Supporting Information

Unraveling a general mechanism of converting ionic B/N complexes into neutral B/N analogues of alkanes: $H^{\delta+}\cdots H^{\delta-}$dihydrogen bonding assisted dehydrogenation

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1. Experimental Section:

1.1. General Remarks.

All manipulations were carried out on a Schlenk line or in a glove box 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 $^{1}H\{^{11}B\}$ NMRspectra was obtained at 600 MHz spectrometer. X-ray diffraction (XRD) data were obtained with a Rigaku D/max2500diffractometer using Cu/Karadiation, λ = 0.1542 nm, 40 kV, 100 mA. IR spectra were measured by a Spectrum 400F.

NH_3, NH_3BH_3 (AB), $NaBH_4$, tetrahydrofuran (THF) solution of $(CH_3)_2NH$ (2 M), diethyl ether solution of HCl were used as received. NaH was washed with THF and hexane and then dried undervacuum. Ammonium chloride (NH_4Cl) was recrystallized in methanol. The $NH_3BH_2NH_2BH_3$, $Na[BH_3NH_2BH_3]$, $Na[BH_3NH_2BH_2NH_2BH_3]$ and $[NH_3BH_2NH_3]Cl$ were prepared according the literature methods.[1] THF and hexane were dried over sodium and freshly distilled prior to use.

The theoretical calculations were performed at the level of density functional theory (DFT) with hybridmeta-GGA functional M06-2X[2-4] using the Gaussian 09 program.[5] Gaussian basis sets 6-311++G(d, p) were used for all atoms involved in the model reaction. The solvent effect was considered by using the SMD model[6] in THF solvent for all kinds of calculations. After the structural optimizations for all the stationary points, vibrational frequency calculations at the same level of theory were carried out to identify all of the stationary points as minima (zero number of imaginary frequency) or transition state (with only one imaginary frequency), and to provide corrections for Gibbs free energies. In order to obtain more accurate energy atthe DFT-optimized structures, the DLPNO-CCSD(T)/def2-TZVP single-point energy calculations[7] have been done using the ORCA program,[8] with the setting of tightscf and grid4.

1.2. Stability of $[NH_3BH_2NH_3]BH_4$.

The $[NH_3BH_2NH_3]BH_4$ was prepared according the literature method.[1b] The $[NH_3BH_2NH_3]BH_4$ (10 mmol, 0.62 g) was placed in a flask, and then 30 mL of THF was injected. The solution was stirred for 2 hours at room temperature and $[NH_2BH_2]_n$ precipitated was formed (0.27 g, 93%, Fig. S1).[9] After the precipitate being filtered out, the THF was removed from the filtrate under a dynamic vacuum to leave white powder product NH_3BH_3 (0.28 g, 91%, Fig. S2 and S3). NH_3BH_3: ^{11}B NMR (128 MH_Z, THF): δ -22.3 (q, $J_{B\text{-}H}$ = 95 Hz) ppm (Fig. S2).

1.3. The determination of the THF·BH_3 intermediate formed in the dehydrogenation process of $[NH_3BH_2NH_3]BH_4$.

The prepared $[NH_3BH_2NH_3]BH_4$ (5 mmol, 0.31 g) was placed in a flask, and then 20 mL of THF and $(CH_3)_2NH$ (3 mmol, 1.5 mL) were injected at -40 °C. Then the reaction solution was warm up to room temperature. After stirred for 10 min, the reaction solution was monitored by ^{11}B NMR (Fig. 2a) and $^{11}B\{^1H\}$ NMR (Fig. S4a).

1.4. The determination of the $THFBH_2NH_2BH_3$ intermediate formed in the dehydrogenation process of $[NH_4][BH_3NH_2BH_3]$.

The $[NH_4][BH_3NH_2BH_3]$ sample was prepared according the literature method.[10] The prepared $[NH_4][BH_3NH_2BH_3]$ (5 mmol, 0.31 g) was placed in a flask, and then 20 mL of THF and $(CH_3)_2NH$ (3 mmol, 1.5 mL) were injected at -40 °C. Then the reaction solution was warm up to room temperature. After stirred for 10 min, the reaction solution was monitored by ^{11}B NMR (Fig. 2b) and $^{11}B\{^1H\}$ NMR (Fig. S4b).

1.5. Synthesis of $NH_3BH_2NH_2BH_2Cl$.

The prepared $NH_3BH_2NH_2BH_3$ (5 mmol, 0.30 g) was added to a flask and then 30 mL of THF was injected. A solution of 1 M HCl in diethyl ether (5 mL, 5 mmol) was added dropwise to the flask at room temperature and stirred for 1 hour (eqn (S1)). Then the THF was removed from the reaction solution under a dynamic vacuum to leave white powder product $NH_3BH_2NH_2BH_2Cl$ (0.40 g, 85%). ^{11}B NMR (128 MHz, THF-d_8): δ -8.4 (*t*, $J_{B\text{-}H}$ = 113 Hz, BH_2Cl), -13.1 (*q*, $J_{B\text{-}H}$ = 103 Hz, BH_2) ppm (Fig. S5a). $^{11}B\{^1H\}$ NMR (128 MHz, THF-d_8): δ -8.4 (*s*, BH_2Cl), -13.1 (*s*, BH_2) ppm (Fig. S5b). ^1H NMR (600 MH_Z, THF-d_8): δ 4.60 (*br t*, 3H of NH_3), 3.07 (*br s*, 2H of NH_2), 2.53 (*q*, 2 H of $ClBH_2$), 2.02 (*q*, 2 H of BH_2) ppm (Fig. S6a). $^1H\{^{11}B\}$ NMR (600 MH_Z, THF-d_8): δ 4.60 (*br t*, 3H of NH_3), 3.07 (*br s*, 2H of NH_2), 2.53 (*m*, 2 H of $ClBH_2$), 2.02 (*m*, 2 H of BH_2) ppm (Figure S6b). IR (cm^{-1}): 3111 (s, br), 2413 (s), 2343 (s), 1585 (m), 1410 (s), 1268 (s), 1212 (s), 1136 (s), 1040 (m), 981 (w), 877 (m), 814 (m), 718 (w) (Fig. S7).

$$HCl + NH_3BH_2NH_2BH_3 \rightarrow NH_3BH_2NH_2BH_2Cl + H_2 \qquad (S1)$$

1.6. Synthesis of $[NH_3BH_2NH_2BH_2NH_3]Cl$.

$NH_3BH_2NH_2BH_2Cl$ (0.47 g, 5 mmol) was placed in a flask, and the 20 mL of THF was injected into the flask. Then excess NH_3 was bubbleed into the flask at 0 °C and more white precipitate produced immediately (eqn (S2)). The solid was filtration, and washed with THF (3 × 20 mL) and dried under a dynamic vacuum to yield $[NH_3BH_2NH_2BH_2NH_3]Cl$ (0.51 g, 91%). ^{11}B NMR (128 MHz, DMF-d_7): δ -13.5 (*t*, $J_{B\text{-}H}$ = 103 Hz, BH_2) ppm (Fig. S8). ^1H NMR (600 MH_Z, DMF-d_7): δ 5.61 (*br s*, 6H of 2 NH_3),

3.83 (*s*, 2H of NH_2), 2.11 (*br*, 4 H of BH_2) ppm (Fig. S9a). $^1H\{^{11}B\}$ NMR (600 MH_Z, DMF-d_7): δ 5.60 (*br s*, 6H of 2 NH_3), 3.83 (*s*, 2H of NH_2), 2.11 (*s*, 4 H of BH_2) ppm (Fig. S9b). IR (cm^{-1}): 3277 (s), 3099 (br, s), 2399 (s), 2345 (s), 2302 (m), 1609 (w), 1554 (w), 1410 (s), 1262 (m), 1214 (s), 1146 (s), 1070 (s), 997 (m), 917 (m), 808 (m), 703 (w), 655 (w) (Fig. S10).

$$NH_3BH_2NH_2BH_2Cl + NH_3 \rightarrow [NH_3BH_2NH_2BH_2NH_3]^+Cl^- \qquad (S2)$$

1.7. Synthesis of $[NH_3BH_2NH_2BH_2NH_3]BH_4$.

The prepared $[NH_3BH_2NH_2BH_2NH_3]Cl$ (4.5 mmol, 0.51 g) and $NaBH_4$ (4.5 mmol, 0.17 g) were added to a flask and then 30 mL of liquid NH_3 was condensed into the flask at -78 °C and stirred for 1 hour (eqn (S3)). Then the reaction was warm up to room temperature and liquid NH_3 was volatilized completely to leave a white product. The solid product was extracted with 100 mL of THF at -78 °C and the THF solution was monitored by ^{11}B NMR at low temperatures (Fig. S11a). Some white precipitate was filtered out and then the resulting residue was dried under a dynamic vacuum to give white product, which was confirmed by XRD to be pure NaCl (Fig. S12). Then the filtrate was warm up to room temperature and stirred for 1 hour. During this time, some white precipitate produced. Then the resulting precipitate was filteredanddried under dynamic vacuum to give the $[NH_2BH_2]_n$ white product, which was confirmed by IR (0.24 g, 91%, Fig. S13). Removal of THF from the filtrate under dynamic vacuum gave NH_3BH_3 as a white product (0.13 g, 93%, Fig. S14). $[NH_3BH_2NH_2BH_2NH_3]BH_4$: ^{11}B NMR (193 MHz, THF): δ -14.3 (*br*, BH_2), -37.7 ppm (*q*, J_{B-H}= 81 Hz, BH_4) (Fig. S11a). $[NH_2BH_2]_n$: IR (cm^{-1}): 3300 (s), 3248 (s), 2399 (s, br), 1560 (s), 1405 (s, br) 1208 (s, br), 1082 (s), 1059 (s), 846 (m), 710 (w) (Fig. S13).

$$NH_3BH_2NH_2BH_2NH_3]^+Cl^- + NaBH_4 \rightarrow [NH_3BH_2NH_2BH_2NH_3]^+[BH_4]^- + NaCl \qquad (S3)$$

1.8. Reaction of $[NH_3BH_2NH_3]Cl$ with $Na[BH_3NH_2BH_3]$.

$Na[BH_3NH_2BH_3]$ (0.34 g, 5 mmol) and $[NH_3BH_2NH_3]Cl$ (0.41 g, 5mmol) were added to a flask and then 30 mL of liquid NH_3 was condensed into the flask at -78 °C and stirred for 2 hours. Then the reaction was warm up to room temperature and liquid NH_3 was volatilized completely to leave a white product. The solid product was extracted with 100 mL of THF at -78 °C. Some white precipitate (NaCl, Fig. S15) was filtered out and then the filtrate was warm up to room temperature and stirred for 1 hour. During this time, some white precipitate produced. Then the resulting precipitate was filtered and dried under dynamic vacuum to give the $[NH_2BH_2]_n$ white product (Fig. S16).[9] Removal of THF from the filtrate under dynamic vacuum gave $NH_3BH_2NH_2BH_3$ as a white product (0.23 g, 76%).[1c] $NH_3BH_2NH_2BH_3$: ^{11}B NMR (193 MHz,THF): δ -11.6 (*t*, J_{B-H} = 103 Hz, BH_2), -22.7 (*q*, J_{B-H} = 92 Hz, BH_3) ppm (Fig. S17a). $^{11}B\{^1H\}$ NMR (193 MHz,THF): δ -11.6 (*s*, BH_2), -22.7 (*q*, BH_3) ppm (Fig.

S17b). $[NH_2BH_2]_n$: IR (cm^{-1}): 3248 (s), 2946 (w), 2342 (s, br), 1402 (s), 1170 (m), 1053 (m), 863 (w), 810 (w) 705 (w) (Fig. S16).

1.9. Reaction of $Na[BH_3NH_2BH_2NH_2BH_3]$ with $[NH_3BH_2NH_3]Cl$.

The prepared $Na[BH_3NH_2BH_2NH_2BH_3]$ (0.48 g, 5 mmol) and $[NH_3BH_2NH_3]Cl$ (0.41 g, 5mmol) were added to a flask and then 30 mL of liquid NH_3 was condensed into the flask at -78 °C and stirred for 2 hours. Then the reaction was warm up to room temperature and liquid NH_3 was volatilized completely to leave a white product. The solid product was extracted with 100 mL of THF. The formed NaCl was filtered out. Then THF was removed from the filtrate under a dynamic vacuum to leave white powderproduct (0.41 g), which was confirmed by XRD (Fig. S18) and ^{11}B NMR (Fig. S19) to be a mixture of $NH_3BH_2NH_2BH_2NH_2BH_3$ and NH_3BH_3.

2. Table:

Table S1. Energies of the stationary points obtained by DLPNO-CCSD(T)/def2-TZVP and M06-2X/6-311++G(d, p)/SMD_{THF} calculations.

	Thermal Correction to Gibbs Free Energy using M06-2X (a.u.)	Single-Point Energy using DLPNO-CCSD(T) (a.u.)
DADB+THF	0.211895	-398.1032104
TS1	0.207625	-398.0707613
THF	0.089014	-232.0212807
$NH_3BH_2NH_2$+BH_3·H_2	0.10153	-166.0508035
pre-TS2	0.214391	-398.082362494
TS2	0.210981	-398.0766076
H_2	-0.001322	-1.168270988
$NH_3BH_2NH_2$+THF·BH_3	0.198304	-396.9317739
TS3	0.199739	-396.9142909
$NH_3BH_2NH_2BH_3$	0.095262	-164.9178262
TS4	0.195469	-396.9282474
NH_2BH_2	0.025576	-81.87207442
NH_3+THF· BH_3	0.148345	-315.0510024
TS5	0.15036	-315.0393899
NH_3BH_3	0.048163	-83.03935266
AADB	0.110629	-166.0650988
TS6	0.104732	-166.0437454
NH_3	0.015341	-56.46050045
$BH_3NH_2BH_2$·H_2	0.069671	-109.5759111
TS7	0.179075	-341.6145166
$THFBH_2NH_2BH_3$	0.16914	-340.4776273
TS8	0.1981	-396.9111914
TS9	0.201121	-396.9260331

* 1 a.u. = 627.503 kcal/mol.

3. Supporting Results:

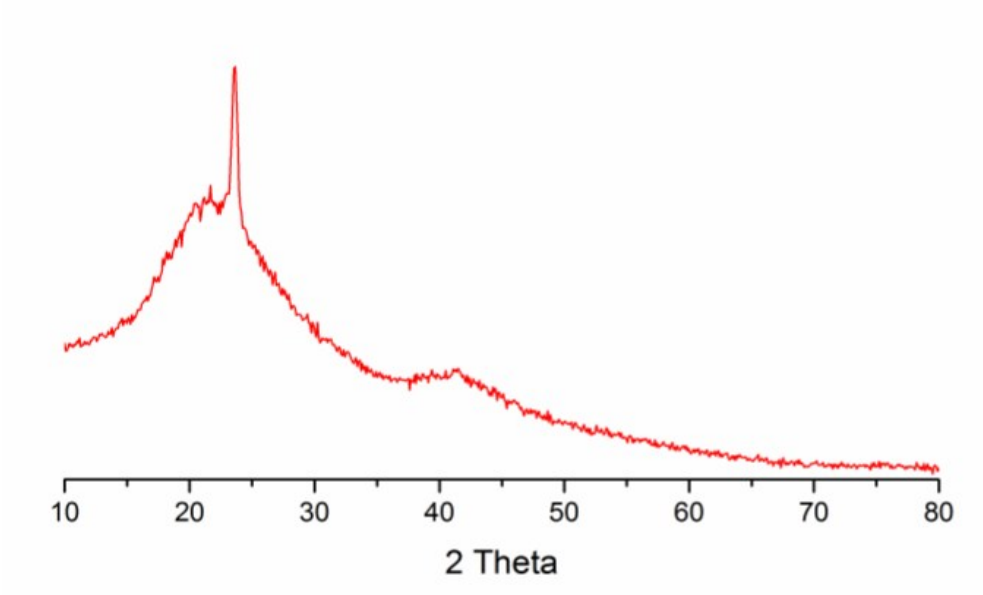

Fig. S1 X-ray powder diffraction data of the formed $[NH_2BH_2]_n$.

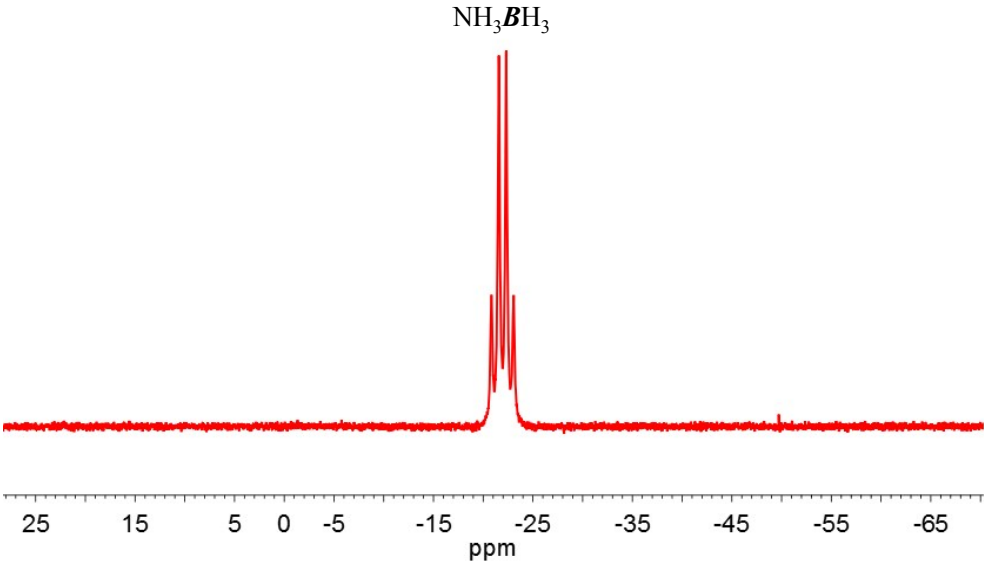

Fig. S2 ^{11}B NMR spectrum of the formed NH_3BH_3.

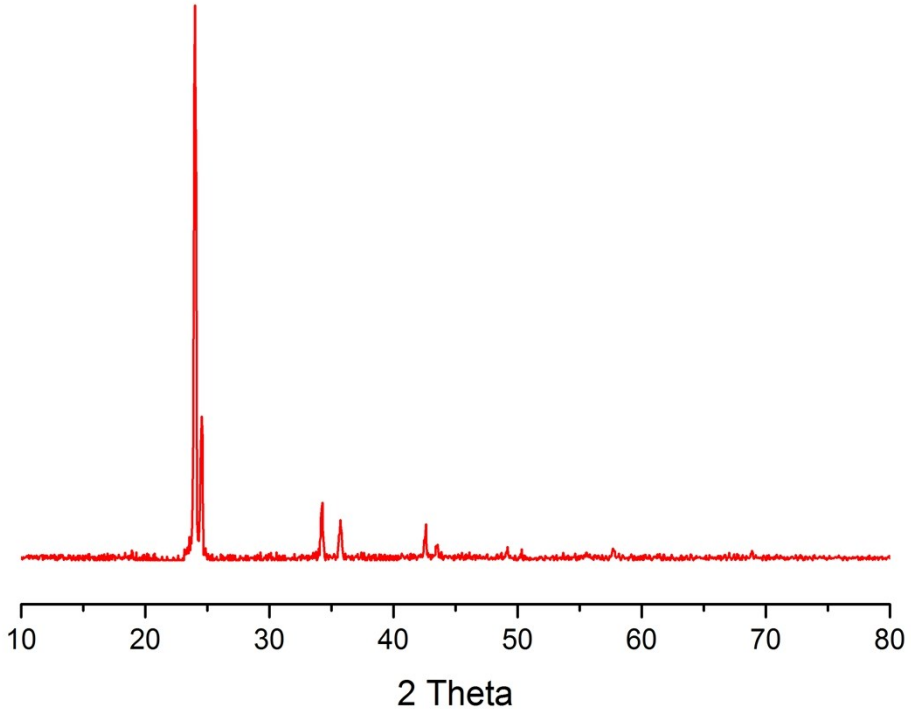

Fig. S3 X-ray powder diffraction data of the formed NH_3BH_3.

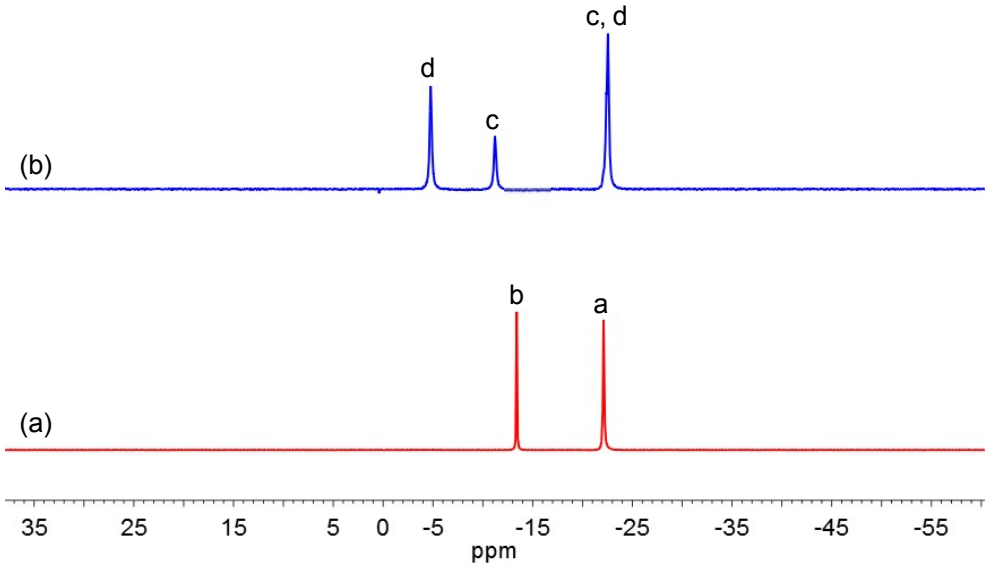

Fig. S4 The $^{11}B\{^1H\}$ NMR spectra of the products when (a) DADB and (b) AADB dehydrogenate in THF with the presence of $(CH_3)_2NH$. a, NH_3BH_3; b, $(CH_3)_2NHBH_3$; c, $NH_3BH_2NH_2BH_3$; d, $(CH_3)_2NHBH_2NH_2BH_3$.

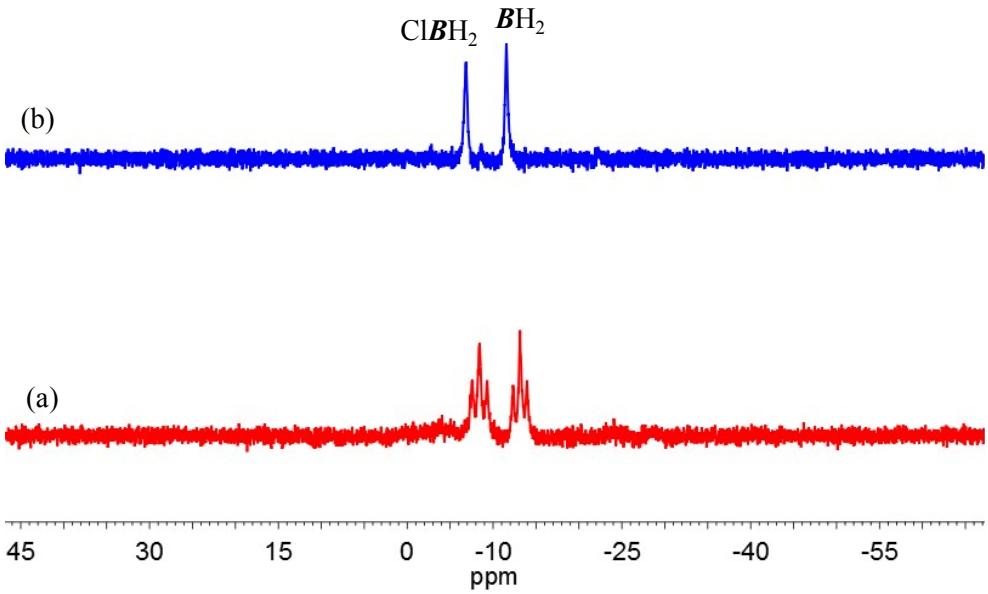

Fig. S5 ^{11}B NMR (a) and ^{11}B{^{1}H} NMR (b) spectra of the prepared $NH_3BH_2NH_2BH_2Cl$ in THF-d_8.

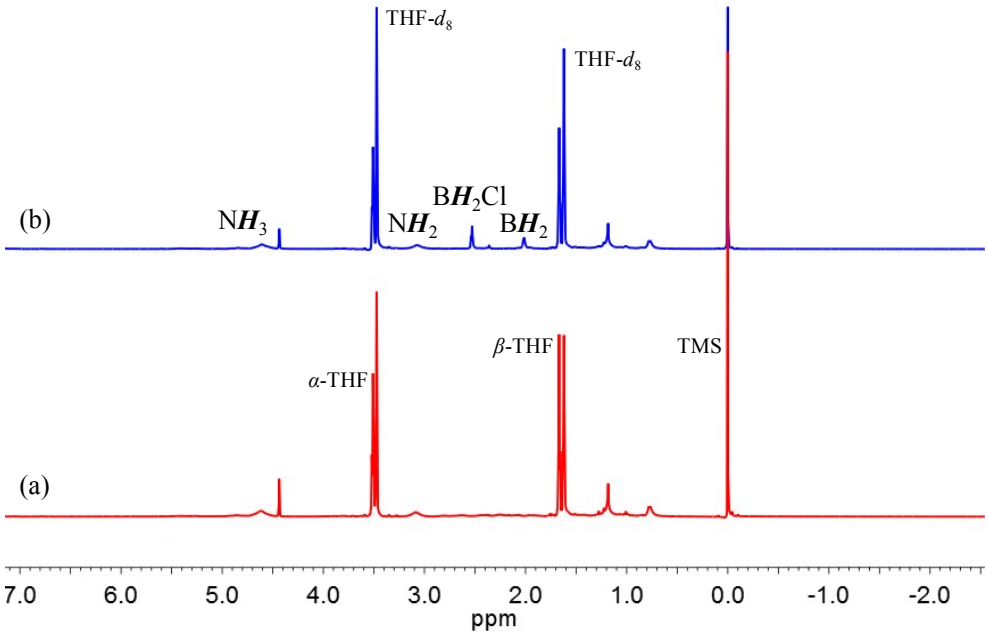

Fig. S6 ^{1}H NMR (a) and ^{1}H{^{11}B} NMR (b) spectra of the prepared $NH_3BH_2NH_2BH_2Cl$ in THF-d_8.

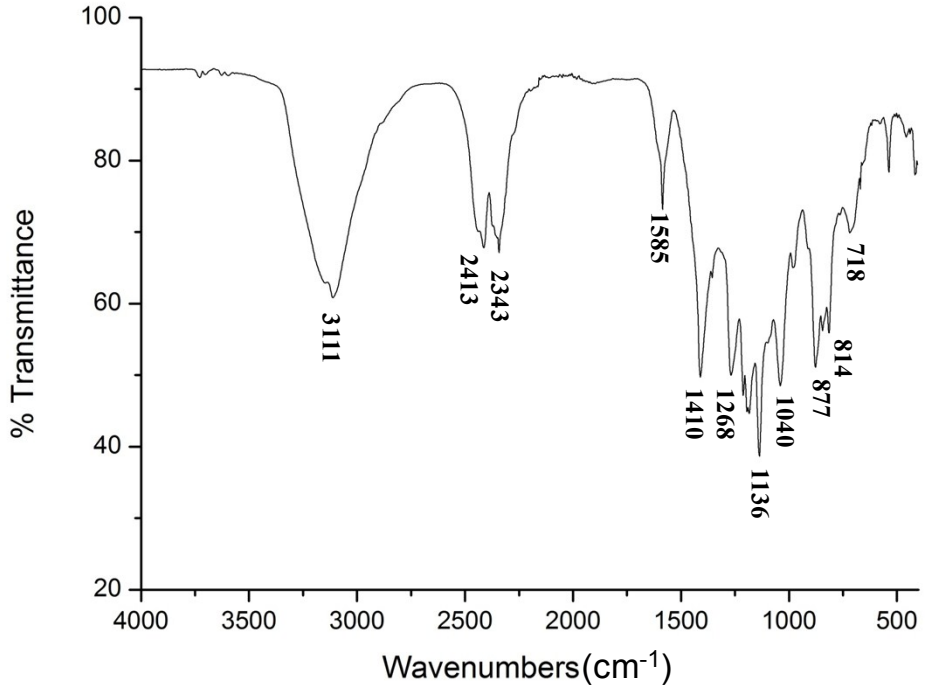

Fig. S7 IR spectrum of the prepared $NH_3BH_2NH_2BH_2Cl$.

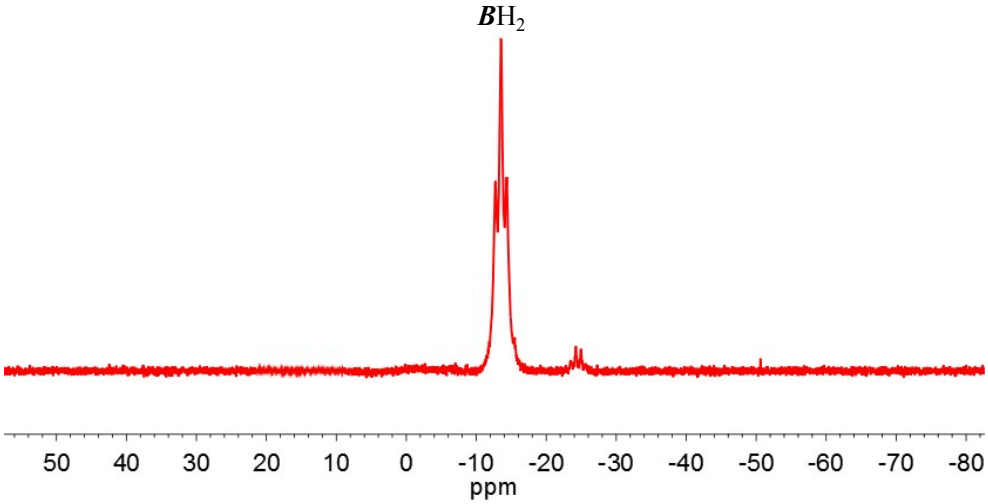

Fig. S8 ^{11}B NMR spectrum of the prepared $[NH_3BH_2NH_2BH_2NH_3]Cl$ in DMF-d_7.

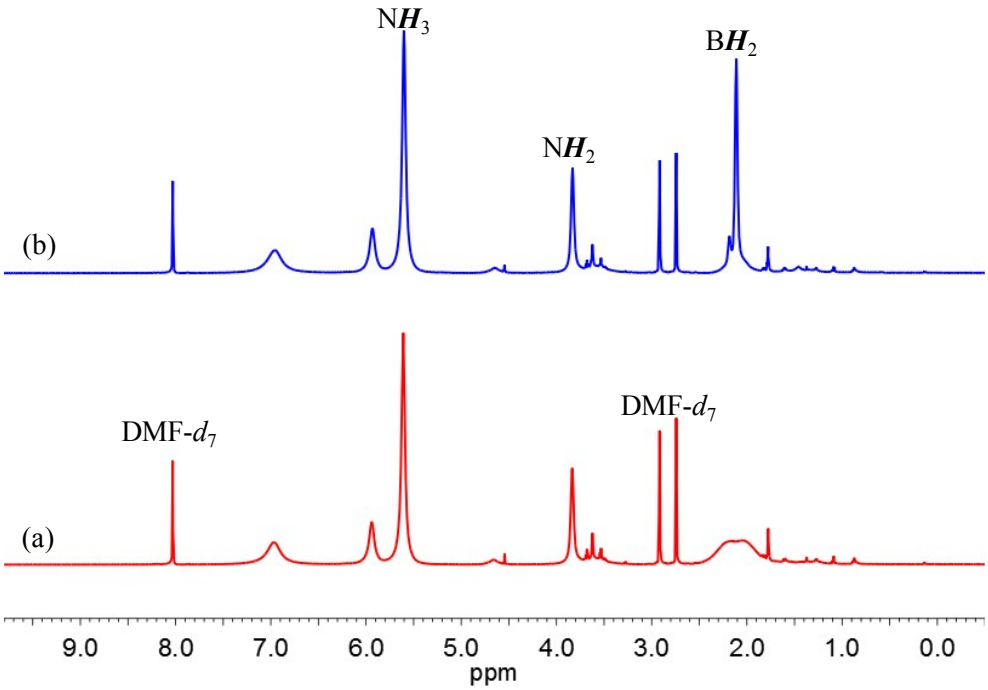

Fig. S9 ^{1}H NMR (a) and ^{1}H{^{11}B} NMR (b) spectra of the prepared $[NH_3BH_2NH_2BH_2NH_3]Cl$ in DMF-d_7.

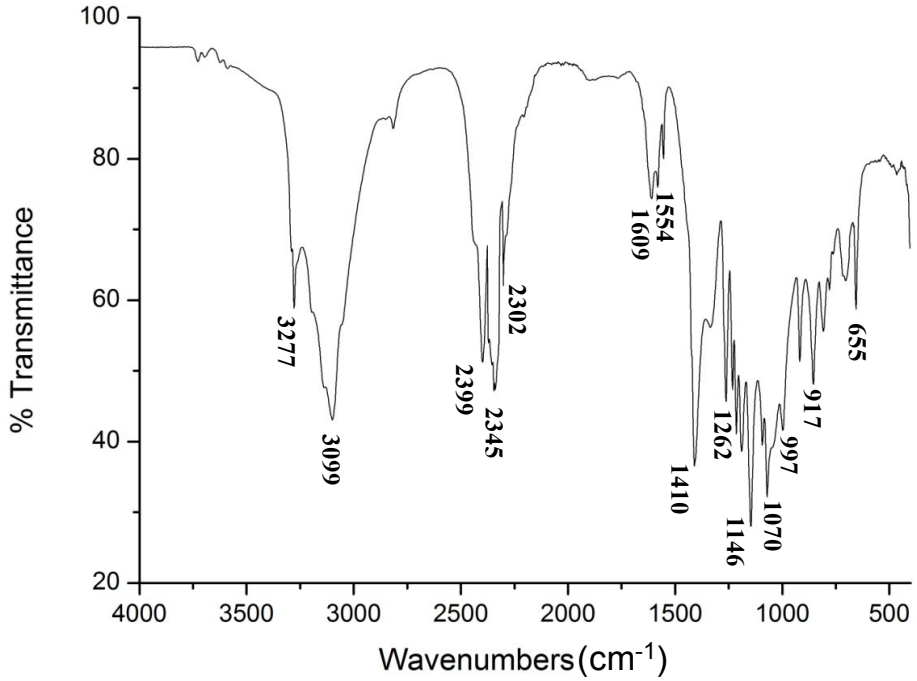

Fig. S10 IR spectrum of the prepared $[NH_3BH_2NH_2BH_2NH_3]Cl$.

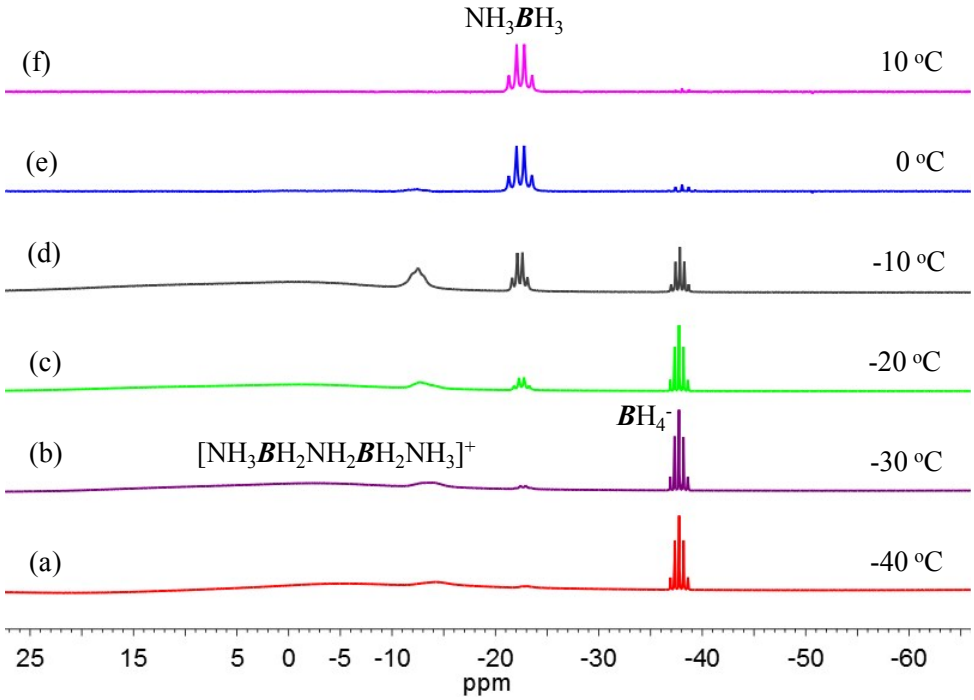

Fig. S11 Variable temperature ^{11}B NMR spectra of the prepared $[NH_3BH_2NH_2BH_2NH_3]^+[BH_4]^-$ in THF.

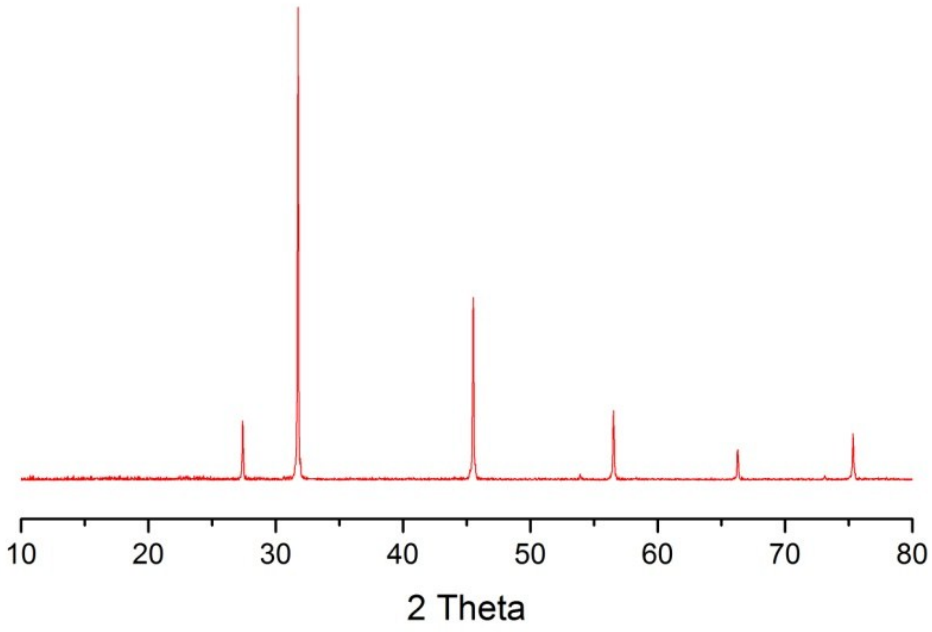

Fig. S12 X-ray powder diffraction data of the NaCl isolated from the reaction of $[NH_3BH_2NH_2BH_2NH_3]Cl$ with $NaBH_4$.

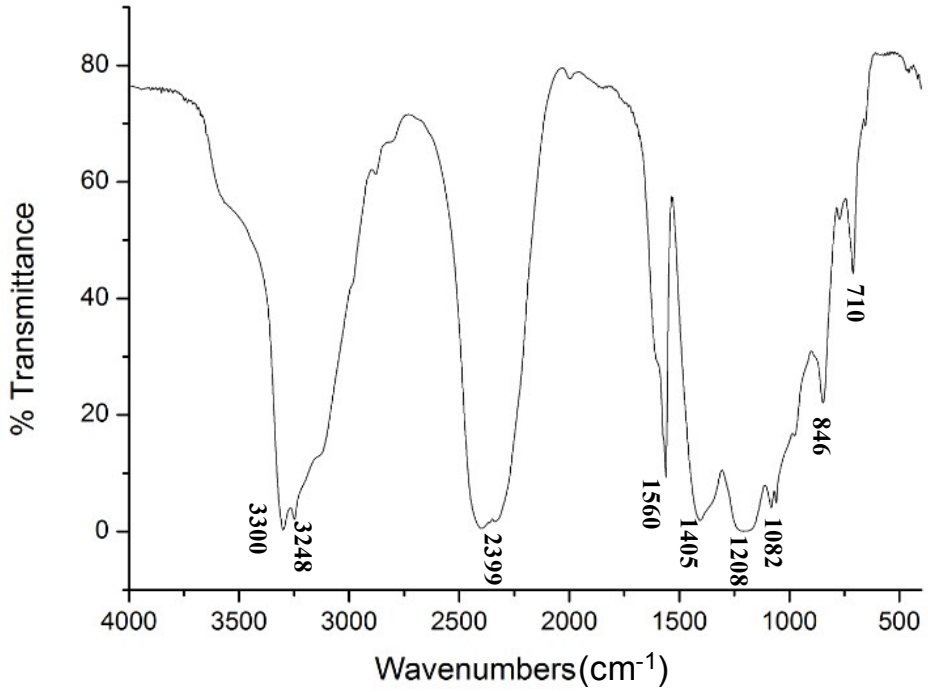

Fig. S13 IR spectrum of the formed $[NH_2BH_2]_n$.

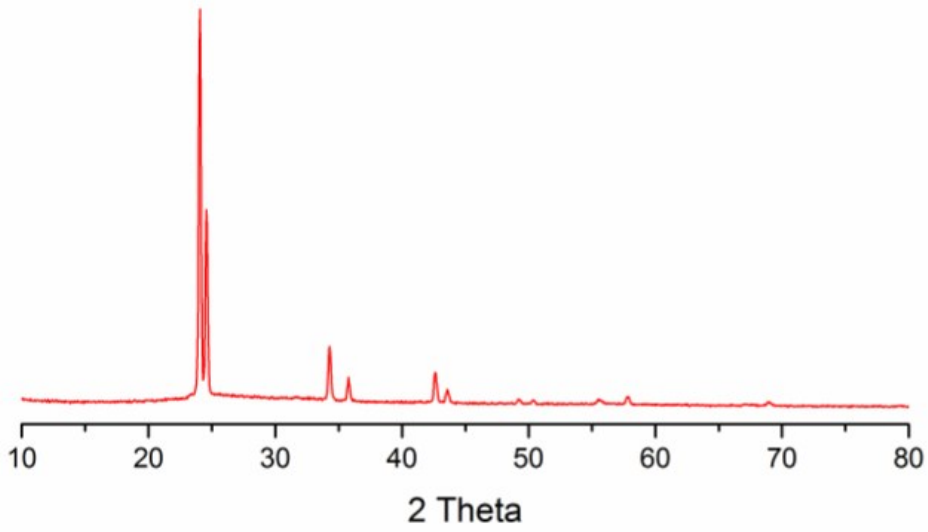

Fig. S14 X-ray powder diffraction data of the formed NH_3BH_3.

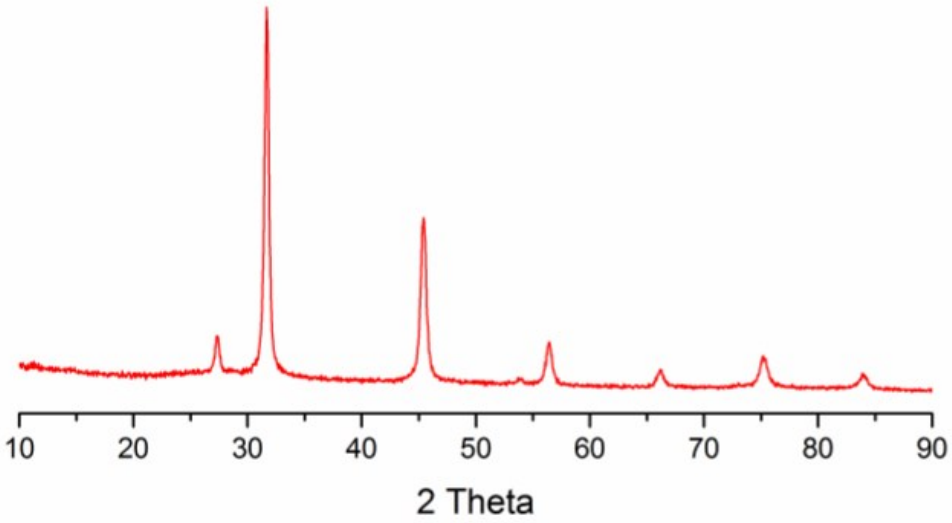

Fig. S15 X-ray powder diffraction data of the NaCl isolated from the reaction of $[NH_3BH_2NH_3]Cl$ with $Na[BH_3NH_2BH_3]$.

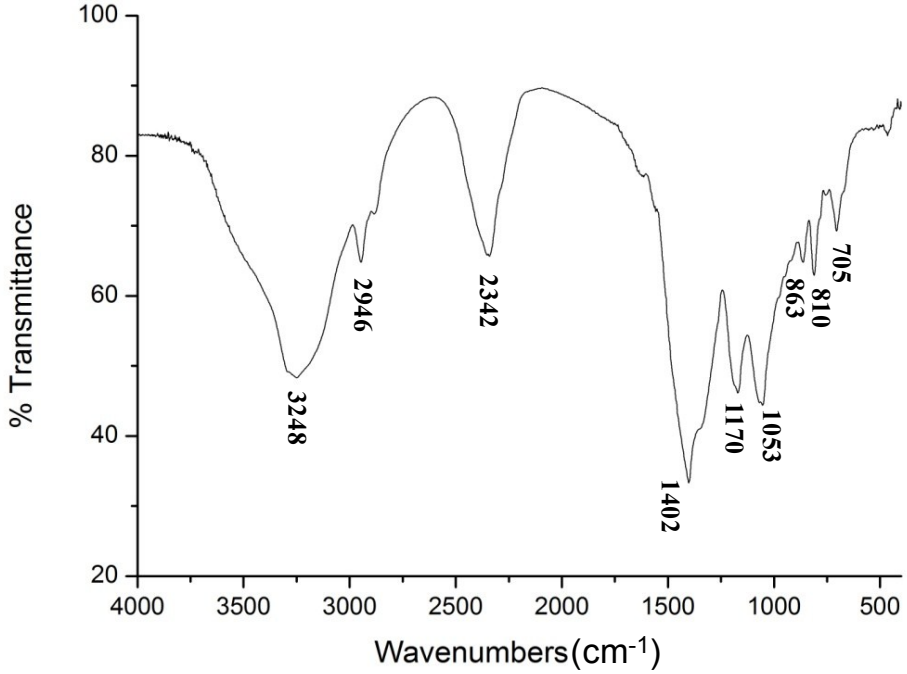

Fig. S16 IR spectrum of the formed $[NH_2BH_2]_n$ isolated from the reaction of $[NH_3BH_2NH_3]Cl$ with $Na[BH_3NH_2BH_3]$.

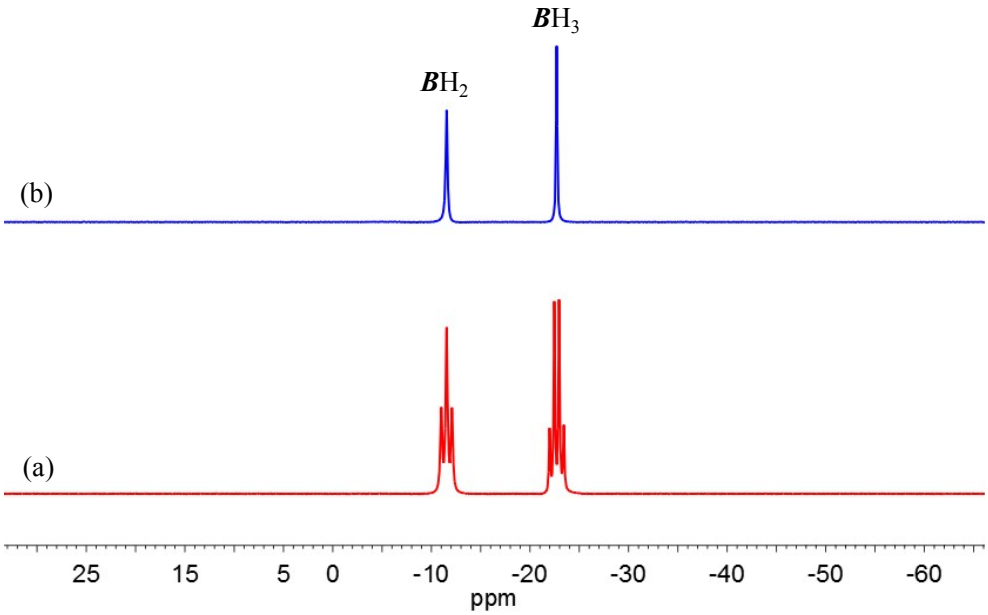

Fig. S17 ^{11}B NMR (a) and $^{11}B\{^{1}H\}$ NMR (b) spectra of the $NH_3BH_2NH_2BH_3$ in THF, which was isolated from the reaction of $[NH_3BH_2NH_3]Cl$ with $Na[BH_3NH_2BH_3]$.

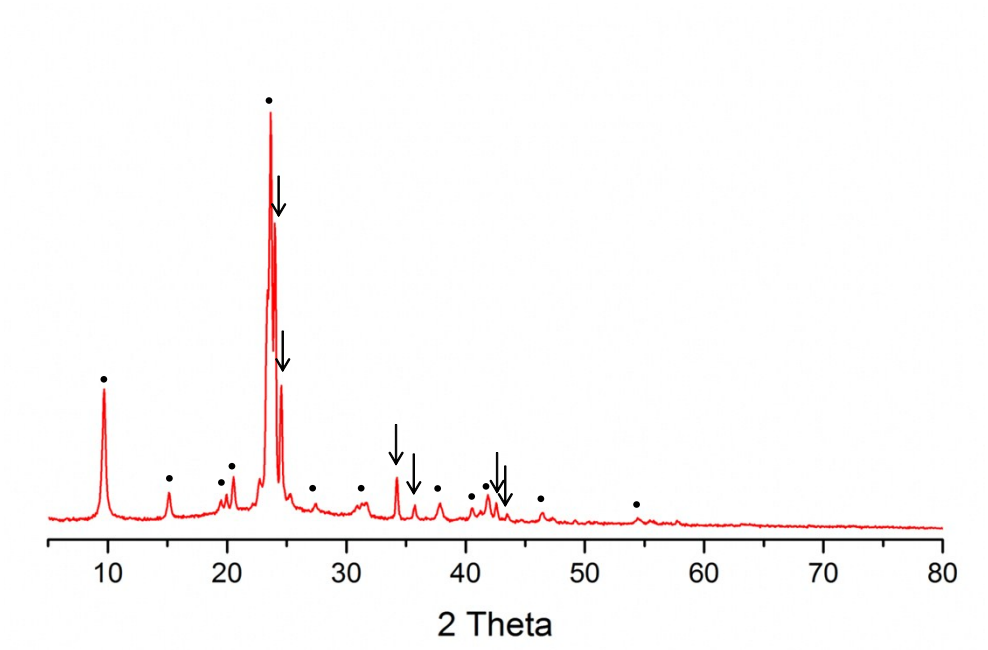

Fig. S18 X-ray powder diffraction data of a mixture of NH_3BH_3 (↓) and $NH_3BH_2NH_2BH_2NH_3$ (•) isolated from the reaction of $[NH_3BH_2NH_3]Cl$ and $Na[BH_3NH_2BH_2NH_2BH_3]$.

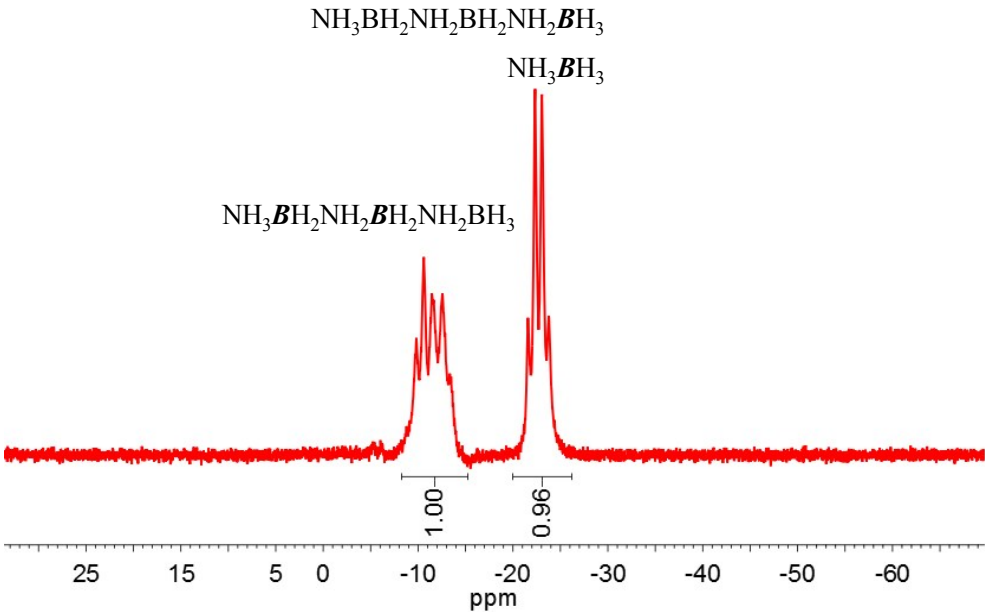

Fig. S19 ^{11}B NMR spectrum of the mixture of NH_3BH_3 and $NH_3BH_2NH_2BH_2NH_3$ in THF.

4. References:

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5. Geometrical Coordinates and Vibrational Frequencies of the Listed Compounds

Formation of NH_3BH_3

DADB+THF

Zero-point correction= 0.260367 (Hartree/Particle)
Thermal correction to Energy= 0.275759
Thermal correction to Enthalpy= 0.276703
Thermal correction to Gibbs Free Energy= 0.2
B 4.93204800 0.13511895
Sum of electronic and zero-point Energies= -398.575993
Sum of electronic and thermal Energies= -398.560601
Sum of electronic and thermal Enthalpies= -398.559656
Sum of electronic and thermal Free Energies= -398.624464
Cartesian coordinates38400 0.39350500

N	4.43720500	-1.10334200	-0.47003600
H	3.46247600	-1.36060000	-0.26391400
H	1.83943900	-0.38430900	1.00064600
H	6.03850200	0.44534900	0.04592100
H	4.83204600	-0.14586200	1.55564200
H	4.49784200	-0.94398600	-1.47672000
H	5.01340800	-1.92084900	-0.26710800
B	1.26928200	-0.73541100	-0.02828900
H	1.63092800	-1.87308300	-0.30907400
H	1.57963900	0.01665600	-0.94639600
H	0.06497900	-0.71821900	0.14027300
N	3.92789800	1.32397700	0.07446200
H	4.14634700	2.13635500	0.65157000
H	3.95991900	1.63279200	-0.89799300
H	2.95809300	1.04895800	0.27344400
C	-4.14485200	-0.75179800	-0.15507900
O	-3.80602100	0.31252300	-1.05253000
C	-2.66311800	1.01455800	-0.55500100
C	-2.58713300	0.67645400	0.92778500
C	-3.05582400	-0.78015200	0.91681500
H	-5.12706700	-0.53932300	0.28107400
H	-4.21039800	-1.68569500	-0.71886400
H	-1.76178600	0.66690100	-1.07431600
H	-2.80127400	2.07840600	-0.75775600
H	-1.58283600	0.80279800	1.33348800
H	-3.28370300	1.29997300	1.49562600
H	-2.23245800	-1.43006800	0.61027400
H	-3.43273200	-1.12505800	1.88023700

Vibrational frequencies

2.1732	21.3854	37.8046
47.4883	56.4819	71.8354

83.7288	103.4589	131.9415
146.0268	198.2343	238.9759
262.4903	279.8453	286.3347
334.2745	364.9833	581.2760
675.8569	694.3770	748.5113
781.2771	797.6357	854.4508
858.7596	890.2356	925.1980
937.8694	948.8810	974.4266
1033.2874	1046.9698	1094.9485
1106.2430	1109.8230	1122.2264
1129.3711	1132.6337	1169.6933
1194.9396	1201.2899	1204.5908
1229.2705	1232.8773	1268.4288
1270.2089	1274.1895	1318.5622
1341.6281	1378.9253	1413.8322
1422.0571	1436.6627	1475.7167
1491.1894	1518.3804	1529.5211
1622.7934	1631.2090	1640.2170
1646.8354	2355.1170	2358.7903
2361.4480	2444.8466	2557.0634
2595.4156	3041.3943	3048.4562
3062.7471	3075.8267	3101.7746
3114.0689	3139.4335	3144.0783
3363.2929	3384.6591	3497.1644
3509.0318	3549.0386	3559.3777

TS1

Zero-point correction= 0.254854 (Hartree/Particle)
Thermal correction to Energy= 0.269995
Thermal correction to Enthalpy= 0.270940
Thermal correction to Gibbs Free Energy= 0.207625
Sum of electronic and zero-point Energies= -398.533578
Sum of electronic and thermal Energies= -398.518437
Sum of electronic and thermal Enthalpies= -398.517492
Sum of electronic and thermal Free Energies= -398.580807
Cartesian coordinates

B	4.51368800	0.40115000	-0.01682700
N	3.23363100	-0.25087500	0.45278100
H	2.05213300	1.20615500	0.33466400
H	0.62551100	0.88191400	-0.93729800
H	4.95541600	1.17173900	0.81055200
H	4.38073600	0.91800100	-1.10763600
H	2.81306500	-0.91874000	-0.18477500
H	3.25333900	-0.66148100	1.37969100
B	0.63725100	1.52626700	0.07272700
H	1.88730600	2.01722300	0.27259600

H	0.26561100	0.97380800	1.06815400
H	0.27423400	2.66487900	-0.04534500
N	5.70308100	-0.71260400	-0.22924800
H	6.57252300	-0.28360200	-0.54555000
H	5.90708600	-1.21238400	0.63543400
H	5.43950700	-1.40962400	-0.92538800
C	-3.75716600	0.88537500	-0.14960600
O	-2.36039800	0.68778800	-0.38188500
C	-2.03455800	-0.69743800	-0.23180400
C	-3.36576000	-1.43871100	-0.12667100
C	-4.24924900	-0.38206800	0.53987300
H	-3.88442500	1.78770400	0.45200300
H	-4.26721100	1.03029500	-1.11005200
H	-1.43206400	-1.01259100	-1.08656300
H	-1.43851000	-0.82537500	0.67883400
H	-3.75121400	-1.67656900	-1.12203000
H	-3.28295200	-2.36390800	0.44498800
H	-5.31724400	-0.55013800	0.39567500
H	-4.04094900	-0.33528800	1.61214500

Vibrational frequencies

-45.0262	11.3543	18.6188
24.6982	43.7609	61.2172
71.7821	75.9302	88.7497
118.4165	168.6861	203.1470
212.9068	276.3647	318.2024
345.2799	429.9496	581.0652
657.1984	664.4861	670.4102
674.3210	749.5948	816.6447
845.1823	858.2403	887.0952
890.0809	924.1775	939.8991
947.0242	974.9841	1000.4800
1042.4602	1044.9400	1048.5447
1098.2958	1131.2909	1134.4599
1153.1439	1170.2096	1182.9372
1195.8347	1198.8744	1199.1829
1205.6380	1225.6900	1266.5923
1271.7431	1315.5438	1341.5452
1371.4517	1376.0492	1409.8671
1477.1274	1488.9156	1519.0432
1530.2685	1598.3812	1631.2885
1637.8474	1750.5466	2447.4183
2457.2693	2537.6433	2608.5412
2627.3390	3034.2282	3045.8125
3061.3552	3067.5469	3103.3568
3115.6422	3125.4636	3133.2899
3202.7271	3453.5048	3540.8102

3552.7952 3562.1706 3623.4319

$NH_3BH_2NH_2+BH_3·H_2$

Zero-point correction= 0.136429 (Hartree/Particle)
Thermal correction to Energy= 0.145699
Thermal correction to Enthalpy= 0.146643
Thermal correction to Gibbs Free Energy= 0.101530
Sum of electronic and zero-point Energies= -166.237474
Sum of electronic and thermal Energies= -166.228205
Sum of electronic and thermal Enthalpies= -166.227260
Sum of electronic and thermal Free Energies= -166.272374
Cartesian coordinates

B	-0.927761000000	0.564616000000	-0.154631000000
N	0.099739000000	-0.537363000000	-0.168941000000
H	1.923417000000	0.387243000000	-0.337861000000
H	2.850140000000	0.001711000000	1.307761000000
H	-1.037745000000	1.106506000000	-1.236086000000
H	-0.730350000000	1.367233000000	0.736216000000
H	0.252756000000	-1.025532000000	0.706949000000
H	0.017312000000	-1.224464000000	-0.909746000000
B	3.228240000000	0.047634000000	0.171515000000
H	2.474280000000	0.962497000000	-0.528704000000
H	3.268834000000	-0.975957000000	-0.452105000000
H	4.144151000000	0.795990000000	-0.023583000000
N	-2.433820000000	-0.027938000000	0.161405000000
H	-3.139113000000	0.707341000000	0.178229000000
H	-2.722981000000	-0.709941000000	-0.538777000000
H	-2.464529000000	-0.496774000000	1.066036000000

Vibrational frequencies

8.2296	40.1995	109.9988
128.1842	198.4229	215.1336
258.8949	348.4416	399.1511
601.9398	632.2000	653.6267
660.4711	802.7678	839.7023
908.6246	1002.0543	1040.0731
1059.6770	1095.4276	1130.5398
1165.9325	1197.1652	1203.0670
1207.5947	1226.4194	1368.0020
1595.4547	1631.4280	1640.5215
1728.3460	2441.5965	2451.6921
2537.6673	2611.9083	2622.9968
3368.3346	3456.9415	3546.2780
3558.6560	3563.0386	3628.7435

THF

Zero-point correction= 0.117331 (Hartree/Particle)
Thermal correction to Energy= 0.122231
Thermal correction to Enthalpy= 0.123175
Thermal correction to Gibbs Free Energy= 0.089014
Sum of electronic and zero-point Energies= -232.296366
Sum of electronic and thermal Energies= -232.291467
Sum of electronic and thermal Enthalpies= -232.290523
Sum of electronic and thermal Free Energies= -232.324683
Cartesian coordinates

C	1.162903000000	0.423464000000	0.137330000000
O	-0.000035000000	1.246856000000	-0.000079000000
C	-1.162959000000	0.423387000000	-0.137229000000
C	-0.726362000000	-0.988827000000	0.239051000000
C	0.726456000000	-0.988746000000	-0.239097000000
H	1.950067000000	0.820955000000	-0.506953000000
H	1.508572000000	0.462911000000	1.177120000000
H	-1.950004000000	0.820793000000	0.507254000000
H	-1.508863000000	0.462876000000	-1.176935000000
H	-0.766691000000	-1.123646000000	1.323403000000
H	-1.342032000000	-1.755530000000	-0.232472000000
H	1.342187000000	-1.755444000000	0.232356000000
H	0.766809000000	-1.123440000000	-1.323465000000

Vibrational frequencies

55.0388	272.9302	578.5435
672.4291	855.8555	890.8293
918.2878	933.3753	945.4841
973.3062	1040.9647	1128.6646
1169.3671	1192.9542	1198.5374
1266.8590	1271.0291	1313.3648
1342.4283	1378.1290	1411.7311
1478.4258	1488.9574	1516.1921
1527.6348	3040.6340	3046.3474
3064.3031	3066.9940	3101.6811
3103.1737	3125.2282	3132.8735

pre-TS2

Zero-point correction= 0.256510 (Hartree/Particle)
Thermal correction to Energy= 0.271718
Thermal correction to Enthalpy= 0.272662
Thermal correction to Gibbs Free Energy= 0.214391
Sum of electronic and zero-point Energies= -398.539047
Sum of electronic and thermal Energies= -398.523839
Sum of electronic and thermal Enthalpies= -398.522895
Sum of electronic and thermal Free Energies= -398.581166
Cartesian coordinates

B	0.69349300	2.36443200	-0.42233500

H	0.08085100	3.30761700	-0.83863600
H	0.38638800	1.31084900	-0.89478200
H	1.73408800	2.93120700	-1.16772000
N	2.67277400	-0.73282300	-1.25968900
H	2.04095900	2.26698300	-0.83641400
H	2.53218600	-1.73332600	-1.33976100
B	3.13963800	-0.24071600	0.08586800
H	0.96599500	2.39793900	0.74104400
H	4.10465700	-0.86106000	0.48918700
H	1.85655000	-0.26581300	-1.63759800
H	3.35045900	0.95881900	0.09403700
N	1.99344400	-0.46360400	1.24670100
H	2.27262400	-0.04960500	2.13594300
H	1.83823100	-1.45664700	1.41895700
H	1.07630200	-0.07139900	1.00142800
C	-1.93520400	0.63378700	0.92143900
O	-0.90812600	-0.37025100	0.87441900
C	-1.10094400	-1.21052800	-0.27193700
C	-2.53353400	-0.96258000	-0.72509900
C	-2.69660600	0.52354300	-0.39572300
H	-2.58571400	0.42043000	1.77596400
H	-1.46674400	1.60913200	1.07065800
H	-0.38787000	-0.92258900	-1.05437200
H	-0.90347700	-2.24356700	0.02142300
H	-2.68156700	-1.19342100	-1.78010000
H	-3.22728900	-1.56350100	-0.13101400
H	-2.21685700	1.13434700	-1.16494400
H	-3.73621100	0.83670100	-0.29748300

Vibrational frequencies

36.2558	58.9569	74.5196
82.1025	96.3644	101.5299
122.9271	147.7356	176.2388
190.0196	202.6040	215.8958
237.4839	254.6190	282.2940
343.6677	370.7977	415.3541
582.2947	600.1361	661.1804
677.8366	684.1956	811.6154
843.6323	861.8756	881.1989
890.3594	930.7838	935.1623
951.4389	979.9816	1002.9393
1027.8783	1035.3634	1050.5385
1095.5128	1123.1939	1135.0239
1167.9848	1171.7333	1193.9337
1198.1473	1198.8477	1204.4892
1213.4216	1243.0340	1272.2728
1277.0561	1319.0687	1345.1322

1383.0737	1391.3304	1417.7102
1475.7905	1487.8788	1517.5857
1535.8704	1600.9473	1633.3368
1658.3901	1760.8918	2425.6963
2450.7244	2565.3009	2643.0268
2666.8700	3040.5839	3060.8190
3068.1672	3072.0102	3115.1931
3123.8251	3132.4417	3141.5026
3380.0831	3505.9248	3551.2300
3558.5437	3619.7285	3633.7855

TS2

Zero-point correction= 0.253837 (Hartree/Particle)
Thermal correction to Energy= 0.268772
Thermal correction to Enthalpy= 0.269716
Thermal correction to Gibbs Free Energy= 0.210981
Sum of electronic and zero-point Energies= -398.536234
Sum of electronic and thermal Energies= -398.521300
Sum of electronic and thermal Enthalpies= -398.520356
Sum of electronic and thermal Free Energies= -398.579090
Cartesian coordinates

B	0.373538000000	1.884876000000	-0.534875000000
H	-0.680765000000	2.304731000000	-0.905546000000
H	0.974810000000	1.130533000000	-1.232832000000
H	0.927961000000	3.464159000000	-1.187507000000
N	3.432542000000	-0.622662000000	-1.019483000000
H	1.588602000000	3.115739000000	-1.057695000000
H	3.498941000000	-1.631192000000	-1.089079000000
B	3.403936000000	-0.044395000000	0.370479000000
H	0.712250000000	2.056977000000	0.593661000000
H	4.328125000000	-0.446277000000	1.053311000000
H	2.706445000000	-0.300110000000	-1.647964000000
H	3.335469000000	1.169469000000	0.361338000000
N	2.058958000000	-0.523291000000	1.204344000000
H	2.033823000000	-0.110205000000	2.136412000000
H	2.047461000000	-1.535054000000	1.327253000000
H	1.180452000000	-0.267930000000	0.740694000000
C	-1.861070000000	0.347328000000	1.098656000000
O	-0.787393000000	-0.111937000000	0.258939000000
C	-1.319648000000	-0.798099000000	-0.890006000000
C	-2.811526000000	-0.961836000000	-0.621337000000
C	-3.108851000000	0.274740000000	0.230331000000
H	-1.940558000000	-0.316060000000	1.966434000000
H	-1.617862000000	1.354785000000	1.440634000000
H	-1.139243000000	-0.179064000000	-1.774618000000
H	-0.788267000000	-1.744958000000	-1.004268000000

H -3.391538000000 -1.005139000000 -1.543080000000
H -2.999090000000 -1.871549000000 -0.045058000000
H -3.177941000000 1.164080000000 -0.402196000000
H -4.021229000000 0.189040000000 0.820686000000
Vibrational frequencies

-439.6335	18.7608	30.7866
51.8041	74.6717	95.4465
123.0028	139.1833	150.9149
181.7501	231.3240	269.8129
274.7511	294.4140	305.5364
317.1538	344.9838	359.2381
420.2759	572.4329	577.6383
648.7610	666.8368	679.8241
803.7752	844.9098	855.9466
868.1210	890.2439	899.9288
923.8398	926.3664	945.1556
971.9355	1002.4218	1044.5282
1052.0866	1093.7428	1111.8526
1128.3919	1139.2150	1165.6797
1167.2714	1168.7380	1173.4404
1196.0723	1202.7837	1222.7554
1269.0247	1271.4401	1314.4431
1341.7515	1375.9002	1383.4263
1406.0306	1476.9082	1488.4514
1512.8560	1525.4763	1597.7053
1639.9441	1661.5258	2435.2406
2445.5634	2592.8549	2695.1280
2711.3134	3053.7039	3062.5937
3069.0281	3074.5572	3114.9173
3121.0436	3135.6470	3143.8206
3397.6120	3512.8103	3552.7377
3561.0121	3636.9176	4211.8234

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

$NH_3BH_2NH_2$+THF·BH_3

Zero-point correction= 0.240618 (Hartree/Particle)
Thermal correction to Energy= 0.254141
Thermal correction to Enthalpy= 0.255085
Thermal correction to Gibbs Free Energy= 0.198304
Sum of electronic and zero-point Energies= -397.407934
Sum of electronic and thermal Energies= -397.394411
Sum of electronic and thermal Enthalpies= -397.393467

Sum of electronic and thermal Free Energies= -397.450248
Cartesian coordinates

B	-0.083648000000	-0.155791000000	-0.321798000000
H	0.083604000000	-0.405182000000	0.855980000000
H	0.403827000000	0.899381000000	-0.653069000000
N	5.314521000000	0.812280000000	-0.070135000000
H	5.274012000000	1.034516000000	-1.057744000000
B	4.702275000000	-0.498111000000	0.344394000000
H	0.222936000000	-1.073841000000	-1.044906000000
H	5.113777000000	-1.430364000000	-0.318673000000
H	5.023705000000	1.628297000000	0.455313000000
H	4.807593000000	-0.698557000000	1.539269000000
N	3.070686000000	-0.509132000000	0.080332000000
H	2.634815000000	-1.386866000000	0.363277000000
H	2.845609000000	-0.369503000000	-0.904412000000
H	2.599806000000	0.234465000000	0.595697000000
C	-2.492589000000	-1.143138000000	-0.291984000000
O	-1.640595000000	0.029668000000	-0.514110000000
C	-2.243443000000	1.213591000000	0.085993000000
C	-3.715142000000	0.864078000000	0.142794000000
C	-3.669944000000	-0.620616000000	0.517867000000
H	-2.777315000000	-1.503322000000	-1.280274000000
H	-1.894863000000	-1.893214000000	0.223497000000
H	-1.807751000000	1.342399000000	1.080302000000
H	-1.986623000000	2.057130000000	-0.551389000000
H	-4.244832000000	1.472534000000	0.874794000000
H	-4.176290000000	1.004045000000	-0.837606000000
H	-3.472029000000	-0.731490000000	1.585930000000
H	-4.588100000000	-1.153786000000	0.274507000000

Vibrational frequencies

30.2398	38.4760	47.5028
60.7111	72.5577	80.6595
92.0042	200.9024	225.7993
256.8262	283.1474	306.3598
333.0465	348.6293	511.9015

563.3836	577.0289	646.6821
660.3260	747.3137	800.0055
836.6530	860.9605	874.8588
912.0357	928.7832	947.0219
948.4906	966.7276	999.4217
1002.9702	1061.3228	1096.3751
1104.9098	1132.7441	1165.1521
1168.0216	1193.7649	1196.8058
1204.6040	1206.1275	1223.5141
1228.7674	1268.8833	1284.0348
1329.2050	1359.2356	1368.7003
1397.1130	1416.7330	1478.8500
1490.9423	1509.8876	1519.8287
1601.0054	1629.3623	1637.0580
2445.9076	2448.9962	2454.1699
2503.5266	2529.7318	3085.0870
3092.7414	3103.1326	3106.3363
3145.8825	3152.4697	3171.3918
3179.3975	3459.0863	3551.3122
3556.0977	3564.7140	3634.7954

TS3

Zero-point correction= 0.239894 (Hartree/Particle)
Thermal correction to Energy= 0.252649
Thermal correction to Enthalpy= 0.253593
Thermal correction to Gibbs Free Energy= 0.199739
Sum of electronic and zero-point Energies= -397.390731
Sum of electronic and thermal Energies= -397.377977
Sum of electronic and thermal Enthalpies= -397.377033

Sum of electronic and thermal Free Energies= -397.430886
Cartesian coordinates

B	0.358627000000	-0.700088000000	-0.459919000000
H	0.334700000000	-0.163235000000	0.610636000000
H	0.566288000000	-0.048387000000	-1.440983000000
N	2.763724000000	-0.838982000000	-0.246283000000
H	2.994602000000	-1.003412000000	-1.219766000000
B	3.226447000000	0.471629000000	0.336484000000
H	0.316719000000	-1.893400000000	-0.527670000000
H	2.836024000000	1.423699000000	-0.309261000000
H	2.998086000000	-1.670728000000	0.283687000000
H	2.954831000000	0.565595000000	1.516130000000
N	4.872519000000	0.595011000000	0.283081000000
H	5.205037000000	1.469216000000	0.689624000000
H	5.215812000000	0.557057000000	-0.676017000000
H	5.318384000000	-0.166627000000	0.793247000000

C	-2.399629000000	-1.087131000000	0.417303000000
O	-1.650421000000	-0.504963000000	-0.667578000000
C	-2.026407000000	0.876007000000	-0.836236000000
C	-3.303746000000	1.051519000000	-0.028291000000
C	-3.061345000000	0.083159000000	1.132125000000
H	-3.140540000000	-1.770522000000	-0.007991000000
H	-1.707308000000	-1.653326000000	1.042211000000
H	-1.218355000000	1.502320000000	-0.444252000000
H	-2.141907000000	1.067298000000	-1.903593000000
H	-3.448442000000	2.084177000000	0.289608000000
H	-4.173373000000	0.737185000000	-0.611580000000
H	-2.367747000000	0.524018000000	1.853165000000
H	-3.971751000000	-0.212451000000	1.653613000000

Vibrational frequencies

-408.6144	36.1730	41.2552
66.1481	83.0284	104.0581
130.8537	171.3533	208.5778
240.9874	272.8220	291.8341
301.6591	349.2962	443.3413
579.8819	629.7743	651.0743
663.0389	669.1474	803.4970
834.3045	854.6176	889.5718
904.8827	911.1487	923.0350
936.6066	948.6584	980.2938
1001.9347	1045.1766	1095.5981
1108.1306	1115.6763	1132.2271
1153.0489	1156.3946	1167.4030
1170.8078	1200.6220	1207.7553
1224.8655	1271.0955	1274.8851
1320.8194	1351.6327	1358.6905
1381.4816	1409.4992	1478.6709
1487.8913	1510.4896	1522.4265
1598.5881	1636.2839	1642.0435
2455.3847	2467.2661	2548.6371
2641.4192	2643.9950	3058.0835
3071.0217	3078.1473	3081.2845
3126.1604	3129.3884	3136.2655
3144.9420	3461.4420	3548.4118
3562.3929	3569.0887	3632.9954

$NH_3BH_2NH_2BH_3$

Zero-point correction= 0.123984 (Hartree/Particle)

Thermal correction to Energy= 0.130379

Thermal correction to Enthalpy= 0.131323

Thermal correction to Gibbs Free Energy= 0.095262

Sum of electronic and zero-point Energies= -165.134112

Sum of electronic and thermal Energies= -165.127717
Sum of electronic and thermal Enthalpies= -165.126773

Sum of electronic and thermal Free Energies= -165.162834
Cartesian coordinates

B	2.124112000000	0.130741000000	-0.000083000000
H	2.901751000000	-0.805953000000	0.000202000000
H	2.251910000000	0.805664000000	1.002359000000
N	0.628106000000	-0.462641000000	0.000077000000
H	0.534628000000	-1.072191000000	0.811790000000
B	-0.487434000000	0.625732000000	0.000074000000
H	2.252186000000	0.805035000000	-1.002897000000
H	-0.437106000000	1.278531000000	1.010237000000
H	0.534177000000	-1.072431000000	-0.811405000000
H	-0.436953000000	1.278551000000	-1.010088000000
N	-1.915211000000	-0.126871000000	-0.000063000000
H	-2.671970000000	0.557336000000	0.000601000000
H	-2.050965000000	-0.715716000000	0.822397000000
H	-2.051320000000	-0.714605000000	-0.823250000000

Vibrational frequencies

104.8762	168.9884	224.5598
230.2338	361.6846	647.2946
712.0362	719.0994	780.9919
847.4276	855.0268	873.1941
1012.7314	1074.9662	1108.8332
1169.2207	1186.7574	1202.9412
1206.6064	1220.0834	1229.3488
1237.9741	1405.3265	1608.5751
1632.8412	1637.5757	2419.0292
2451.9615	2460.0951	2533.2854
2561.2266	3443.5786	3478.7555
3534.4778	3539.5873	3541.5293

TS4

Zero-point correction= 0.237305 (Hartree/Particle)
Thermal correction to Energy= 0.251333
Thermal correction to Enthalpy= 0.252277
Thermal correction to Gibbs Free Energy= 0.195469
Sum of electronic and zero-point Energies= -397.397419
Sum of electronic and thermal Energies= -397.383392
Sum of electronic and thermal Enthalpies= -397.382447

Sum of electronic and thermal Free Energies= -397.439256
Cartesian coordinates

B	-0.430681000000	-1.997003000000	0.878642000000
H	-1.133672000000	-2.121291000000	1.859076000000
H	0.733018000000	-1.805138000000	1.143073000000

N	3.090245000000	0.537915000000	1.007620000000
H	2.841925000000	1.460941000000	1.328669000000
B	3.477467000000	0.259135000000	-0.316893000000
H	-0.599667000000	-2.866599000000	0.056354000000
H	3.705138000000	1.174621000000	-1.049494000000
H	2.936737000000	-0.181432000000	1.698150000000
H	3.869967000000	-0.837701000000	-0.579013000000
N	1.518888000000	-0.341368000000	-1.600771000000
H	1.904015000000	-0.637986000000	-2.493315000000
H	0.730762000000	0.267900000000	-1.802855000000
H	1.143232000000	-1.167928000000	-1.142687000000
C	-2.230781000000	-0.634781000000	-0.446108000000
O	-0.900745000000	-0.667626000000	0.160681000000
C	-0.596002000000	0.604719000000	0.796059000000
C	-1.430074000000	1.583532000000	-0.002614000000
C	-2.723889000000	0.790701000000	-0.223459000000
H	-2.090709000000	-0.886284000000	-1.497728000000
H	-2.838542000000	-1.395460000000	0.042913000000
H	-0.909756000000	0.543946000000	1.842285000000
H	0.483288000000	0.734690000000	0.727674000000
H	-1.590358000000	2.516312000000	0.536754000000
H	-0.940763000000	1.805571000000	-0.955053000000
H	-3.346621000000	0.836765000000	0.671889000000
H	-3.305414000000	1.148563000000	-1.072090000000

Vibrational frequencies

-152.1645	25.3675	42.4550
58.0956	68.5193	76.8742
101.6150	134.4010	186.1148
212.4442	227.6205	240.3780
277.9645	292.1384	299.0048
370.1450	477.4938	487.6108
497.3602	580.4229	726.3226
754.7400	853.8936	874.3919
877.9784	907.4757	935.5317
944.4977	946.2306	961.7521
999.1992	1013.4423	1062.9361
1099.2581	1113.6179	1115.1532
1129.2102	1164.1459	1194.8767
1198.4323	1200.4349	1205.5446
1223.9491	1262.0774	1282.2390
1308.4180	1326.5300	1354.4134
1393.3496	1411.5475	1478.5790
1489.1639	1513.1790	1522.4979
1610.4863	1635.9427	1644.7648
2474.1154	2505.2704	2524.5228
2598.1088	2654.6767	3070.5177

3085.8158	3092.6162	3102.0888
3141.8417	3148.7097	3167.4920
3175.0672	3484.1962	3606.9528
3612.7192	3614.6245	3713.4532

NH_2BH_2

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	0.610231000000	-0.000001000000	0.000036000000
H	1.164555000000	0.844173000000	-0.000106000000
H	1.164515000000	-0.844206000000	-0.000109000000
B	-0.776533000000	-0.000002000000	0.000016000000
H	-1.358976000000	1.040282000000	-0.000060000000
H	-1.359045000000	-1.040230000000	-0.000058000000

Vibrational frequencies

605.7851	737.8214	840.3543
1011.1225	1117.6854	1160.3313
1358.8005	1619.9571	2620.6165
2684.6208	3602.9197	3700.3977

NH_3+ THF· BH_3

Zero-point correction= 0.186755 (Hartree/Particle)
Thermal correction to Energy= 0.197949
Thermal correction to Enthalpy= 0.198893
Thermal correction to Gibbs Free Energy= 0.148345
Sum of electronic and zero-point Energies= -315.418617
Sum of electronic and thermal Energies= -315.407423
Sum of electronic and thermal Enthalpies= -315.406479

Sum of electronic and thermal Free Energies= -315.457026
Cartesian coordinates

B	1.301940000000	0.108569000000	-0.174420000000
H	1.437342000000	-0.085935000000	1.017220000000
H	1.664884000000	1.208700000000	-0.517786000000
H	1.755415000000	-0.782842000000	-0.852010000000
N	4.587252000000	-0.149660000000	0.174298000000
H	5.193449000000	0.604340000000	0.491999000000
H	4.160796000000	0.194683000000	-0.681567000000
H	3.833631000000	-0.192235000000	0.855774000000

C	-0.958386000000	-1.183308000000	-0.231480000000
O	-0.257666000000	0.085280000000	-0.445301000000
C	-1.041099000000	1.189379000000	0.088690000000
C	-2.460242000000	0.667136000000	0.019974000000
C	-2.275821000000	-0.797591000000	0.430814000000
H	-1.083126000000	-1.630722000000	-1.216916000000
H	-0.320782000000	-1.812809000000	0.388032000000
H	-0.713249000000	1.368783000000	1.116650000000
H	-0.830502000000	2.056439000000	-0.533609000000
H	-3.125910000000	1.216209000000	0.684653000000
H	-2.838081000000	0.739620000000	-1.002603000000
H	-2.188802000000	-0.874649000000	1.516331000000
H	-3.090910000000	-1.440752000000	0.100271000000

Vibrational frequencies

30.6438	52.3198	54.9451
74.8703	88.4776	129.8981
178.5159	225.7753	241.5223
282.6394	302.1395	504.2312
579.9267	751.1988	858.5786
877.2337	913.9342	927.9791
944.6030	951.6547	971.4585
998.4170	1061.6818	1108.0517
1132.4371	1166.5124	1190.8516
1197.0277	1204.1328	1205.9610
1224.6173	1269.5337	1282.5509
1327.0478	1354.2288	1394.7221
1416.1022	1478.0830	1489.7063
1512.4015	1527.6212	1639.0956
1649.3506	2459.5303	2502.2044
2530.2426	3077.0942	3084.3909
3089.1976	3127.1737	3141.2335
3148.2822	3177.9294	3191.4230
3484.7679	3586.1624	3603.6733

TS5

Zero-point correction= 0.185990 (Hartree/Particle)
Thermal correction to Energy= 0.196220
Thermal correction to Enthalpy= 0.197164
Thermal correction to Gibbs Free Energy= 0.150360
Sum of electronic and zero-point Energies= -315.402300
Sum of electronic and thermal Energies= -315.392070
Sum of electronic and thermal Enthalpies= -315.391126

Sum of electronic and thermal Free Energies= -315.437931
Cartesian coordinates

B	1.669595000000	0.043150000000	-0.249615000000

H	1.402415000000	-0.238786000000	0.883179000000
H	1.815009000000	1.189450000000	-0.555155000000
H	1.892390000000	-0.823762000000	-1.040647000000
N	3.965247000000	-0.014202000000	0.343469000000
H	4.253598000000	-0.923028000000	0.693678000000
H	4.540848000000	0.190109000000	-0.468192000000
H	4.201098000000	0.669686000000	1.056514000000
C	-1.008007000000	-1.140532000000	-0.438066000000
O	-0.327670000000	0.093055000000	-0.741172000000
C	-1.005130000000	1.194264000000	-0.106750000000
C	-2.354810000000	0.643180000000	0.330991000000
C	-1.990798000000	-0.803130000000	0.674858000000
H	-1.524537000000	-1.476635000000	-1.342024000000
H	-0.258223000000	-1.881659000000	-0.156714000000
H	-0.409480000000	1.514812000000	0.754354000000
H	-1.067722000000	2.012869000000	-0.824653000000
H	-2.773411000000	1.198809000000	1.170279000000
H	-3.065885000000	0.668751000000	-0.498992000000
H	-1.490503000000	-0.845920000000	1.646116000000
H	-2.846464000000	-1.478162000000	0.689222000000

Vibrational frequencies

-404.7745	44.8637	90.6107
108.5150	126.8301	156.6146
183.9380	201.9581	247.0738
278.1680	360.6238	369.7174
573.7652	668.9480	853.1521
886.1309	904.9577	909.6130
922.1062	932.5445	947.3058
976.4168	1043.7144	1091.7423
1112.3058	1115.9538	1152.1269
1157.4984	1169.6052	1197.5128
1208.0898	1272.0307	1273.8888
1316.8833	1347.9421	1381.4363
1408.7211	1474.7321	1485.7934
1514.8586	1526.3973	1635.8936
1636.7009	2552.4384	2642.4987
2651.1886	3064.1257	3065.6312
3069.9717	3073.8990	3122.8275
3126.2757	3135.8358	3141.9319
3491.8490	3613.8390	3620.1262

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

AADB
Zero-point correction= 0.141839 (Hartree/Particle)
Thermal correction to Energy= 0.150226
Thermal correction to Enthalpy= 0.151170
Thermal correction to Gibbs Free Energy= 0.110629
Sum of electronic and zero-point Energies= -166.266445
Sum of electronic and thermal Energies= -166.258058
Sum of electronic and thermal Enthalpies= -166.257114

Sum of electronic and thermal Free Energies= -166.297655
Cartesian coordinates

N	-1.524641000000	-0.019826000000	-0.000143000000
B	-0.726941000000	1.350948000000	-0.002473000000
B	-0.658012000000	-1.354433000000	0.000240000000
N	2.256087000000	0.019518000000	0.000747000000
H	-1.395051000000	-2.323115000000	-0.046625000000
H	2.299151000000	-0.258991000000	-0.981530000000
H	-2.148246000000	-0.037366000000	0.804747000000
H	-2.147554000000	-0.034970000000	-0.805646000000
H	0.073981000000	-1.330370000000	-0.976985000000
H	0.003517000000	-1.374251000000	1.026796000000
H	1.403596000000	0.589397000000	0.146484000000
H	3.090541000000	0.551859000000	0.252412000000
H	2.179051000000	-0.819861000000	0.579416000000
H	-1.495047000000	2.291846000000	0.048622000000

H	0.000555000000	1.364380000000	0.982979000000
H	-0.059855000000	1.401028000000	-1.023732000000

Vibrational frequencies

107.2438	135.8355	151.9818
177.5601	184.4813	239.1825
274.6556	334.0483	358.9186
625.3949	734.8658	826.6585
831.6494	908.9857	1019.8689
1063.0113	1160.9404	1194.4758
1201.4512	1207.7604	1213.0639
1222.8995	1227.8187	1263.7824
1416.5847	1441.2316	1471.9759
1605.3475	1676.9710	1698.0208
2363.2544	2390.9846	2391.7991
2407.5064	2416.4990	2438.4485
3258.5322	3459.8037	3501.1542
3538.5960	3555.8172	3561.0707

TS6

Zero-point correction= 0.136987 (Hartree/Particle)
Thermal correction to Energy= 0.145153
Thermal correction to Enthalpy= 0.146097
Thermal correction to Gibbs Free Energy= 0.104732
Sum of electronic and zero-point Energies= -166.238105
Sum of electronic and thermal Energies= -166.229939
Sum of electronic and thermal Enthalpies= -166.228995

Sum of electronic and thermal Free Energies= -166.270360
Cartesian coordinates

B	2.229573000000	-0.513453000000	0.268347000000
H	2.652473000000	-1.527215000000	-0.252847000000
H	2.027063000000	-0.676765000000	1.454646000000
N	0.808794000000	-0.164788000000	-0.416909000000
H	0.189543000000	-0.961719000000	-0.275618000000
B	0.190449000000	1.128435000000	0.142815000000
H	2.970551000000	0.427932000000	0.071703000000
H	-0.108052000000	1.060957000000	1.296862000000
H	0.948202000000	-0.094772000000	-1.423365000000
H	0.765637000000	2.118615000000	-0.202019000000
N	-2.419775000000	-0.379003000000	0.077032000000
H	-2.567022000000	-1.049117000000	-0.673642000000
H	-3.313619000000	0.074950000000	0.249218000000
H	-2.190950000000	-0.908294000000	0.915286000000
H	-0.893971000000	1.462327000000	-0.599542000000
H	-1.303098000000	0.804730000000	-0.237352000000

Vibrational frequencies

-218.5199	33.1745	67.3755
112.2590	184.3643	249.2954
288.8665	363.0523	419.6994
648.6799	662.2754	774.0189
808.8191	852.6311	915.6500
993.6443	1016.6255	1069.4010
1143.5396	1161.5811	1177.9983
1186.9158	1199.4802	1201.6977
1218.3227	1228.7608	1238.3003
1612.6933	1627.2293	1633.4288
1782.7727	2440.3735	2455.8139
2464.8249	2598.6123	2661.1815
2892.8024	3488.4584	3490.4550
3550.0811	3606.7368	3608.4694

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

$BH_3NH_2BH_2 \cdot H_2$

Zero-point correction= 0.098524 (Hartree/Particle)
Thermal correction to Energy= 0.104625
Thermal correction to Enthalpy= 0.105569
Thermal correction to Gibbs Free Energy= 0.069671
Sum of electronic and zero-point Energies= -109.717220
Sum of electronic and thermal Energies= -109.711118
Sum of electronic and thermal Enthalpies= -109.710174

Sum of electronic and thermal Free Energies= -109.746073
Cartesian coordinates

B	-1.446004000000	-0.275087000000	-0.000354000000
H	-2.341806000000	0.541968000000	0.004860000000

H	-1.456403000000	-0.960561000000	1.000029000000
N	-0.043308000000	0.547572000000	0.000121000000
H	-0.036514000000	1.156117000000	0.816511000000
B	1.122976000000	-0.428152000000	0.001211000000
H	-1.460177000000	-0.952374000000	-1.006227000000
H	1.307062000000	-1.012569000000	1.021222000000
H	-0.036022000000	1.155598000000	-0.816660000000
H	1.303039000000	-1.019479000000	-1.015625000000
H	2.320001000000	0.383076000000	-0.396236000000
H	2.319114000000	0.391416000000	0.387001000000

Vibrational frequencies

12.3635	198.0645	285.3546
296.0367	532.4162	649.5178
652.5858	779.8479	798.5683
880.5971	977.1522	1024.2298
1081.7558	1122.2010	1168.8285
1196.0752	1197.6505	1202.9590
1206.3863	1220.2431	1443.7488
1611.5504	2454.3251	2471.6671
2479.5298	2642.8472	2708.5539
3509.6759	3570.9213	3871.3914

TS7

Zero-point correction= 0.217281 (Hartree/Particle)
Thermal correction to Energy= 0.228892
Thermal correction to Enthalpy= 0.229836
Thermal correction to Gibbs Free Energy= 0.179075
Sum of electronic and zero-point Energies= -342.018868
Sum of electronic and thermal Energies= -342.007257
Sum of electronic and thermal Enthalpies= -342.006313
Sum of electronic and thermal Free Energies= -342.057075
Cartesian coordinates

B	3.77116400	-0.05851100	-0.17902300
H	4.23193700	-0.88061700	-0.93869200
H	4.22580000	-0.15104700	0.93985700
N	2.16581200	-0.37886900	-0.05605100
H	2.05641700	-1.28061200	0.40325000
B	1.27930500	0.67294900	0.56814000
H	3.85239900	1.07394600	-0.61001300
H	1.03793200	1.63413700	-0.08560000
H	1.82022700	-0.50812700	-1.00670300
H	0.63716900	0.40580900	1.53385200
C	-1.26755000	-1.26404000	0.16736600
O	-0.56507400	-0.41915400	-0.74334900
C	-1.48844800	0.59088000	-1.13951500
C	-2.19836600	0.97971900	0.15435300

C	-2.25761000	-0.35597900	0.92658200
H	-1.79504700	-2.04287700	-0.39590700
H	-0.52796200	-1.74070000	0.81459300
H	-0.92251400	1.39979200	-1.60344300
H	-2.19330000	0.17813800	-1.87412200
H	-1.59381100	1.70939500	0.69718800
H	-3.18340200	1.41242200	-0.02485000
H	-1.96388300	-0.22516700	1.96875500
H	-3.26059800	-0.78526300	0.91175700
H	2.34428500	1.34763300	1.81467300
H	2.61375300	1.68278300	1.19625000

Vibrational frequencies

-399.9580	20.1142	53.2715
87.2843	108.4651	131.1116
144.0582	185.4321	225.3746
287.7003	317.2933	336.4208
368.1683	557.3865	614.9631
671.2088	690.4722	716.7151
792.7267	813.8481	877.4591
895.1025	927.4887	936.4205
952.2845	960.9396	975.8860
991.9876	1035.2365	1055.2190
1058.1101	1118.3798	1130.4271
1149.7053	1174.7641	1191.9240
1202.0319	1207.9989	1217.1252
1224.9085	1242.4591	1243.3017
1249.0844	1292.2305	1313.0123
1327.6092	1376.2624	1410.5322
1470.8347	1488.0577	1509.9475
1523.8837	1619.5945	2448.5745
2475.6613	2487.4858	2658.1287
2742.0544	3041.4115	3046.0593
3072.3837	3078.5069	3107.0637
3122.9802	3133.2422	3140.2425
3502.5492	3566.2085	4280.7565

THF$BH_2NH_2BH_3$

Zero-point correction= 0.204239 (Hartree/Particle)
Thermal correction to Energy= 0.213807
Thermal correction to Enthalpy= 0.214752
Thermal correction to Gibbs Free Energy= 0.169140
Sum of electronic and zero-point Energies= -340.899714
Sum of electronic and thermal Energies= -340.890145
Sum of electronic and thermal Enthalpies= -340.889201

Sum of electronic and thermal Free Energies= -340.934812

Cartesian coordinates

B	2.654295000000	-0.209235000000	1.137700000000
H	3.697123000000	-0.817927000000	1.295016000000
H	1.736970000000	-0.772224000000	1.700670000000
N	2.336285000000	-0.177303000000	-0.438299000000
H	2.245428000000	-1.132654000000	-0.783090000000
B	1.141094000000	0.697808000000	-0.912524000000
H	2.757190000000	0.942222000000	1.514156000000
H	0.842671000000	0.479346000000	-2.064225000000
H	3.161758000000	0.183555000000	-0.916841000000
H	1.327336000000	1.854407000000	-0.649322000000
C	-1.175515000000	1.215945000000	0.102012000000
O	-0.080873000000	0.258897000000	-0.044606000000
C	-0.598372000000	-1.105175000000	-0.192931000000
C	-2.110530000000	-0.938057000000	-0.211926000000
C	-2.322120000000	0.353448000000	0.583895000000
H	-0.835107000000	1.975375000000	0.802529000000
H	-1.366658000000	1.657547000000	-0.879212000000
H	-0.185825000000	-1.516474000000	-1.114194000000
H	-0.237324000000	-1.662278000000	0.670981000000
H	-2.465555000000	-0.811956000000	-1.236818000000
H	-2.609599000000	-1.799387000000	0.229907000000
H	-3.285009000000	0.823326000000	0.387312000000
H	-2.228136000000	0.167232000000	1.655886000000

Vibrational frequencies

36.1421	57.1418	119.8321
161.8307	219.1945	258.5444
271.0312	312.9644	381.6547
532.3238	576.7147	654.0644
732.1676	756.3849	826.9796
865.1333	876.7411	918.4587
929.1692	935.0576	946.8106
956.4247	964.0969	1003.2715
1054.2591	1059.6663	1090.6340
1153.5469	1168.2641	1182.5918
1203.3231	1205.7863	1214.8821
1218.8602	1224.7702	1233.2843
1243.5394	1269.9718	1283.0694
1328.3147	1355.9988	1393.3437
1414.1911	1475.7023	1486.7664
1509.4961	1519.5602	1603.8844
2421.0757	2440.7105	2457.6627
2498.4926	2581.3661	3081.8436
3086.5058	3103.2027	3113.7211
3146.6478	3154.2513	3179.7548
3183.4996	3481.3416	3534.5584

TS8

Zero-point correction= 0.238162 (Hartree/Particle)
Thermal correction to Energy= 0.251581
Thermal correction to Enthalpy= 0.252525
Thermal correction to Gibbs Free Energy= 0.198100
Sum of electronic and zero-point Energies= -397.377109
Sum of electronic and thermal Energies= -397.363691
Sum of electronic and thermal Enthalpies= -397.362746

Sum of electronic and thermal Free Energies= -397.417171
Cartesian coordinates

B	-2.451266000000	0.281208000000	0.016376000000
H	-3.225080000000	1.066946000000	0.477419000000
H	-1.687651000000	-0.299257000000	0.727668000000
N	-0.976844000000	2.008113000000	-0.319600000000
H	-1.524858000000	2.629484000000	0.261701000000
B	0.478878000000	1.988130000000	0.063666000000
H	-2.471555000000	0.049226000000	-1.156549000000
H	0.700300000000	2.427970000000	1.166777000000
H	-1.157446000000	2.260748000000	-1.284020000000
H	1.250277000000	2.386200000000	-0.788874000000
N	-4.006515000000	-1.373230000000	0.340242000000
H	-4.851976000000	-1.192833000000	-0.193268000000
H	-4.276070000000	-1.436845000000	1.317585000000
H	-3.665069000000	-2.288620000000	0.062089000000
C	2.194499000000	0.178497000000	0.871088000000
O	0.915251000000	0.430389000000	0.220775000000
C	0.812736000000	-0.404159000000	-0.958477000000
C	1.494386000000	-1.679102000000	-0.511173000000
C	2.699234000000	-1.139393000000	0.272554000000
H	2.853522000000	1.022119000000	0.659249000000
H	1.988325000000	0.130988000000	1.939166000000
H	-0.244335000000	-0.492052000000	-1.194625000000
H	1.350246000000	0.090667000000	-1.774716000000
H	0.824181000000	-2.245868000000	0.139053000000
H	1.784694000000	-2.306008000000	-1.353664000000
H	3.039720000000	-1.825993000000	1.046373000000
H	3.531092000000	-0.945918000000	-0.406217000000

Vibrational frequencies

-480.8744	40.1405	54.5918
79.2404	99.0033	111.9270
130.4847	166.2198	180.3823
204.4435	215.7467	231.1000
314.0906	328.9692	349.4781
387.4576	453.4948	531.1033

599.1291	721.0984	767.6422
792.7472	833.0943	895.7461
903.7561	909.1776	916.9641
934.7519	952.4416	974.2086
981.2195	1005.0742	1064.9470
1083.0331	1101.1307	1105.9817
1139.1737	1156.8789	1160.2759
1163.0119	1182.5652	1212.5572
1233.3969	1236.2139	1260.6052
1285.9482	1326.3319	1343.1684
1388.4688	1411.2633	1481.2502
1493.7577	1511.1367	1524.2187
1610.1974	1632.6730	1639.8577
2433.5014	2516.6585	2549.0569
2639.6863	2654.0453	3079.2253
3085.6263	3087.7640	3100.8633
3140.4750	3153.9198	3165.9932
3188.2890	3491.4423	3564.1751
3616.3495	3617.8299	3643.2678

TS9

Zero-point correction= 0.240143 (Hartree/Particle)
Thermal correction to Energy= 0.252894
Thermal correction to Enthalpy= 0.253838
Thermal correction to Gibbs Free Energy= 0.201121
Sum of electronic and zero-point Energies= -397.398653
Sum of electronic and thermal Energies= -397.385903
Sum of electronic and thermal Enthalpies= -397.384959

Sum of electronic and thermal Free Energies= -397.437676
Cartesian coordinates

B	-2.469295000000	-1.637024000000	0.788976000000
H	-2.906034000000	-2.679399000000	0.334430000000
H	-3.369852000000	-0.930989000000	1.199500000000
N	-1.731061000000	-0.846633000000	-0.400957000000
H	-2.391154000000	-0.696449000000	-1.161438000000
B	-1.101454000000	0.513353000000	-0.042271000000
H	-1.645886000000	-1.845256000000	1.656284000000
H	-1.203754000000	0.902316000000	1.074158000000
H	-1.019842000000	-1.458916000000	-0.797643000000
H	-0.634869000000	1.173281000000	-0.919728000000
N	-3.145175000000	1.559751000000	-0.406006000000
H	-3.592002000000	1.587953000000	-1.319110000000
H	-2.998119000000	2.523647000000	-0.120068000000
H	-3.813267000000	1.154236000000	0.244524000000
C	1.576218000000	0.613823000000	1.101228000000

O	0.724216000000	-0.290914000000	0.366086000000
C	1.436844000000	-0.813047000000	-0.776144000000
C	2.884459000000	-0.369856000000	-0.602433000000
C	2.718092000000	0.948815000000	0.154808000000
H	0.978181000000	1.474939000000	1.398680000000
H	1.930431000000	0.094795000000	1.996064000000
H	1.312557000000	-1.897186000000	-0.792345000000
H	0.992530000000	-0.380364000000	-1.679619000000
H	3.432424000000	-1.091082000000	0.008515000000
H	3.393256000000	-0.262278000000	-1.560253000000
H	3.616333000000	1.258557000000	0.688917000000
H	2.419056000000	1.747632000000	-0.529084000000

Vibrational frequencies

-456.1421	41.3469	53.5504
98.2970	121.6037	124.7510
135.0987	159.5828	193.6255
225.2532	252.0966	279.1868
312.3564	337.1096	386.8099
417.9890	579.8271	648.3711
676.6838	737.3965	847.0849
860.3871	889.1068	904.9992
933.7180	937.7766	947.9866
953.7449	969.1793	986.8887
1020.3067	1053.5847	1091.0347
1113.5274	1121.6926	1170.7907
1172.2593	1193.8369	1195.6216
1202.6933	1207.8537	1215.2051
1217.9326	1251.9382	1277.9230
1281.4355	1323.7772	1349.3271
1387.0827	1416.7788	1475.3993
1486.4916	1517.4490	1529.2300
1599.2345	1635.2254	1639.6402
2413.3843	2447.6623	2458.8281
2616.7598	2708.4150	3050.3206
3066.3727	3073.7064	3077.1879
3122.8433	3136.5917	3142.8353
3160.8151	3485.0505	3511.2308
3561.4767	3604.7515	3613.3185