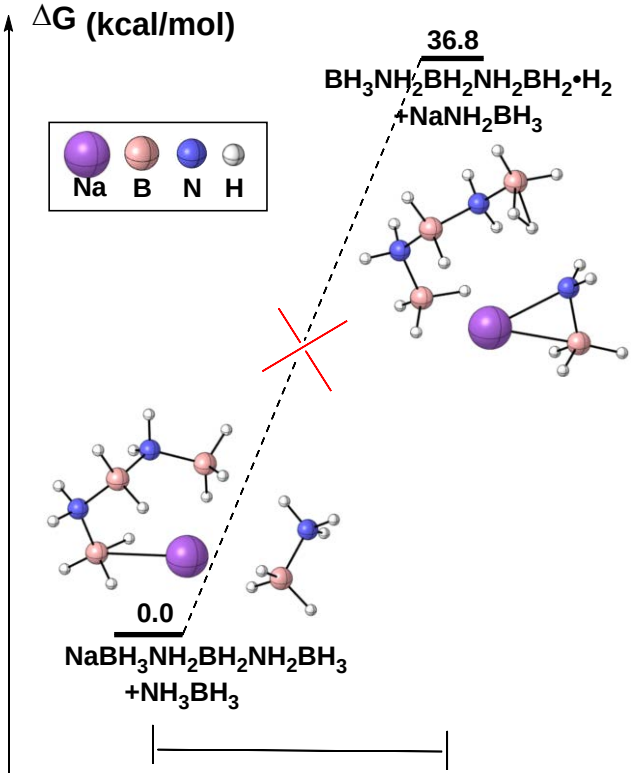

Fig. S14 High Gibbs free energy difference ΔG.

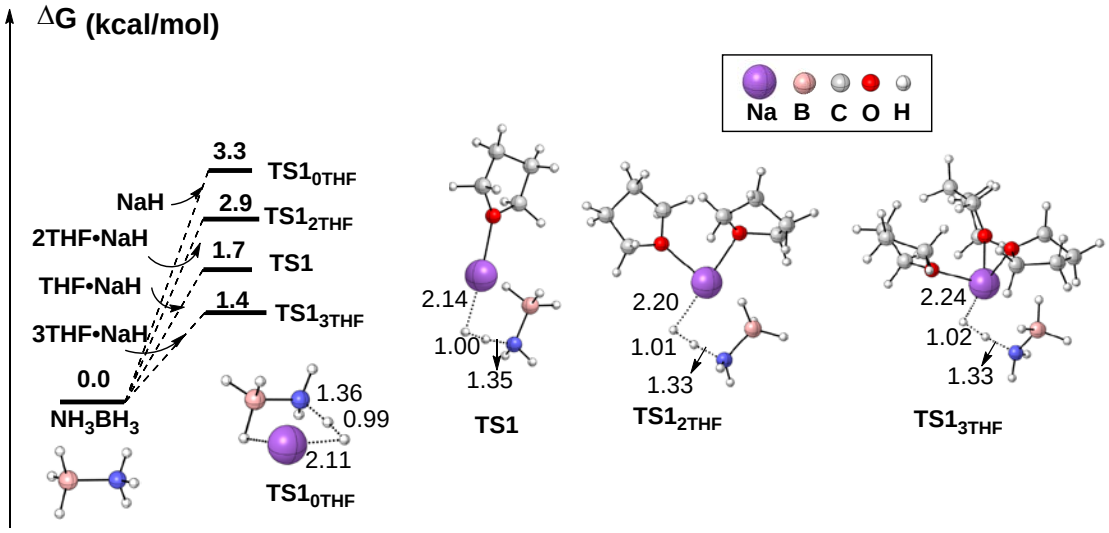

Fig. S15 Transition state TS1 with zero, one, two or three THF moleculars.

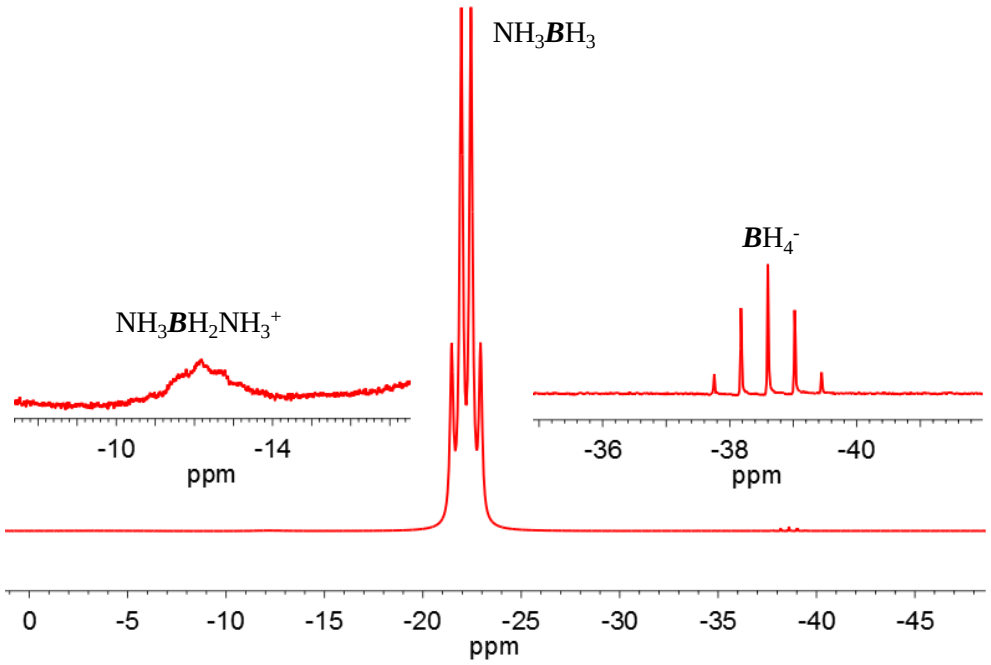

Fig. S16 ^{11}B NMR spectrum of the solution of the NH_3BH_3 in THF, the formed DADB.

4. References:

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S4. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378−6396.

5. Cartesian coordinates and vibrational frequencies of the studied models:

THF·NaH

Zero-point correction= 0.122617 (Hartree/Particle)

Thermal correction to Energy = 0.130395

Thermal correction to Enthalpy = 0.131339

Thermal correction to Gibbs Free Energy = 0.088178

Sum of electronic and zero-point Energies = -395.147423

Sum of electronic and thermal Energies = -395.139645

Sum of electronic and thermal Enthalpies = -395.138701

Sum of electronic and thermal Free Energies = -395.181862

Cartesian coordinates

Na	-2.634921000000	0.000130000000	0.006424000000
H	-4.646346000000	-0.006230000000	0.005323000000
C	0.434812000000	-1.179396000000	-0.143302000000
O	-0.406136000000	-0.011847000000	-0.014680000000
C	0.409334000000	1.171096000000	0.132712000000
C	1.821041000000	0.735628000000	-0.233790000000
C	1.830806000000	-0.715943000000	0.248283000000
H	0.036781000000	-1.963432000000	0.501991000000
H	0.403163000000	-1.516631000000	-1.183286000000
H	0.008657000000	1.949525000000	-0.518065000000
H	0.353189000000	1.505261000000	1.173006000000
H	1.961615000000	0.777194000000	-1.316643000000
H	2.578371000000	1.357133000000	0.243649000000
H	2.608091000000	-1.322325000000	-0.216231000000
H	1.953742000000	-0.755462000000	1.333608000000

Vibrational frequencies

7.7087	66.7333	115.4733
231.3742	272.5041	341.8362
344.1687	577.577	687.353

863.564 888.3547 923.1979

923.7594 946.2413 977.4647

1047.916 1094.1354 1098.5556

1168.0141 1195.5685 1201.6686

1274.2182 1276.4759 1318.2764

1348.3589 1386.1054 1416.7198

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1524.5822 3066.4968 3072.242

3074.6669 3075.979 3125.2914

3127.5383 3136.7157 3144.1093

NH_3BH_3

Zero-point correction= 0.070504 (Hartree/Particle)

Thermal correction to Energy= 0.074203

Thermal correction to Enthalpy= 0.075147

Thermal correction to Gibbs Free Energy= 0.048163

Sum of electronic and zero-point Energies= -83.137892

Sum of electronic and thermal Energies= -83.134193

Sum of electronic and thermal Enthalpies= -83.133249

Sum of electronic and thermal Free Energies= -83.160234

Cartesian coordinates

N	0.000000000000	0.000000000000	0.713715000000
H	0.000000000000	0.945663000000	1.092759000000
H	0.818968000000	-0.472831000000	1.092759000000
H	-0.818968000000	-0.472831000000	1.092759000000
B	0.000000000000	0.000000000000	-0.902502000000
H	0.000000000000	-1.159431000000	-1.253924000000
H	-1.004096000000	0.579715000000	-1.253924000000
H	1.004096000000	0.579715000000	-1.253924000000

Vibrational frequencies

281.9080 708.0780 714.3194

765.1036 1075.8939 1077.9102

1191.6924 1207.1700 1209.4486

1396.7021 1643.9385 1646.9041

2465.6374 2484.8311 2487.1770

3468.7239 3561.0580 3561.3555

TS1

Zero-point correction= 0.189510 (Hartree/Particle)

Thermal correction to Energy= 0.201563

Thermal correction to Enthalpy= 0.202507

Thermal correction to Gibbs Free Energy= 0.149652

Sum of electronic and zero-point Energies= -478.299487

Sum of electronic and thermal Energies= -478.287435

Sum of electronic and thermal Enthalpies= -478.286491

Sum of electronic and thermal Free Energies= -478.339346

Cartesian coordinates

N	4.050049000000	0.210553000000	0.052111000000
H	4.618236000000	0.339579000000	0.885267000000
H	4.640619000000	0.429180000000	-0.746212000000
B	2.720175000000	1.039779000000	0.079644000000
H	2.888096000000	2.241021000000	0.152937000000
H	2.094826000000	0.783587000000	-0.949999000000
H	2.064421000000	0.664754000000	1.052123000000
Na	1.258074000000	-1.122841000000	-0.075508000000
H	3.219204000000	-1.977883000000	-0.081555000000
H	3.645786000000	-1.077872000000	-0.025089000000
C	-1.104163000000	0.971001000000	-0.275925000000
O	-0.856436000000	-0.438853000000	-0.080473000000
C	-2.091042000000	-1.122969000000	0.212461000000
C	-3.194677000000	-0.127246000000	-0.117237000000
C	-2.521941000000	1.203501000000	0.227455000000

H	-0.343202000000	1.532469000000	0.268074000000
H	-1.017434000000	1.192940000000	-1.343870000000
H	-2.130594000000	-2.035232000000	-0.384697000000
H	-2.099143000000	-1.388547000000	1.274175000000
H	-3.434731000000	-0.165131000000	-1.182969000000
H	-4.102734000000	-0.318645000000	0.454519000000
H	-2.990734000000	2.063186000000	-0.251053000000
H	-2.520217000000	1.360185000000	1.309201000000

Vibrational frequencies

-1482.2540	33.9397	41.4009
57.8606	78.4348	89.9072
126.0285	132.9052	175.0396
242.6552	276.8454	278.8526
364.1042	520.7635	581.9224
658.2496	688.4001	775.7914
815.6523	869.3816	872.5715
890.7813	927.8307	928.8178
947.5972	981.7670	1033.8708
1049.9669	1103.5688	1117.9522
1172.6994	1184.7193	1197.8937
1207.1070	1230.3982	1260.7804
1276.0080	1278.8919	1321.8654
1350.9431	1386.5519	1417.5353
1480.5368	1491.4964	1505.7033
1520.4420	1529.4668	1531.6903
1541.6196	1601.8449	2318.5988
2327.8593	2444.0245	3064.5401
3072.5842	3076.8613	3079.1705
3132.0087	3133.4953	3140.1945
3146.7743	3508.5225	3589.7584

$[NH_2BH_3]^-$

Zero-point correction= 0.054151 (Hartree/Particle)

Thermal correction to Energy= 0.057816

Thermal correction to Enthalpy= 0.058761

Thermal correction to Gibbs Free Energy= 0.030989

Sum of electronic and zero-point Energies= -82.644980

Sum of electronic and thermal Energies= -82.641314

Sum of electronic and thermal Enthalpies= -82.640369

Sum of electronic and thermal Free Energies= -82.668141

Cartesian coordinates

N	0.760806000000	0.000000000000	-0.123429000000
H	1.174423000000	-0.805817000000	0.336786000000
H	1.174419000000	0.805817000000	0.336790000000
B	-0.792216000000	0.000000000000	0.014586000000
H	-1.197597000000	0.000031000000	1.191392000000
H	-1.257905000000	0.998067000000	-0.536978000000
H	-1.257903000000	-0.998098000000	-0.536921000000

Vibrational frequencies

274.1631	704.5898	758.9311
878.1751	981.3057	1113.7002
1169.1331	1200.8485	1203.6363
1588.1596	2167.4735	2301.0704
2324.2427	3516.2479	3587.6504

THF·Na^+

Zero-point correction= 0.118851 (Hartree/Particle)

Thermal correction to Energy= 0.125687

Thermal correction to Enthalpy= 0.126632

Thermal correction to Gibbs Free Energy= 0.086830

Sum of electronic and zero-point Energies= -394.471103

Sum of electronic and thermal Energies= -394.464266

Sum of electronic and thermal Enthalpies= -394.463322

Sum of electronic and thermal Free Energies= -394.503124

Cartesian coordinates

Na	-2.686713000000	0.000016000000	0.061831000000
C	0.322609000000	1.185724000000	0.068136000000
O	-0.507358000000	0.007120000000	-0.087683000000
C	0.326888000000	-1.168976000000	-0.209227000000
C	1.687669000000	-0.738780000000	0.311323000000
C	1.750716000000	0.712772000000	-0.167785000000
H	-0.011135000000	1.938867000000	-0.646959000000
H	0.188094000000	1.564319000000	1.084869000000
H	-0.132549000000	-1.974875000000	0.364935000000
H	0.374237000000	-1.455633000000	-1.263743000000
H	1.706937000000	-0.782556000000	1.403223000000
H	2.492420000000	-1.359229000000	-0.081895000000
H	2.473346000000	1.318188000000	0.378500000000
H	1.994062000000	0.749337000000	-1.232297000000

Vibrational frequencies

49.4345	73.6539	141.6737
252.4629	269.8019	575.0928
688.2976	863.7755	885.9335
919.0656	930.2584	947.7510
978.9617	1051.5422	1087.1580
1167.6129	1196.0056	1205.7173
1273.0700	1278.9980	1322.2322
1351.8582	1387.6081	1417.0170
1473.2204	1485.0214	1514.5429
1527.9660	3070.5745	3072.0658
3078.6980	3081.1032	3131.8103
3132.0994	3140.1479	3147.4152

H_2

Zero-point correction= 0.010160 (Hartree/Particle)

Thermal correction to Energy= 0.012520

Thermal correction to Enthalpy= 0.013465

Thermal correction to Gibbs Free Energy= -0.001322

Sum of electronic and zero-point Energies= -1.157686

Sum of electronic and thermal Energies= -1.155326

Sum of electronic and thermal Enthalpies= -1.154382

Sum of electronic and thermal Free Energies= -1.169168

Cartesian coordinates

H	0.000000000000	0.000000000000	0.370405000000
H	0.000000000000	0.000000000000	-0.370405000000

Vibrational frequencies

4459.6822

TS2

Zero-point correction= 0.123637 (Hartree/Particle)

Thermal correction to Energy= 0.132144

Thermal correction to Enthalpy= 0.133088

Thermal correction to Gibbs Free Energy= 0.092033

Sum of electronic and zero-point Energies= -165.754336

Sum of electronic and thermal Energies= -165.745828

Sum of electronic and thermal Enthalpies= -165.744884

Sum of electronic and thermal Free Energies= -165.785939

Cartesian coordinates

N	1.536740000000	0.627052000000	-0.002732000000
H	1.707942000000	1.208167000000	0.813198000000
H	1.728219000000	1.219285000000	-0.805995000000
B	2.411148000000	-0.659598000000	0.000177000000
H	2.118694000000	-1.350972000000	0.976053000000
H	2.185968000000	-1.309605000000	-1.020436000000

H	3.632350000000	-0.439689000000	0.045167000000
B	-0.714003000000	0.216131000000	0.003129000000
H	-0.907271000000	1.400824000000	-0.080972000000
H	-0.565869000000	-0.286319000000	1.083814000000
H	-0.542178000000	-0.437797000000	-0.989090000000
N	-2.752024000000	-0.193738000000	-0.000809000000
H	-3.229794000000	0.224592000000	0.792215000000
H	-2.909302000000	-1.196619000000	0.040072000000
H	-3.197499000000	0.152271000000	-0.845768000000

Vibrational frequencies

-506.1919	86.1687	110.2467
134.0270	170.9155	196.5577
225.0881	241.6261	364.8106
474.6471	508.0996	736.3359
780.3043	884.9255	990.5850
1005.3239	1009.5986	1097.5936
1119.7000	1128.6803	1134.4471
1137.3104	1178.8495	1201.0578
1203.7749	1587.8228	1632.9399
1636.0093	2209.6950	2288.8504
2316.1983	2499.0998	2576.6660
2594.1324	3488.1107	3504.8874
3582.3274	3615.0121	3617.8849

$[BH_3NH_2BH_3]^-$

Zero-point correction= 0.089064 (Hartree/Particle)

Thermal correction to Energy= 0.094353

Thermal correction to Enthalpy= 0.095297

Thermal correction to Gibbs Free Energy= 0.061937

Sum of electronic and zero-point Energies= -109.290970

Sum of electronic and thermal Energies= -109.285681

Sum of electronic and thermal Enthalpies= -109.284737

Sum of electronic and thermal Free Energies= -109.318097

Cartesian coordinates

N	0.000005000000	0.530371000000	-0.000044000000
H	0.000000000000	1.153445000000	-0.805016000000
H	-0.000021000000	1.153582000000	0.804821000000
B	-1.357780000000	-0.300065000000	0.000039000000
H	-1.381924000000	-0.994003000000	-1.001855000000
H	-1.382270000000	-0.993196000000	1.002484000000
H	-2.302655000000	0.477711000000	-0.000442000000
B	1.357775000000	-0.300064000000	0.000010000000
H	2.302669000000	0.477695000000	0.000349000000
H	1.382257000000	-0.993371000000	-1.002312000000
H	1.381929000000	-0.993818000000	1.002033000000

Vibrational frequencies

47.7882	214.3608	301.1290
614.4216	729.8536	815.8002
821.0114	901.7417	1014.2794
1056.4649	1156.6548	1184.7962
1190.0049	1194.5892	1194.9296
1200.9412	1201.2976	1224.6631
1605.7075	2358.8765	2368.4940
2399.2487	2404.4234	2411.9054
2416.5492	3504.4663	3560.2042

NH_3

Zero-point correction= 0.034409 (Hartree/Particle)

Thermal correction to Energy= 0.037277

Thermal correction to Enthalpy= 0.038221

Thermal correction to Gibbs Free Energy= 0.015341

Sum of electronic and zero-point Energies= -56.516885

Sum of electronic and thermal Energies= -56.514018

Sum of electronic and thermal Enthalpies= -56.513074

Sum of electronic and thermal Free Energies= -56.535954

Cartesian coordinates

N	-0.000024000000	0.000023000000	-0.113781000000
H	-0.929789000000	0.148294000000	0.265542000000
H	0.593512000000	0.730672000000	0.265495000000
H	0.336447000000	-0.879128000000	0.265433000000

Vibrational frequencies

1058.2805	1637.7081	1640.1328
3507.4871	3629.5186	3630.8310

$NH_2B_2H_5$

Zero-point correction= 0.084059 (Hartree/Particle)

Thermal correction to Energy= 0.088042

Thermal correction to Enthalpy= 0.088986

Thermal correction to Gibbs Free Energy= 0.059182

Sum of electronic and zero-point Energies= -108.593576

Sum of electronic and thermal Energies= -108.589594

Sum of electronic and thermal Enthalpies= -108.588649

Sum of electronic and thermal Free Energies= -108.618454

Cartesian coordinates

N	0.000645000000	0.785310000000	0.000064000000
H	0.000862000000	1.360153000000	-0.833467000000
H	0.000866000000	1.360111000000	0.833618000000
B	-0.951009000000	-0.435631000000	-0.000038000000
H	-1.517910000000	-0.616688000000	-1.032048000000
H	-1.516655000000	-0.617526000000	1.032497000000
B	0.950326000000	-0.436523000000	-0.000055000000
H	1.516684000000	-0.618563000000	-1.032165000000
H	1.515681000000	-0.619193000000	1.032496000000

H	-0.000630000000	-1.384702000000	-0.000917000000

Vibrational frequencies

318.9603	661.1028	704.2701
747.6607	777.7039	877.1174
918.6764	955.6769	1011.5677
1036.7532	1081.7446	1090.9862
1132.9688	1194.3449	1214.6037
1609.8977	1745.9842	2024.8230
2596.1703	2612.8299	2674.2323
2680.5448	3574.8690	3654.1646

TS3

Zero-point correction= 0.138542 (Hartree/Particle)

Thermal correction to Energy= 0.147140

Thermal correction to Enthalpy= 0.148084

Thermal correction to Gibbs Free Energy= 0.105821

Sum of electronic and zero-point Energies= -191.233123

Sum of electronic and thermal Energies= -191.224524

Sum of electronic and thermal Enthalpies= -191.223580

Sum of electronic and thermal Free Energies= -191.265843

Cartesian coordinates

N	-1.379302000000	0.639430000000	0.151638000000
H	-1.213233000000	1.016200000000	1.077160000000
H	-1.339093000000	1.387381000000	-0.530006000000
N	1.627935000000	0.616083000000	-0.135614000000
H	1.748152000000	1.014390000000	-1.063210000000
H	1.729157000000	1.397254000000	0.507057000000
B	2.679949000000	-0.498071000000	0.151464000000
H	2.542524000000	-0.899135000000	1.307394000000
H	2.495069000000	-1.446451000000	-0.612379000000
H	3.858162000000	-0.130199000000	0.016905000000

B	-0.569229000000	-0.592301000000	-0.192044000000
H	-0.154301000000	-1.251955000000	0.701817000000
H	-0.324888000000	-0.792794000000	-1.335852000000
B	-2.623155000000	-0.337487000000	0.023157000000
H	-3.176418000000	-0.491112000000	1.078591000000
H	-3.316572000000	-0.045211000000	-0.913723000000
H	-2.026819000000	-1.407669000000	-0.258807000000

Vibrational frequencies

-433.9553	51.3497	93.5651
110.2234	157.6412	160.4651
253.5806	299.1539	383.8286
704.2042	730.2829	760.0876
773.2646	781.6771	860.9476
882.9240	898.1735	965.4823
979.4450	1025.3123	1047.4218
1087.3792	1111.1759	1123.3640
1176.9139	1178.8741	1183.6393
1189.0331	1200.7088	1211.5064
1342.4570	1587.3498	1614.4288
2211.0527	2236.5222	2301.9157
2326.3348	2530.3233	2579.4193
2653.9803	2746.1237	3508.5109
3567.3087	3583.2105	3642.1836

$[BH_3NH_2BH_2NH_2BH_3]^-$

Zero-point correction= 0.143344 (Hartree/Particle)

Thermal correction to Energy= 0.151277

Thermal correction to Enthalpy= 0.152221

Thermal correction to Gibbs Free Energy= 0.111928

Sum of electronic and zero-point Energies= -191.292619

Sum of electronic and thermal Energies= -191.284687

Sum of electronic and thermal Enthalpies= -191.283743

Sum of electronic and thermal Free Energies= -191.324036

Cartesian coordinates

N	1.284621000000	-0.453357000000	-0.000444000000
H	1.260105000000	-1.072969000000	0.808547000000
H	1.260008000000	-1.071712000000	-0.810398000000
B	2.690978000000	0.309357000000	0.000147000000
H	3.582845000000	-0.523806000000	-0.001701000000
H	2.747849000000	0.998480000000	-1.001233000000
H	2.748678000000	0.995165000000	1.003734000000
N	-1.284603000000	-0.453317000000	0.000499000000
H	-1.259877000000	-1.072846000000	-0.808557000000
H	-1.260146000000	-1.071761000000	0.810384000000
B	-2.691034000000	0.309336000000	-0.000372000000
H	-2.748137000000	0.998304000000	1.001124000000
H	-2.748426000000	0.995310000000	-1.003857000000
H	-3.582853000000	-0.523877000000	0.001054000000
B	0.000004000000	0.466919000000	0.000203000000
H	-0.000271000000	1.134353000000	-1.009512000000
H	0.000355000000	1.134021000000	1.010138000000

Vibrational frequencies

65.4363	97.4079	177.4807
180.3099	211.2591	323.4673
341.5701	627.0499	641.8658
770.7886	776.5156	798.8838
864.4258	879.3680	880.1031
922.2237	998.0016	1067.6964
1092.0963	1134.2528	1174.4988
1185.3647	1188.5088	1199.5698
1202.1022	1203.6698	1204.7025
1216.5975	1229.0588	1239.2037

1243.1295	1600.0906	1606.9786
2405.9465	2407.0025	2426.5036
2426.8809	2432.8051	2433.2065
2479.7798	2494.7621	3487.1945
3487.7766	3547.1892	3548.0797

TS4

Zero-point correction= 0.259888 (Hartree/Particle)

Thermal correction to Energy= 0.275442

Thermal correction to Enthalpy= 0.276386

Thermal correction to Gibbs Free Energy= 0.215472

Sum of electronic and zero-point Energies= -585.734507

Sum of electronic and thermal Energies= -585.718953

Sum of electronic and thermal Enthalpies= -585.718009

Sum of electronic and thermal Free Energies= -585.778922

Cartesian coordinates

N	-3.524238000000	0.669644000000	-1.153912000000
H	-3.252902000000	0.978206000000	-2.081686000000
H	-4.322184000000	0.046777000000	-1.233240000000
Na	-0.011439000000	-1.469398000000	-0.857189000000
N	-2.710619000000	-0.828751000000	0.810383000000
H	-2.980889000000	-1.710867000000	0.376753000000
H	-3.521983000000	-0.508455000000	1.341082000000
B	-1.501635000000	-1.087236000000	1.838888000000
H	-0.582890000000	-1.610008000000	1.226414000000
H	-1.159600000000	-0.012209000000	2.280862000000
H	-1.889602000000	-1.839687000000	2.704401000000
B	-2.389785000000	0.167074000000	-0.308015000000
H	-1.946992000000	-1.501538000000	-1.581757000000
H	-1.288408000000	0.553900000000	-0.513409000000
B	-3.645636000000	1.817531000000	-0.051954000000

H	-2.674834000000	1.505772000000	0.684284000000
H	-3.414450000000	2.898967000000	-0.512429000000
H	-4.649483000000	1.687698000000	0.593772000000
C	3.133059000000	-0.328396000000	-1.009509000000
O	1.849516000000	-0.362172000000	-0.352815000000
C	1.869305000000	0.482392000000	0.819702000000
C	3.126802000000	1.327911000000	0.680684000000
C	4.074128000000	0.358154000000	-0.028636000000
H	3.424670000000	-1.351701000000	-1.251791000000
H	3.035101000000	0.246061000000	-1.935963000000
H	0.946396000000	1.063903000000	0.839749000000
H	1.907721000000	-0.154711000000	1.708206000000
H	2.929630000000	2.197803000000	0.048441000000
H	3.498862000000	1.671404000000	1.645803000000
H	4.903415000000	0.852505000000	-0.534548000000
H	4.477634000000	-0.366531000000	0.683314000000

Vibrational frequencies

-777.5264	25.5725	45.7984
52.4493	68.6223	84.1979
101.4350	128.8535	133.3751
137.6090	143.3975	187.8950
219.8273	242.4044	286.4014
288.9142	384.4244	429.6435
534.9808	584.0459	585.5890
666.2429	688.8910	740.9735
750.2140	784.6500	841.6253
867.8933	869.7243	891.3547
894.0345	926.2569	930.3071
932.5748	948.6287	980.0097
982.3577	995.3281	1041.3590
1047.3411	1053.7083	1090.9126

1100.0602	1108.0029	1165.9282
1171.4993	1173.5291	1192.1282
1196.9590	1199.2805	1202.0810
1203.0861	1206.7810	1220.0752
1273.9291	1276.4869	1276.8728
1325.8701	1331.9497	1351.7497
1384.5751	1414.6271	1482.6362
1493.4768	1515.9256	1529.9517
1576.3675	1603.7742	2222.0203
2420.6590	2472.2688	2491.1772
2547.9768	2610.4359	2706.8523
3061.7714	3073.1504	3076.5317
3093.7706	3130.6289	3136.6229
3151.0256	3159.7465	3474.1996
3531.9901	3539.3617	3609.9513

$BH_3NH_2BH(\mu\text{-}H)BH_2NH_2$

Zero-point correction= 0.137173 (Hartree/Particle)

Thermal correction to Energy= 0.144017

Thermal correction to Enthalpy= 0.144961

Thermal correction to Gibbs Free Energy= 0.107281

Sum of electronic and zero-point Energies= -190.584615

Sum of electronic and thermal Energies= -190.577772

Sum of electronic and thermal Enthalpies= -190.576828

Sum of electronic and thermal Free Energies= -190.614508

Cartesian coordinates

N	1.593429000000	-0.577540000000	-0.043574000000
H	2.283233000000	-0.954763000000	0.595796000000
H	1.569266000000	-1.116835000000	-0.902559000000
B	1.545370000000	0.967865000000	-0.198600000000
H	1.306244000000	1.329577000000	-1.307506000000

H	0.384604000000	1.155640000000	0.452237000000
H	2.307525000000	1.566595000000	0.489195000000
B	0.240775000000	-0.167368000000	0.571238000000
N	-0.983503000000	-0.495898000000	-0.282279000000
H	-0.776156000000	-0.388752000000	-1.276198000000
H	-1.219282000000	-1.480584000000	-0.155683000000
B	-2.290559000000	0.392056000000	0.068134000000
H	-2.525993000000	0.232311000000	1.247326000000
H	-2.008128000000	1.546774000000	-0.176557000000
H	-3.201843000000	-0.002504000000	-0.629381000000
H	0.133114000000	-0.336163000000	1.740441000000

Vibrational frequencies

75.4329	167.0983	213.7298
246.7955	373.7891	557.7566
624.7888	707.1324	726.3172
752.6727	780.8835	858.0146
885.1672	892.4481	943.4899
978.4727	1018.1142	1057.1827
1076.2154	1079.1106	1144.6619
1152.7138	1191.3332	1198.5766
1203.0665	1204.0722	1208.6204
1258.4224	1601.3976	1608.4390
1763.6243	2035.9914	2452.2333
2468.0857	2476.9339	2620.7800
2699.6780	2704.5357	3474.2041
3532.8401	3557.7873	3639.5271

TS5

Zero-point correction= 0.192651 (Hartree/Particle)

Thermal correction to Energy= 0.203547

Thermal correction to Enthalpy= 0.204491

Thermal correction to Gibbs Free Energy= 0.156943

Sum of electronic and zero-point Energies= -273.234666

Sum of electronic and thermal Energies= -273.223771

Sum of electronic and thermal Enthalpies= -273.222827

Sum of electronic and thermal Free Energies= -273.270374

Cartesian coordinates

N	2.887984000000	-0.263827000000	0.424667000000
H	3.627228000000	-0.781462000000	-0.042377000000
H	3.126246000000	-0.288063000000	1.412313000000
B	2.782406000000	1.194666000000	-0.107689000000
H	1.786988000000	1.741162000000	0.385700000000
H	3.758094000000	1.911287000000	0.139870000000
H	2.630155000000	1.171477000000	-1.330831000000
N	0.247046000000	-0.417409000000	-0.810690000000
H	0.620861000000	-0.907962000000	-1.615420000000
H	0.568567000000	0.549925000000	-0.831182000000
B	0.483962000000	-1.087589000000	0.525596000000
H	0.450852000000	-0.393218000000	1.488481000000
H	-1.141860000000	-1.395350000000	0.553218000000
H	0.782569000000	-2.235001000000	0.540675000000
B	-1.265744000000	-0.690877000000	-0.480757000000
N	-1.994191000000	0.610005000000	-0.071920000000
H	-1.443079000000	1.108788000000	0.628430000000
H	-2.039633000000	1.237947000000	-0.874092000000
B	-3.481976000000	0.397568000000	0.498762000000
H	-4.137236000000	-0.135429000000	-0.375394000000
H	-3.399267000000	-0.315251000000	1.480208000000
H	-3.938594000000	1.488471000000	0.786391000000
H	-1.831010000000	-1.327548000000	-1.319953000000

Vibrational frequencies

-395.6031	52.1373	79.0463

99.9995	168.6753	183.9785
211.2067	220.2309	234.9596
271.5031	291.6950	364.6563
385.9769	634.5699	715.9694
740.6318	751.5086	771.6267
781.7537	791.1496	848.3961
880.8844	891.8003	916.9112
941.3494	981.0123	993.8384
1042.1730	1050.4267	1069.7830
1103.6975	1121.3943	1133.1496
1170.7063	1189.2142	1192.0217
1197.1806	1198.7603	1208.1283
1211.2959	1218.7210	1229.0376
1247.1582	1348.9540	1593.6210
1604.3505	1610.0896	2229.4160
2241.0933	2274.2214	2310.8782
2436.5847	2445.1181	2450.5352
2615.8232	2663.7087	2758.4621
3470.4255	3486.2922	3514.9097
3533.1003	3588.7957	3599.3248

$[BH_3(NH_2BH_2)_2NH_2BH_3]^-$

Zero-point correction= 0.197734 (Hartree/Particle)

Thermal correction to Energy= 0.208050

Thermal correction to Enthalpy= 0.208994

Thermal correction to Gibbs Free Energy= 0.162814

Sum of electronic and zero-point Energies= -273.296800

Sum of electronic and thermal Energies= -273.286484

Sum of electronic and thermal Enthalpies= -273.285540

Sum of electronic and thermal Free Energies= -273.331720

Cartesian coordinates

N	0.000138000000	-0.304498000000	-0.129117000000
H	-0.029147000000	-0.097936000000	-1.129164000000
H	0.020529000000	0.612359000000	0.320072000000
B	1.329819000000	-1.076383000000	0.211092000000
H	1.403360000000	-1.217607000000	1.410702000000
H	1.331740000000	-2.134808000000	-0.382962000000
N	-2.561617000000	-0.222022000000	-0.227135000000
H	-2.669980000000	-0.361917000000	-1.230733000000
H	-3.394418000000	-0.645143000000	0.178714000000
B	-2.586959000000	1.346572000000	0.083171000000
H	-2.378533000000	1.495523000000	1.273475000000
H	-1.712590000000	1.883112000000	-0.573580000000
H	-3.679611000000	1.789726000000	-0.229313000000
B	-1.319550000000	-1.052548000000	0.297875000000
H	-1.369627000000	-1.092761000000	1.506210000000
H	-1.328446000000	-2.157428000000	-0.203616000000
N	2.560654000000	-0.200037000000	-0.264141000000
H	3.399553000000	-0.646614000000	0.101750000000
H	2.660601000000	-0.263277000000	-1.276230000000
B	2.579045000000	1.340759000000	0.163880000000
H	1.710511000000	1.923275000000	-0.460777000000
H	2.356407000000	1.399418000000	1.359762000000
H	3.673651000000	1.807977000000	-0.101645000000

Vibrational frequencies

61.4149	91.5033	127.0112
136.4608	169.6384	241.2646
251.4686	265.6702	289.0113
384.7639	424.4377	639.8039
654.8771	669.6656	726.1524
745.8107	786.9706	837.3546
853.0565	876.2411	893.9476

912.5575	916.5943	944.0658
991.2834	1052.9344	1054.0177
1101.2010	1117.7967	1153.7775
1181.9590	1188.5524	1197.7381
1206.8108	1207.1753	1212.1747
1215.2661	1221.6085	1223.7579
1227.7062	1238.5141	1243.7657
1246.7910	1250.2307	1607.1131
1608.4473	1610.5268	2410.0215
2414.5714	2422.2670	2427.3491
2429.2552	2441.4560	2453.4647
2474.3100	2491.3867	2505.9472
3459.9110	3493.3363	3493.8765
3516.3637	3551.1655	3551.6003

TS6

Zero-point correction= 0.192099 (Hartree/Particle)

Thermal correction to Energy= 0.203023

Thermal correction to Enthalpy= 0.203968

Thermal correction to Gibbs Free Energy= 0.156865

Sum of electronic and zero-point Energies= -273.234379

Sum of electronic and thermal Energies= -273.223455

Sum of electronic and thermal Enthalpies= -273.222511

Sum of electronic and thermal Free Energies= -273.269614

Cartesian coordinates

N	-0.253754000000	-1.452724000000	-0.279636000000
H	-1.126936000000	-1.726482000000	0.163094000000
H	-0.403603000000	-1.386229000000	-1.281362000000
B	1.070952000000	-2.199610000000	0.183593000000
H	1.751410000000	-2.493711000000	-0.762534000000
H	1.648223000000	-1.258679000000	0.786232000000

H	0.848630000000	-3.058649000000	0.989692000000
B	0.371831000000	-0.250926000000	0.364112000000
N	1.242415000000	0.652641000000	-0.506789000000
H	1.810061000000	0.097412000000	-1.147368000000
H	0.600504000000	1.194607000000	-1.083605000000
B	2.194954000000	1.667443000000	0.303853000000
H	1.472217000000	2.387837000000	0.962816000000
H	2.918355000000	0.998438000000	1.014429000000
H	2.837508000000	2.305610000000	-0.508293000000
H	0.131073000000	0.002511000000	1.492172000000
N	-1.563816000000	1.134127000000	-0.085587000000
H	-1.691380000000	1.697184000000	-0.924028000000
H	-1.445359000000	1.809099000000	0.666199000000
B	-2.812605000000	0.228012000000	0.160122000000
H	-2.962751000000	-0.522456000000	-0.806384000000
H	-2.623954000000	-0.464641000000	1.161993000000
H	-3.863572000000	0.855249000000	0.322632000000

Vibrational frequencies

-518.5354	75.8547	79.3578
126.6797	151.1122	195.4931
208.1669	233.9010	244.6848
253.9693	275.6802	373.8208
405.5963	479.6773	653.7563
736.8387	746.4057	761.6346
782.7916	795.7142	849.2330
874.7143	887.8069	895.6752
956.0789	987.5196	1001.2139
1032.5590	1041.9758	1062.7832
1105.7776	1124.3728	1166.9729
1177.8289	1189.4530	1190.9663
1197.8627	1199.0619	1205.2893

1208.8185	1213.7861	1216.0303
1276.2715	1343.5885	1575.8195
1590.2069	1607.7861	2225.7420
2260.6914	2293.7798	2325.5579
2437.2047	2449.9147	2456.1856
2540.4816	2599.3707	2759.0353
3487.5073	3492.0065	3519.6677
3549.7143	3568.0198	3596.2157

$[BH(NH_2BH_3)_3]^-$

Zero-point correction= 0.196622 (Hartree/Particle)

Thermal correction to Energy= 0.207201

Thermal correction to Enthalpy= 0.208146

Thermal correction to Gibbs Free Energy= 0.161659

Sum of electronic and zero-point Energies= -273.302839

Sum of electronic and thermal Energies= -273.292259

Sum of electronic and thermal Enthalpies= -273.291315

Sum of electronic and thermal Free Energies= -273.337802

Cartesian coordinates

N	1.461029000000	-0.579211000000	0.091795000000
H	1.766696000000	-1.276804000000	0.769552000000
H	1.272145000000	-1.112414000000	-0.758241000000
B	2.677543000000	0.431902000000	-0.176657000000
H	2.406193000000	1.099179000000	-1.156981000000
H	2.799324000000	1.140551000000	0.806020000000
H	3.684910000000	-0.222135000000	-0.372592000000
B	0.130754000000	0.059595000000	0.617825000000
N	-0.314008000000	1.207305000000	-0.339387000000
H	0.408160000000	1.925640000000	-0.304649000000
H	-0.310190000000	0.875541000000	-1.304966000000
B	-1.735308000000	1.878645000000	-0.026945000000

H	-2.606639000000	1.074141000000	-0.304328000000
H	-1.764171000000	2.152358000000	1.158942000000
H	-1.849206000000	2.878869000000	-0.710520000000
H	0.312993000000	0.504842000000	1.724404000000
N	-0.999352000000	-1.032753000000	0.630271000000
H	-1.873281000000	-0.552262000000	0.846316000000
H	-0.845215000000	-1.660459000000	1.417368000000
B	-1.207494000000	-1.902332000000	-0.700623000000
H	-0.265625000000	-2.667790000000	-0.803960000000
H	-2.248767000000	-2.522755000000	-0.601104000000
H	-1.248478000000	-1.142935000000	-1.652011000000

Vibrational frequencies

63.2328	85.4829	98.6629
165.0340	198.6049	209.2537
235.9501	268.8040	293.9154
340.1515	396.8877	464.7961
639.2859	650.2034	672.8507
733.3601	783.2435	795.1624
859.2384	882.5593	890.2014
912.1622	922.0831	932.4183
993.9914	1025.8512	1052.3645
1121.9753	1123.3836	1175.5416
1181.1270	1188.8214	1191.9535
1196.3149	1201.9706	1203.0422
1208.3303	1217.9471	1221.0090
1229.1005	1234.7990	1250.4759
1256.6262	1271.7705	1596.7024
1600.1165	1605.5030	2414.3465
2427.5187	2431.0386	2432.9919
2435.2731	2436.6873	2440.4928
2441.9234	2442.9342	2521.0232

3473.3098 3477.0408 3481.5399

3532.7360 3535.5673 3540.2226

NH_3BH_3+NH_3BH_3

Zero-point correction= 0.142032 (Hartree/Particle)

Thermal correction to Energy= 0.151310

Thermal correction to Enthalpy= 0.152254

Thermal correction to Gibbs Free Energy= 0.106918

Sum of electronic and zero-point Energies= -166.273296

Sum of electronic and thermal Energies= -166.264019

Sum of electronic and thermal Enthalpies= -166.263075

Sum of electronic and thermal Free Energies= -166.308411

Cartesian coordinates

N	-1.887073000000	-0.499687000000	0.046286000000
H	-2.176468000000	-1.476427000000	0.082920000000
H	-1.295393000000	-0.331065000000	0.858785000000
H	-1.303270000000	-0.389801000000	-0.782188000000
B	-3.156086000000	0.505151000000	0.009276000000
H	-2.707359000000	1.630344000000	-0.034862000000
H	-3.789675000000	0.228979000000	-0.985396000000
H	-3.788554000000	0.306500000000	1.022688000000
N	1.748866000000	-0.014549000000	-0.167997000000
H	1.570956000000	-0.077895000000	-1.169207000000
H	1.213730000000	0.777662000000	0.184274000000
H	1.367663000000	-0.856680000000	0.261181000000
B	3.329461000000	0.144976000000	0.145614000000
H	3.441645000000	0.208441000000	1.349617000000
H	3.875637000000	-0.834428000000	-0.310867000000
H	3.691664000000	1.163387000000	-0.399418000000

Vibrational frequencies

39.0168 52.1822 56.8689

78.9810	101.1402	113.9720
278.3678	292.4242	705.0888
714.1555	719.2775	730.2541
758.5908	761.9723	1074.5155
1077.9655	1080.4758	1084.1782
1184.5163	1189.1238	1199.7584
1199.8876	1202.1477	1204.1000
1382.8878	1403.3404	1641.2835
1642.5111	1647.7756	1649.5231
2463.3628	2473.6387	2483.5467
2489.4909	2496.2145	2499.3194
3462.6724	3465.5691	3555.3126
3562.1875	3562.5207	3564.8369

TS7

Zero-point correction= 0.138045 (Hartree/Particle)

Thermal correction to Energy= 0.147408

Thermal correction to Enthalpy= 0.148352

Thermal correction to Gibbs Free Energy= 0.104725

Sum of electronic and zero-point Energies= -166.238866

Sum of electronic and thermal Energies= -166.229503

Sum of electronic and thermal Enthalpies= -166.228559

Sum of electronic and thermal Free Energies= -166.272186

Cartesian coordinates

N	2.015299000000	-0.816003000000	0.004532000000
H	1.628059000000	-1.167672000000	0.880155000000
H	2.946648000000	-1.216663000000	-0.099287000000
B	2.051139000000	0.781425000000	-0.027051000000
H	2.723654000000	1.161520000000	0.899688000000
H	2.455994000000	1.131221000000	-1.107661000000
H	0.897817000000	1.188209000000	0.133748000000

N	-2.998225000000	-0.213561000000	-0.017776000000
H	-3.145510000000	-1.218174000000	-0.045494000000
H	-3.471851000000	0.179518000000	-0.825749000000
H	-3.477601000000	0.135518000000	0.806811000000
B	-0.656230000000	0.543162000000	0.042098000000
H	-0.504936000000	-0.127459000000	1.020280000000
H	-0.500793000000	0.056551000000	-1.038270000000
H	-1.081008000000	1.653407000000	0.139071000000
H	1.435463000000	-1.191963000000	-0.745821000000

Vibrational frequencies

-375.6448	62.8619	81.5890
88.5482	150.5887	166.7642
210.2510	216.8936	262.4305
319.5580	360.2480	701.7141
717.1119	795.5619	857.1050
887.2793	1006.8665	1075.8179
1079.9178	1099.6726	1148.5969
1154.9948	1160.0301	1194.9070
1248.4927	1405.8952	1632.2900
1633.4196	1637.2421	1645.0186
2310.0876	2505.9395	2538.7676
2569.0380	2659.3961	2672.1392
3469.4700	3495.8483	3554.5107
3576.7801	3620.1150	3621.0475

AaDB+NH_3

Zero-point correction= 0.139538 (Hartree/Particle)

Thermal correction to Energy= 0.148843

Thermal correction to Enthalpy= 0.149787

Thermal correction to Gibbs Free Energy= 0.106522

Sum of electronic and zero-point Energies= -166.256177

Sum of electronic and thermal Energies= -166.246873

Sum of electronic and thermal Enthalpies= -166.245929

Sum of electronic and thermal Free Energies= -166.289193

Cartesian coordinates

B	2.775068000000	0.077531000000	0.133113000000
H	2.809361000000	0.978620000000	-0.667631000000
H	3.724620000000	-0.660812000000	0.104306000000
H	2.435252000000	0.401763000000	1.237157000000
N	0.030467000000	0.639083000000	-0.104477000000
H	0.235094000000	1.162136000000	-0.955530000000
H	-1.007108000000	0.527708000000	-0.032000000000
B	0.683318000000	-0.787283000000	-0.110453000000
H	1.927740000000	-0.753283000000	-0.450217000000
H	0.296585000000	-1.402267000000	-1.068467000000
H	0.353722000000	1.204655000000	0.680035000000
H	0.541918000000	-1.338178000000	0.940244000000
N	-2.777159000000	-0.057795000000	0.077286000000
H	-2.751566000000	-1.028100000000	0.380724000000
H	-3.251246000000	-0.048257000000	-0.821796000000
H	-3.379463000000	0.435762000000	0.730212000000

Vibrational frequencies

51.0553	72.3082	98.8314
138.8372	190.9051	225.4946
290.2084	290.7114	323.5401
431.5503	476.5085	702.5024
747.4683	860.2455	871.5268
932.9936	1028.4244	1072.3856
1114.8135	1132.5774	1139.2014
1183.8218	1202.9841	1212.8250
1458.4567	1598.1162	1632.0469
1637.1803	1643.6835	1671.4992

2211.5985	2504.9683	2558.9039
2562.2182	2578.7825	2628.4206
3005.4586	3491.1362	3500.3572
3560.2361	3605.9435	3609.4868

$BH_3NH_2BH_2NH_2BH_2 \cdot H_2$

Zero-point correction= 0.154214 (Hartree/Particle)

Thermal correction to Energy= 0.162438

Thermal correction to Enthalpy= 0.163382

Thermal correction to Gibbs Free Energy= 0.122653

Sum of electronic and zero-point Energies= -191.713341

Sum of electronic and thermal Energies= -191.705117

Sum of electronic and thermal Enthalpies= -191.704173

Sum of electronic and thermal Free Energies= -191.744902

Cartesian coordinates

N	1.342061000000	-0.471882000000	0.027883000000
H	1.346594000000	-1.052496000000	0.865831000000
H	1.362723000000	-1.124999000000	-0.754649000000
B	2.710495000000	0.373139000000	0.001476000000
H	3.640910000000	-0.408334000000	0.079733000000
H	2.743990000000	0.988583000000	-1.046069000000
H	2.695849000000	1.130183000000	0.952122000000
N	-1.240350000000	-0.565086000000	-0.054189000000
H	-1.226816000000	-1.120448000000	-0.908819000000
H	-1.171207000000	-1.231106000000	0.716021000000
B	-2.585007000000	0.171094000000	0.086585000000
H	-3.422004000000	-0.075260000000	-0.722652000000
H	-2.955136000000	0.324080000000	1.208266000000
B	0.051210000000	0.400149000000	-0.022209000000
H	-0.038986000000	1.074575000000	0.975683000000
H	0.023816000000	1.049278000000	-1.039464000000

H -2.232762000000 1.570077000000 0.148421000000

H -2.362434000000 1.412732000000 -0.619550000000

Vibrational frequencies

82.7922	102.2228	146.5934
160.1481	201.3584	326.4073
339.0614	635.5708	650.7227
678.8633	698.8766	778.7320
782.9569	814.6947	861.8807
869.2810	887.0144	956.6646
976.2215	1027.0069	1079.3643
1105.8896	1126.9481	1148.9993
1175.3556	1189.3438	1198.5481
1206.4690	1207.6328	1220.2393
1231.5567	1237.2404	1245.0427
1602.5402	1608.5778	1638.6178
2424.2883	2437.9565	2446.9998
2507.4779	2531.6581	2640.2022
2703.1608	3485.7379	3486.2449
3547.8648	3549.5265	3731.4961

NaH+NH_3BH_3

Zero-point correction= 0.075372 (Hartree/Particle)

Thermal correction to Energy= 0.081365

Thermal correction to Enthalpy= 0.082309

Thermal correction to Gibbs Free Energy= 0.047339

Sum of electronic and zero-point Energies= -245.988250

Sum of electronic and thermal Energies= -245.982257

Sum of electronic and thermal Enthalpies= -245.981313

Sum of electronic and thermal Free Energies= -246.016284

Cartesian coordinates

N -1.425221000000 -0.517040000000 -0.000143000000

H	-2.010802000000	-0.665011000000	-0.820642000000
H	-2.011445000000	-0.664976000000	0.819908000000
B	-0.736041000000	0.926350000000	0.000183000000
H	-1.588700000000	1.777963000000	0.000270000000
H	-0.052677000000	0.994658000000	1.008408000000
H	-0.052491000000	0.995062000000	-1.007929000000
Na	1.734882000000	-0.024675000000	-0.000113000000
H	0.980036000000	-1.926987000000	0.001198000000
H	-0.690874000000	-1.251753000000	0.000122000000

Vibrational frequencies

149.5917	167.3843	258.1307
327.2155	404.0817	404.8648
730.9434	762.6666	807.7415
886.5889	1092.1637	1109.0301
1185.1702	1236.4472	1278.3850
1426.8836	1635.7175	1654.0621
2412.9737	2421.8901	2541.1091
3137.3850	3496.3237	3557.7850

$TS1_{0THF}$

Zero-point correction= 0.070319 (Hartree/Particle)

Thermal correction to Energy= 0.075873

Thermal correction to Enthalpy= 0.076817

Thermal correction to Gibbs Free Energy= 0.042559

Sum of electronic and zero-point Energies= -245.983327

Sum of electronic and thermal Energies= -245.977773

Sum of electronic and thermal Enthalpies= -245.976829

Sum of electronic and thermal Free Energies= -246.011086

Cartesian coordinates

N	1.354643000000	-0.509701000000	0.000003000000
H	1.930906000000	-0.693551000000	0.817233000000

H	1.930554000000	-0.693594000000	-0.817465000000
B	0.729726000000	0.925423000000	0.000093000000
H	1.543670000000	1.824207000000	-0.000029000000
H	0.023071000000	1.027312000000	-1.005287000000
H	0.023185000000	1.027249000000	1.005546000000
Na	-1.663114000000	-0.032766000000	-0.000086000000
H	-0.575014000000	-1.841406000000	0.000285000000
H	0.286757000000	-1.348999000000	0.000174000000

Vibrational frequencies

-1477.5428	139.8265	145.3402
301.7087	396.6092	519.5567
656.4081	771.3754	813.9807
875.6016	1035.2922	1117.0754
1186.8718	1245.6229	1283.5858
1503.1437	1529.9989	1544.8576
1601.0597	2307.5518	2321.8779
2469.2750	3509.6124	3590.1880

2THF·NaH

Zero-point correction= 0.241323 (Hartree/Particle)

Thermal correction to Energy= 0.255445

Thermal correction to Enthalpy= 0.256390

Thermal correction to Gibbs Free Energy= 0.198203

Sum of electronic and zero-point Energies= -627.461694

Sum of electronic and thermal Energies= -627.447572

Sum of electronic and thermal Enthalpies= -627.446628

Sum of electronic and thermal Free Energies= -627.504814

Cartesian coordinates

Na	0.014482000000	2.292018000000	-0.012638000000
C	-2.614328000000	0.374080000000	-0.806785000000
O	-1.550047000000	0.677760000000	0.114866000000

C	-1.411580000000	-0.383363000000	1.078943000000
C	-2.237715000000	-1.540611000000	0.532834000000
C	-3.364751000000	-0.798878000000	-0.190340000000
H	-3.226121000000	1.268322000000	-0.933764000000
H	-2.174676000000	0.100829000000	-1.771995000000
H	-0.348155000000	-0.610582000000	1.187348000000
H	-1.801268000000	-0.033860000000	2.040084000000
H	-1.649762000000	-2.127112000000	-0.179039000000
H	-2.590303000000	-2.202507000000	1.323675000000
H	-3.871062000000	-1.403287000000	-0.942734000000
H	-4.104316000000	-0.439562000000	0.529831000000
C	2.659101000000	0.425954000000	0.712719000000
O	1.532839000000	0.639181000000	-0.161236000000
C	1.357092000000	-0.496788000000	-1.027385000000
C	2.209980000000	-1.603128000000	-0.422456000000
C	3.374646000000	-0.801945000000	0.164560000000
H	3.272380000000	1.327979000000	0.712229000000
H	2.284089000000	0.249012000000	1.726120000000
H	0.291404000000	-0.730867000000	-1.072076000000
H	1.705597000000	-0.230908000000	-2.030513000000
H	1.662574000000	-2.116529000000	0.373466000000
H	2.519460000000	-2.337525000000	-1.166049000000
H	3.924193000000	-1.336017000000	0.939593000000
H	4.071094000000	-0.513540000000	-0.626786000000
H	0.178559000000	4.336503000000	0.148049000000

Vibrational frequencies

16.9077	46.3112	64.8084
80.4505	89.0675	99.9059
118.8737	150.6518	174.1458
189.0257	212.4234	229.9943
285.8752	296.1900	297.0981

582.0747	585.3333	685.9633
690.5326	843.9890	864.1684
866.8754	891.2397	893.4974
926.0150	929.7061	931.7817
937.5192	948.9500	949.7239
975.8277	978.5231	1048.5753
1051.8219	1109.8568	1111.2771
1168.3301	1170.0719	1194.8631
1196.6661	1200.5903	1202.3974
1269.4638	1270.9176	1272.0498
1273.9994	1317.3321	1320.3961
1346.7215	1347.3204	1380.6767
1381.4044	1411.7536	1413.4713
1479.2919	1480.4809	1489.8787
1491.1535	1513.7688	1519.6553
1529.1071	1535.4841	3050.1031
3056.1837	3061.9220	3065.4975
3069.1387	3070.7121	3077.9096
3082.7706	3116.7131	3119.5750
3122.7971	3135.3871	3136.1420
3138.5947	3144.0986	3148.8543

TS1$_{2THF}$

Zero-point correction= 0.309073 (Hartree/Particle)

Thermal correction to Energy= 0.327160

Thermal correction to Enthalpy= 0.328104

Thermal correction to Gibbs Free Energy= 0.261235

Sum of electronic and zero-point Energies= -710.612659

Sum of electronic and thermal Energies= -710.594571

Sum of electronic and thermal Enthalpies= -710.593627

Sum of electronic and thermal Free Energies= -710.660497

Cartesian coordinates

N	-2.720329000000	3.207732000000	0.478646000000
H	-3.002301000000	3.330528000000	1.447726000000
H	-3.157929000000	3.953249000000	-0.056467000000
B	-3.022520000000	1.774849000000	-0.078555000000
H	-4.203557000000	1.481437000000	-0.075512000000
H	-2.601013000000	1.727173000000	-1.235143000000
H	-2.400334000000	0.969075000000	0.609743000000
Na	-0.462979000000	1.215124000000	-0.643087000000
H	-0.391354000000	3.220507000000	0.256817000000
H	-1.392279000000	3.293383000000	0.382430000000
C	-2.046510000000	-1.615279000000	-0.951289000000
O	-0.772319000000	-1.035009000000	-0.607981000000
C	-0.350763000000	-1.507016000000	0.683969000000
C	-1.240468000000	-2.704110000000	0.991555000000
C	-2.551005000000	-2.291251000000	0.317421000000
H	-2.704575000000	-0.820789000000	-1.308312000000
H	-1.887338000000	-2.340472000000	-1.755442000000
H	0.713021000000	-1.747573000000	0.632637000000
H	-0.499376000000	-0.709420000000	1.422948000000
H	-0.837218000000	-3.605705000000	0.522536000000
H	-1.338804000000	-2.879761000000	2.062863000000
H	-3.211009000000	-3.131264000000	0.100230000000
H	-3.087670000000	-1.571155000000	0.940180000000
C	2.440104000000	1.189132000000	0.745101000000
O	1.713381000000	0.720252000000	-0.407096000000
C	2.450147000000	-0.325652000000	-1.066080000000
C	3.532674000000	-0.741078000000	-0.078931000000
C	3.833696000000	0.586420000000	0.620592000000
H	2.427779000000	2.279848000000	0.740674000000
H	1.932702000000	0.831305000000	1.647727000000

H	1.750513000000	-1.122526000000	-1.324921000000
H	2.886247000000	0.079372000000	-1.985130000000
H	3.135601000000	-1.464887000000	0.638530000000
H	4.398646000000	-1.178615000000	-0.575795000000
H	4.318898000000	0.467998000000	1.589434000000
H	4.463272000000	1.214624000000	-0.014955000000

Vibrational frequencies

-1442.7940	40.5983	48.4450
55.2342	57.4690	69.3898
78.5394	93.5370	102.2970
104.6039	109.6693	133.6520
167.9229	177.9053	180.1221
197.6295	249.6176	277.0008
280.6848	291.5604	367.0736
524.1045	577.4001	584.3952
625.3704	680.2663	688.6290
785.0613	815.3674	859.4931
868.5043	876.8342	886.4668
894.5043	925.5926	928.8874
930.0479	935.7198	947.1186
947.7470	979.1976	979.9436
1036.8376	1049.2614	1051.2178
1109.5280	1111.2001	1122.2260
1168.4619	1171.7575	1194.1241
1198.7411	1200.3003	1201.6451
1205.0890	1231.4238	1251.4913
1273.1898	1273.6331	1276.3314
1277.7581	1319.7742	1324.0432
1346.2960	1356.2027	1384.7948
1385.3157	1413.9178	1417.0009
1472.1853	1481.5878	1485.4209

1493.3535	1513.1972	1514.8954
1520.0928	1522.6392	1527.8261
1533.3197	1536.3908	1599.1680
2319.1665	2366.9827	2431.8522
3039.4867	3051.3856	3060.2700
3062.8318	3064.0230	3071.0420
3081.7750	3092.7306	3117.6632
3119.7716	3120.3506	3122.6762
3132.6941	3139.2968	3139.7282
3153.5068	3511.6648	3593.1389

3THF·NaH

Zero-point correction= 0.360535 (Hartree/Particle)

Thermal correction to Energy= 0.381062

Thermal correction to Enthalpy= 0.382006

Thermal correction to Gibbs Free Energy= 0.308484

Sum of electronic and zero-point Energies= -859.773966

Sum of electronic and thermal Energies= -859.753439

Sum of electronic and thermal Enthalpies= -859.752495

Sum of electronic and thermal Free Energies= -859.826018

Cartesian coordinates

Na	0.145355000000	-0.334611000000	-1.571519000000
C	1.919869000000	-2.320194000000	0.280528000000
O	1.469314000000	-0.954486000000	0.192014000000
C	2.599149000000	-0.064278000000	0.210038000000
C	3.803969000000	-0.936402000000	-0.111926000000
C	3.415816000000	-2.249746000000	0.570917000000
H	1.349974000000	-2.822580000000	1.064310000000
H	1.725439000000	-2.813222000000	-0.677744000000
H	2.427893000000	0.728522000000	-0.523295000000
H	2.683853000000	0.383156000000	1.207019000000

H	3.880127000000	-1.078480000000	-1.193018000000
H	4.736689000000	-0.511775000000	0.259911000000
H	3.948903000000	-3.116655000000	0.180831000000
H	3.592893000000	-2.183496000000	1.647712000000
C	-0.565377000000	1.604388000000	0.784673000000
O	-0.243817000000	1.672752000000	-0.617916000000
C	0.441289000000	2.902345000000	-0.906403000000
C	0.967422000000	3.389789000000	0.435417000000
C	-0.159879000000	2.953375000000	1.374955000000
H	-1.632542000000	1.395111000000	0.889192000000
H	0.002178000000	0.777003000000	1.221144000000
H	1.219926000000	2.694462000000	-1.642977000000
H	-0.270788000000	3.615672000000	-1.335353000000
H	1.896336000000	2.871356000000	0.687163000000
H	1.149567000000	4.464446000000	0.444524000000
H	0.151536000000	2.867909000000	2.416215000000
H	-0.990513000000	3.661367000000	1.316866000000
C	-3.010079000000	-0.295278000000	-0.886566000000
O	-1.787474000000	-1.007769000000	-0.621499000000
C	-1.923578000000	-1.800193000000	0.567810000000
C	-3.422644000000	-1.889519000000	0.819985000000
C	-3.893993000000	-0.515362000000	0.336604000000
H	-2.765263000000	0.753951000000	-1.068861000000
H	-3.465180000000	-0.715594000000	-1.788549000000
H	-1.449628000000	-2.767304000000	0.391749000000
H	-1.409626000000	-1.295074000000	1.393194000000
H	-3.861880000000	-2.679764000000	0.205423000000
H	-3.656213000000	-2.086119000000	1.866442000000
H	-4.954427000000	-0.483219000000	0.086203000000
H	-3.692239000000	0.241578000000	1.099477000000
H	1.248122000000	-0.578054000000	-3.337860000000

Vibrational frequencies

30.6062	36.6384	49.6550
53.1087	59.5854	72.7144
77.2661	81.1683	88.3981
92.1512	100.7435	112.1685
122.2272	150.5481	177.4343
209.1149	224.3550	228.6161
249.9940	276.8272	279.1676
281.2917	287.2646	577.1395
581.1799	582.5985	678.8256
687.9350	689.4232	778.8839
859.0191	861.3573	863.1752
888.5984	889.3072	891.3552
927.1886	927.5820	928.4196
930.6447	936.2765	941.8809
947.1925	947.4630	948.4774
978.9855	984.3663	986.4427
1049.4013	1052.0557	1053.6307
1112.1319	1114.5199	1117.0887
1170.3326	1171.2125	1171.9808
1198.3545	1199.1509	1200.0955
1205.4445	1208.9775	1211.0553
1269.9916	1272.1673	1273.3291
1274.7174	1276.2566	1278.3893
1320.5594	1321.2182	1321.5105
1347.1097	1348.0786	1350.3905
1380.5834	1381.5607	1383.0112
1411.8685	1413.4257	1415.2983
1473.1684	1476.0008	1479.4308
1485.5120	1488.8899	1491.9617
1519.1780	1520.4855	1524.7749

1530.5242	1533.3413	1534.4949
3051.2282	3059.5742	3060.8408
3063.7302	3065.9123	3066.2739
3068.1542	3068.9674	3069.2486
3073.7214	3075.3874	3075.5408
3116.5743	3116.8673	3118.7423
3122.5309	3123.1927	3129.5956
3132.9512	3133.7191	3140.3498
3141.5505	3146.7855	3147.6591

$TS1_{3THF}$

Zero-point correction= 0.427961 (Hartree/Particle)

Thermal correction to Energy= 0.452497

Thermal correction to Enthalpy= 0.453441

Thermal correction to Gibbs Free Energy= 0.370604

Sum of electronic and zero-point Energies= -942.926643

Sum of electronic and thermal Energies= -942.902107

Sum of electronic and thermal Enthalpies= -942.901162

Sum of electronic and thermal Free Energies= -942.984000

Cartesian coordinates

N	-2.217217000000	2.087748000000	3.036303000000
H	-2.612263000000	1.736330000000	3.905036000000
H	-2.306436000000	3.100469000000	3.058207000000
B	-2.855330000000	1.439226000000	1.757415000000
H	-4.048981000000	1.655905000000	1.647720000000
H	-2.266409000000	1.885508000000	0.776054000000
H	-2.670625000000	0.224432000000	1.817688000000
Na	-0.526274000000	0.330447000000	0.957011000000
H	0.025182000000	1.449824000000	2.814388000000
H	-0.933758000000	1.762954000000	2.972694000000
C	-2.213059000000	-1.930640000000	-0.537199000000

O	-1.369191000000	-0.805662000000	-0.846233000000
C	-2.034016000000	0.040965000000	-1.793868000000
C	-3.515953000000	-0.192653000000	-1.548247000000
C	-3.539899000000	-1.698934000000	-1.270571000000
H	-1.714484000000	-2.848885000000	-0.857534000000
H	-2.347419000000	-1.962565000000	0.547970000000
H	-1.704954000000	1.065400000000	-1.612007000000
H	-1.748209000000	-0.256324000000	-2.810615000000
H	-3.836440000000	0.368767000000	-0.667136000000
H	-4.132630000000	0.096339000000	-2.399923000000
H	-4.395326000000	-2.011016000000	-0.671531000000
H	-3.554976000000	-2.254144000000	-2.211398000000
C	1.395905000000	0.793128000000	-1.542668000000
O	0.684629000000	1.524225000000	-0.531503000000
C	1.365200000000	2.758112000000	-0.238907000000
C	2.433169000000	2.904070000000	-1.318058000000
C	2.771990000000	1.441983000000	-1.620363000000
H	1.408333000000	-0.259843000000	-1.254654000000
H	0.860913000000	0.891234000000	-2.494158000000
H	0.630458000000	3.565287000000	-0.237445000000
H	1.809418000000	2.682998000000	0.759118000000
H	2.013738000000	3.383963000000	-2.206095000000
H	3.288313000000	3.487265000000	-0.976437000000
H	3.243878000000	1.297660000000	-2.592716000000
H	3.430834000000	1.036502000000	-0.846718000000
C	2.350743000000	-0.818144000000	1.394402000000
O	1.019310000000	-1.307892000000	1.150922000000
C	1.074032000000	-2.567398000000	0.462904000000
C	2.515748000000	-3.041197000000	0.597418000000
C	3.275510000000	-1.712402000000	0.576825000000
H	2.388486000000	0.235776000000	1.105876000000

H	2.560408000000	-0.895734000000	2.465574000000
H	0.347083000000	-3.240772000000	0.920424000000
H	0.799054000000	-2.407281000000	-0.585511000000
H	2.661350000000	-3.546004000000	1.556107000000
H	2.804270000000	-3.719709000000	-0.205520000000
H	4.274881000000	-1.775200000000	1.007569000000
H	3.358295000000	-1.341131000000	-0.448837000000

Vibrational frenquencies

-1423.5232	21.2991	33.9724
40.1688	48.1280	54.5147
63.4902	69.4121	75.7885
82.3529	90.0349	91.9988
101.3447	104.5190	113.6476
118.0724	125.9151	136.2357
156.6506	176.6558	184.1771
199.8807	237.9359	244.4715
277.8641	284.4569	286.8111
295.4614	332.0757	521.3094
581.5016	586.8266	586.9856
588.1730	683.7122	686.4304
690.1387	776.1342	815.6250
844.2130	856.8231	862.4249
870.2779	888.8528	890.2606
892.9377	927.1567	928.8808
929.5418	933.1312	936.5005
941.9449	944.6694	947.8109
949.7256	969.9142	976.2960
979.3598	1040.0328	1044.4324
1048.6852	1056.1417	1113.5241
1115.1978	1116.7204	1117.5875
1165.2925	1166.1292	1168.6539

1183.2334	1199.3146	1199.7222
1201.4805	1201.9718	1203.4871
1220.8030	1223.8328	1237.9295
1266.1796	1268.6016	1271.0384
1273.4185	1276.4614	1280.9813
1319.0725	1320.3687	1323.6262
1343.3821	1345.5950	1350.3231
1376.4541	1378.3530	1380.1989
1409.2813	1410.9407	1412.7444
1477.0200	1477.8056	1480.0538
1488.3320	1488.8220	1490.0998
1491.8826	1513.5083	1516.0800
1520.7305	1524.1876	1526.1662
1527.2130	1528.5168	1532.3981
1600.4541	2344.6994	2364.2703
2424.0725	3035.9596	3051.1652
3054.7723	3060.8489	3064.2228
3065.1731	3065.6097	3069.1259
3071.1860	3074.2055	3075.1711
3084.7738	3108.0852	3116.9288
3120.7549	3121.8606	3123.9788
3132.3939	3138.0986	3139.9330
3142.8745	3145.2335	3149.7719
3150.7382	3513.1725	3594.5128