Supporting Information

Experimental and Computational Study of the Formation Mechanism of the Diammoniate of Diborane: The Role of Dihydrogen Bonds

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Supporting Information

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General experimental details

All manipulations were carried out using a high vacuum line or in a nitrogen-filled glovebox or glove bag, unless indicated otherwise. All reactions were monitored using ^{11}B NMR spectroscopy which is the most easily applied technique to distinguish ammonia borane (AB) from the diammoniate of diborane (DADB). The product ratios were calculated based upon the integrated values of the corresponding boron signals in ^{11}B or $^{11}B\{^1H\}$ NMR spectra. The ^{11}B and $^{11}B\{^1H\}$ NMR spectra were obtained at 160 MHz and externally referenced to $BF_3{\cdot}OEt_2$ in C_6D_6 (δ = 0.00 ppm). Ammonia (Matheson), deutero ammonia, ND_3 (Aldrich), trimethylamine borane (Aldrich), and ammonia borane (AB, GFS Chemicals) were used as received without further purification. Tetrahydrofuran borane ($THF{\cdot}BH_3$) (Aldrich) was redistilled prior to use and tetrahydrofuran (THF) (Aldrich) was dried over sodium/benzophenone freshly distilled prior to use.

Reaction of THF·BH_3 with NH_3 at -78 °C

A THF·BH_3 (1M) tetrahydrofuran solution was condensed at −78 °C (20 ml in a 50 ml flask) and maintained at that temperature. Ammonia was passed over the solution with stirring. The reaction process was monitored by ^{11}B and $^{11}B\{^1H\}$ NMR spectra immediately after NH_3 was introduced. Samples of the reaction mixture were withdrawn at one-minute intervals using a syringe and were stored at −78 °C. Their $^{11}B\{^1H\}$ and ^{11}B NMR spectra were obtained rapidly as each sample was warmed from −78 °C to room temperature (Figures 1 and S1). For each sample, it took about one minute to collect a $^{11}B\{^1H\}$ NMR spectrum (scanned 16 times) and two more minutes for ^{11}B NMR spectrum (scanned 16 times).

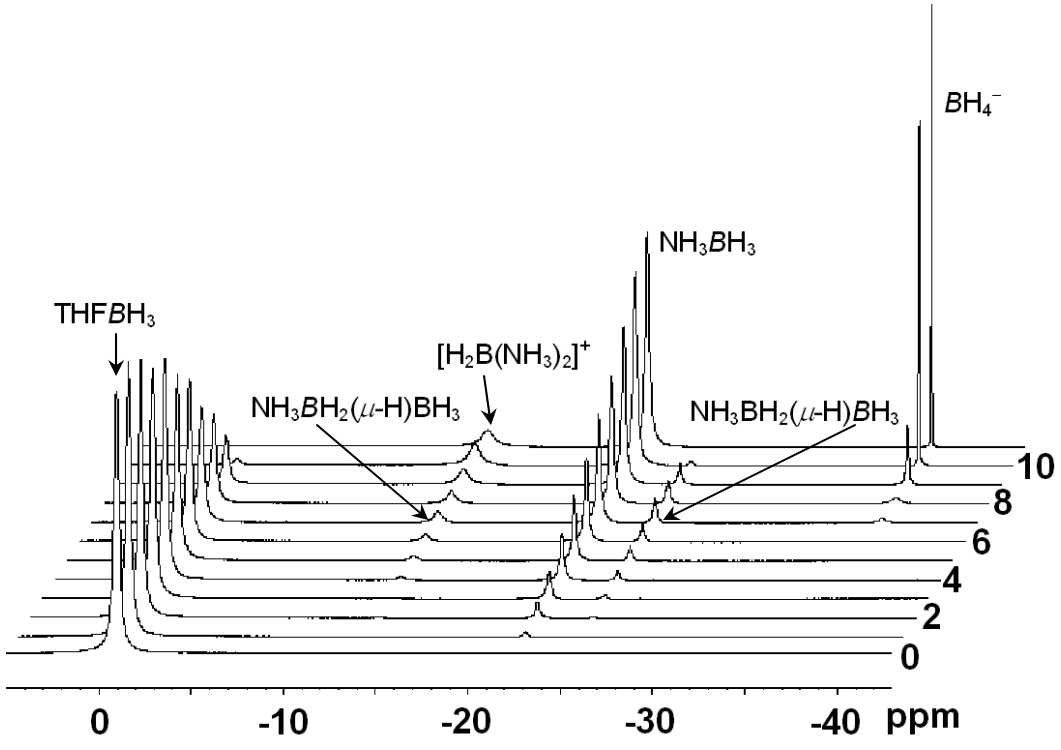


Figure S1. $^{11}B\{^1H\}$ NMR spectra of the reaction of NH_3 with a THF·BH_3 solution at − 78 °C (Samples extracted at one minute interval and stored at −78 °C. After the reaction was complete, spectra were rapidly recorded individually as each sample was warmed to ambient temperature)

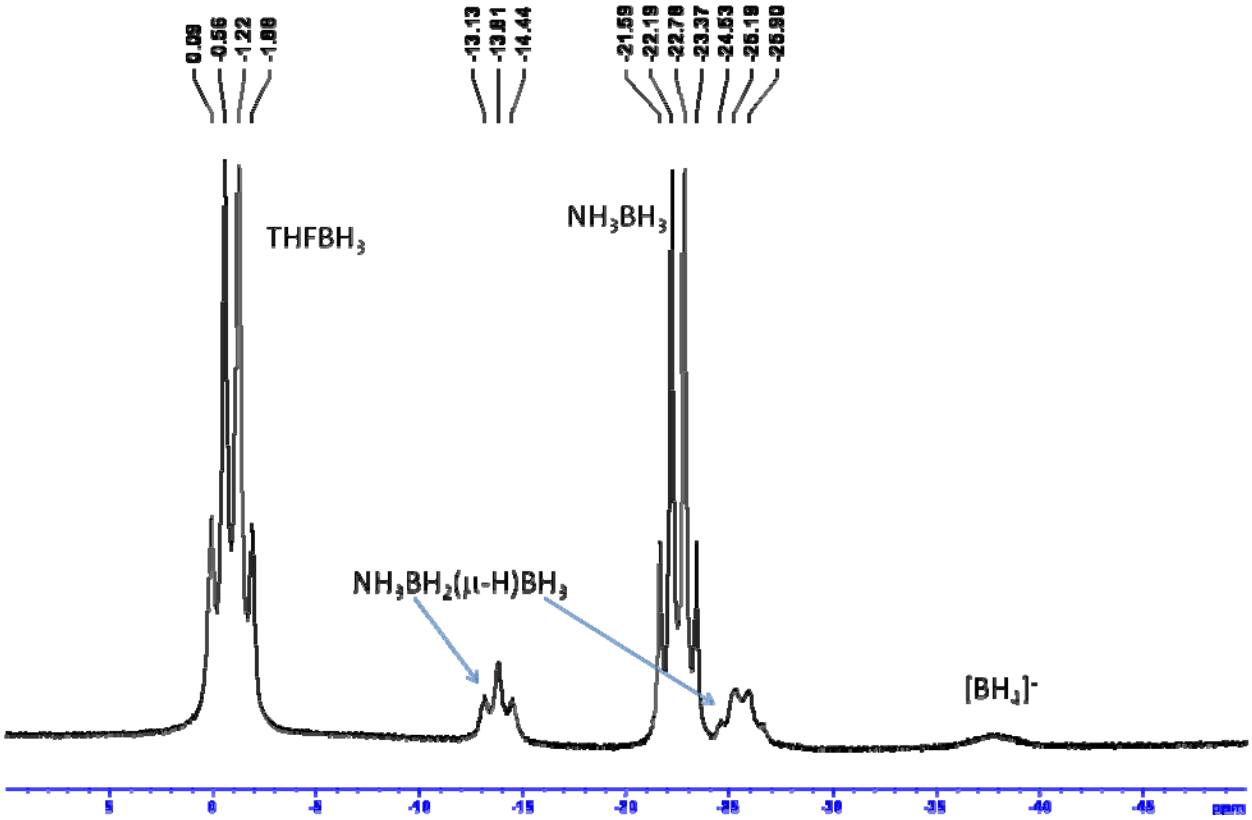


Figure S2. ^{11}B NMR spectrum taken from Figure 1 of the 7-min sample, in which a triplet and a quartet of B_aH_2 group and B_bH_3 group in AaDB are clearly observed. A broad peak emerged at about δ -38 ppm indicates that the $[BH_4]^-$ anion came into being.

Reaction of $THF{\cdot}BH_3$ and $NH_2B_2H_5$ with NH_3 at -78 °C

To a 50 ml flask, 0.1 ml $NH_2B_2H_5$ tetrahydrofuran solution (the ratio of $NH_2B_2H_5$:THF being about 1:1) was added and then 20 ml $THF{\cdot}BH_3$ (1M) tetrahydrofuran solution was condensed at −78 °C, ammonia was passed over the mixture. The reaction process was monitored by ^{11}B and $^{11}B\{^1H\}$ NMR and the spectra were recorded every two minutes. The ^{11}B and $^{11}B\{^1H\}$ NMR spectra were rapidly recorded individually as each sample was warmed to room temperature (Figures S3 and S4).

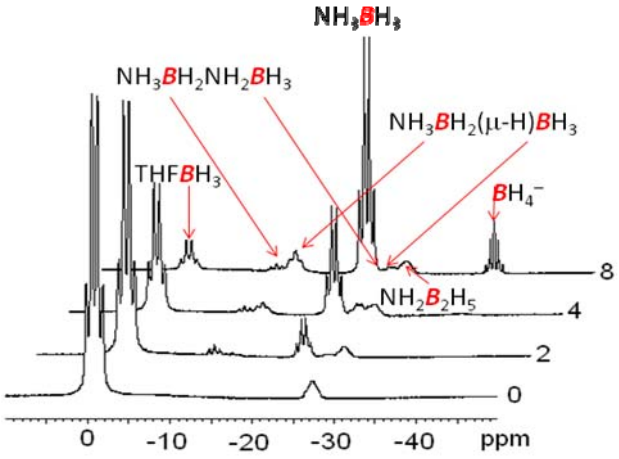


Figure S3. ^{11}B NMR spectra monitoring the progression of the reaction between $THF{\cdot}BH_3$ and $NH_2B_2H_5$ with NH_3 (two minute interval).

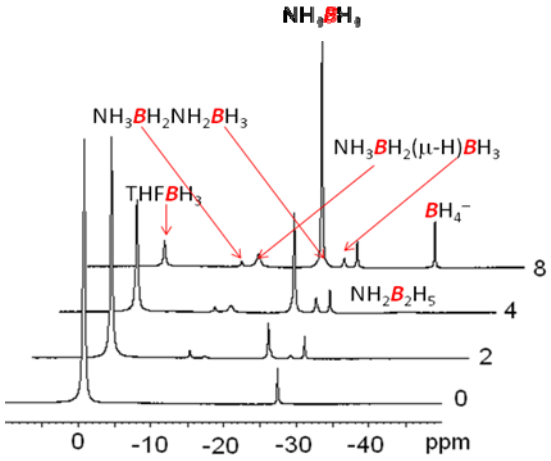


Figure S4. $^{11}B\{^1H\}$ NMR spectra monitoring the progression of the reaction between $THF{\cdot}BH_3$ and $NH_2B_2H_5$ with NH_3 (two minute interval).

Compound $NH_3BH_2NH_2BH_3$ also has a triplet at δ −11.6 and a quartet at δ −22.8 ppm,[S1] which is similar to that of AaDB, a triplet at δ −13.8 and a quartet at δ −25.5 ppm. In order to distinguish these two compounds, a small amount of $NH_2B_2H_5$ was added to $THFBH_3$ solution. Thus, NH_3 will react with both $NH_2B_2H_5$ and $THF{\cdot}BH_3$ at the same time when NH_3 was passed over the mixture. All products from the following four reactions were reflected in ^{11}B and $^{11}B\{^1H\}$ NMR spectra.

$$NH_3 + NH_2B_2H_5 \rightarrow NH_3BH_2NH_2BH_3 \quad (1)$$

$$NH_3 + THF{\cdot}BH_3 \rightarrow NH_3BH_3 + THF \quad (2)$$

$$NH_3BH_3 + THF{\cdot}BH_3 \rightarrow NH_3BH_2(\mu\text{-}H)BH_3 \quad (3)$$

$$NH_3 + NH_3BH_2(\mu\text{-}H)BH_3 \rightarrow [H_2B(NH_3)_2][BH_4] \quad (4)$$

The signal of BH_3 group in $NH_3BH_2NH_2BH_3$ compound overlaps with the signal of BH_3 group in NH_3BH_3 since both groups have very close chemical shift. The boron signal of cation $[H_2B(NH_3)_2]^+$ is not labeled in the spectra because the change from $NH_3BH_2(\mu\text{-}H)BH_3$ to cation of $[H_2B(NH_3)_2]$ is not observed as discussed in the main paper.

Two sets of separated resonances are from $NH_3BH_2NH_2BH_3$ and AaDB compounds, respectively. This observation clearly proves that the resonances at δ −13.8 and −25.5 ppm are not from the $NH_3BH_2NH_2BH_3$ compound.

Computational methods and results on the ^{11}B chemical shifts of AB, DADB, and AaDB

The ^{11}B NMR chemical shifts of AB, DADB, and AaDB were calculated at the B3LYP[S2]/6-311++G(d,p) level of theory with the GIAO method[S3] implemented in the Gaussian 03 program[S4]. The $BF_3{\cdot}OEt_2$ molecule was employed as the reference compound, for which the calculated absolute shielding constant is 101.7 at the B3LYP/6-311++G(d,p) level.

The calculated ^{11}B NMR chemical shift of AB monomer is –20.8 ppm. The ^{11}B NMR of AB dimer shifts slightly to higher field, –24.8 ppm (Figure S5). The predicted ^{11}B NMR of AB is consistent with the experimentally observed data. The ^{11}B NMR chemical shifts of the $[BH_4]^-$ anion group and the $[H_2B(NH_3)_2]^+$ cation group in DADB are predicted as –37.9 and –16.3 ppm, respectively, which also agree well with the experimental data.

The calculated ^{11}B NMR chemical shifts of AaDB are –16.0 ppm for B_a and –10.4 ppm for B_b, respectively. Apparently, the predicted results are not consistent with the experimental data (δ –13.8 and –25.5 ppm). Interestingly, when a AB molecule binds AaDB to form a complex through dihydrogen bonds, the ^{11}B NMR chemical shift of B_b in AaDB shifts to a significantly higher field, –19.8 ppm. When two AB molecules interact with AaDB, the calculated B_b NMR signal shifts further to –24.4 ppm (Figure S5). Thus, computational result indicates that the dihydrogen bonding interaction between AaDB and AB can cause a significant shift for B_b of AaDB in its ^{11}B NMR. The calculated chemical shifts for B_a of AaDB in ^{11}B NMR only changes slightly (from –16.0 to –18.1 ppm), but a bit further away from the experimental value (–13.8 ppm).

The effect of THF solvent on the ^{11}B NMR chemical shifts of AaDB was also considered computationally. One to three THF molecules were explicitly H-bonded to AaDB through N-H...O H-bonds. The calculated ^{11}B NMR for B_b in AaDB shifts considerably (from –10.4 to –17.9 ppm) when three THF molecules are surrounding the AaDB; but the THF solvation effect alone is insufficient to shift the

^{11}B NMR of B_b all the way to –25.5 ppm, due to the lack of dihydrogen bonding interactions between THF and AaDB. The THF solvation effect on the ^{11}B NMR for B_a in AaDB is very small (from –16.0 to –17.7 ppm).

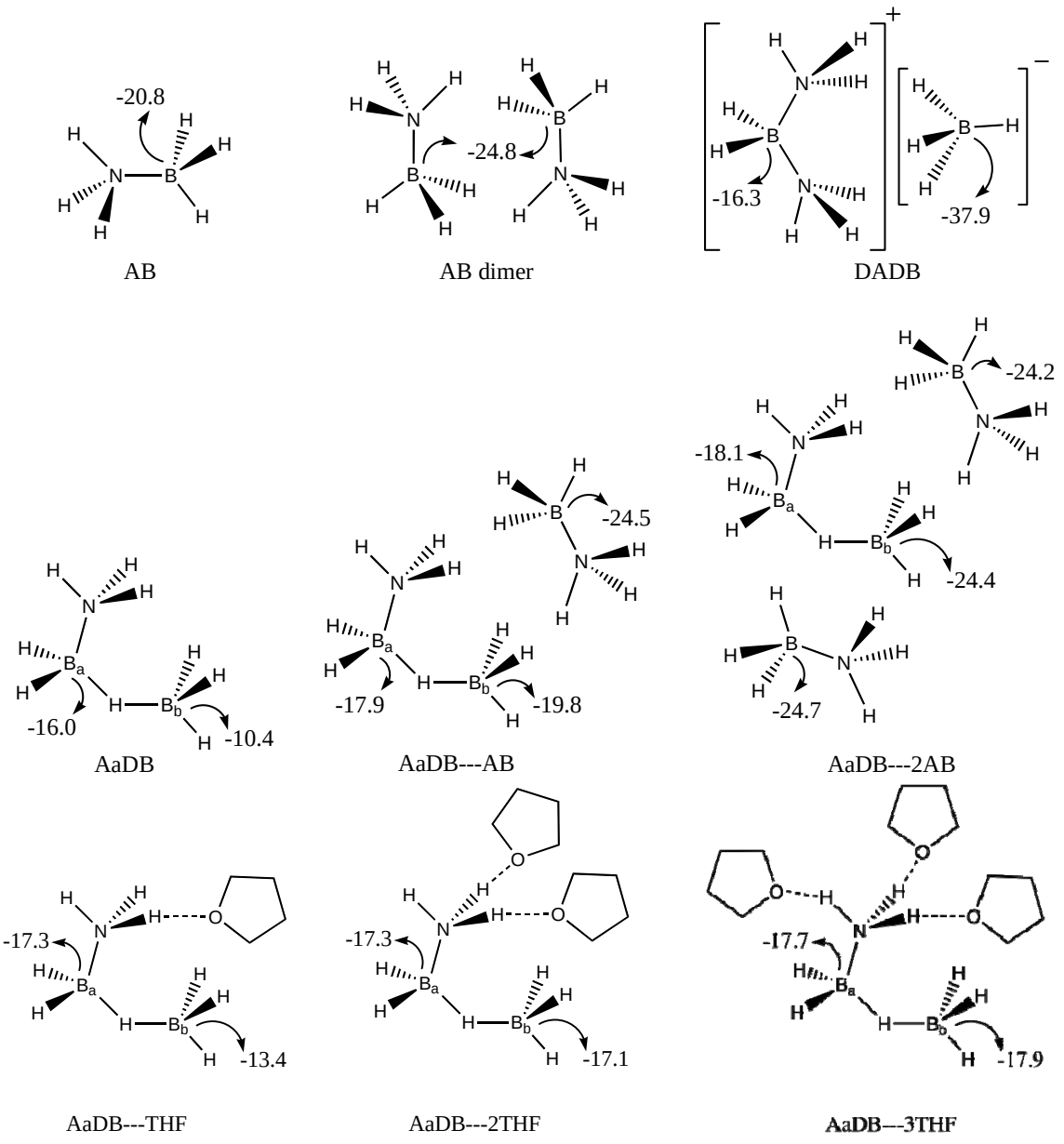


Figure S5. The calculated ^{11}B NMR chemical shifts of AB, DADB, and AaDB at the B3LYP/6-311++G(d,p) level of theory (in ppm). The influence of AB and THF on the ^{11}B NMR signal of AaDB is also shown.

The chemical shift of the cation $[H_2B(NH_3)_2]^+$

When $THF{\cdot}BH_3$ was completely consumed and the reaction solution was warmed to room temperature, the peak at δ -13.8 ppm shifted to δ -12.5 ppm. This process was recorded by the $^{11}B\{^1H\}$ NMR spectra (Figures S6, S7).

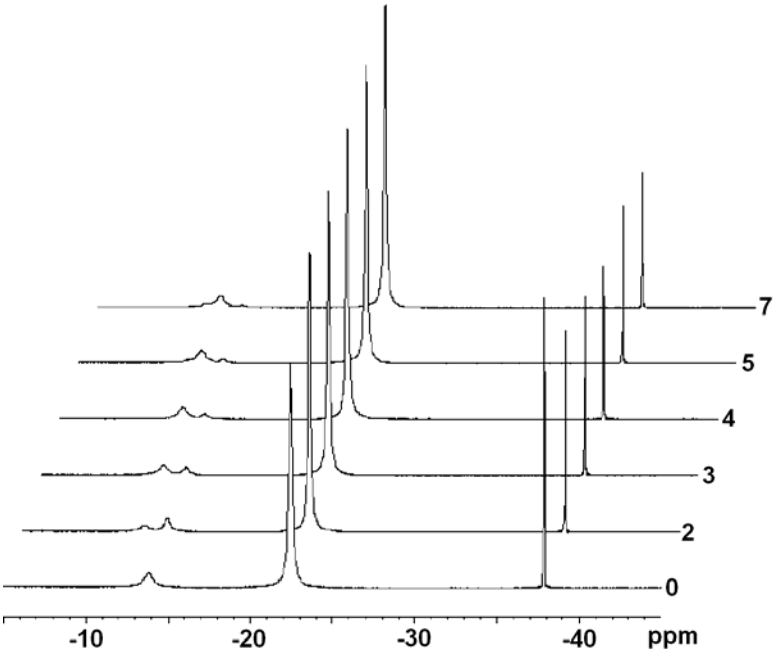


Figure S6. $^{11}B\{^1H\}$ NMR spectra showing the chemical shift of the cation $[H_2B(NH_3)_2]^+$ changing with time at room temperature (numbers on the right are in minutes).

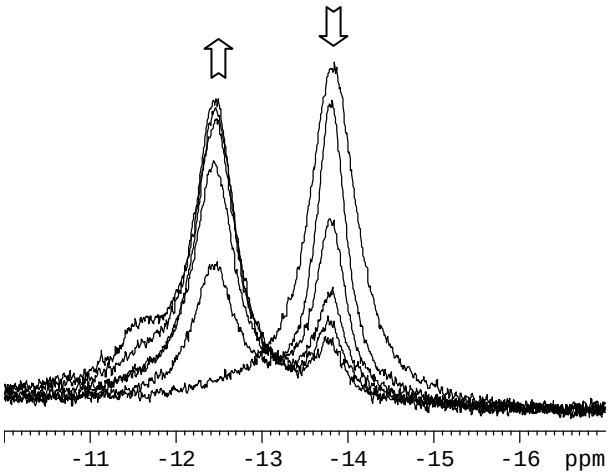


Figure S7. $^{11}B\{^1H\}$ NMR spectra monitoring the chemical shift change of the cation $[H_2B(NH_3)_2]^+$.

Chemical shift change of signal associated with the $[H_2B(NH_3)_2]^+$ cation of DADB was observed at ambient temperature. When the final reaction solution consisting of both AB and DADB (after $THF{\cdot}BH_3$ was completely consumed) was warmed to room temperature, the triplet at δ –13.8 ppm shifted to low frequency field (see the 11-minute spectrum in Figure 1). Further experimentation found that the triplet could shift to δ –12.5 ppm after several minutes and the intensity of the BH_4^- anion peak decreased at the same time (Figures S6, S7). The decomposition of DADB at room temperature to form a polymeric species might cause such a chemical shift change. Further study is in progress.

Reaction of $THF{\cdot}BH_3$ with NH_3 (large excess) at -78 °C

A THF solution of $THF{\cdot}BH_3$ (1ml, 1M) was condensed in a 50 ml flask at -196 °C and then about 15 ml liquid NH_3 was condensed into the flask at –78 °C. The mixture was stirred for 5 min at -78 °C. After NH_3 and THF were removed under vacuum, a white powder was produced. ^{11}B NMR spectrum showed that the white powder is pure AB (Figure S8). This observation differs from the results when NH_3 gas was passed over a $THF{\cdot}BH_3$ (1M) solution at -78 °C where a mixture of AB and DADB was produced (Figures 1 and S1)

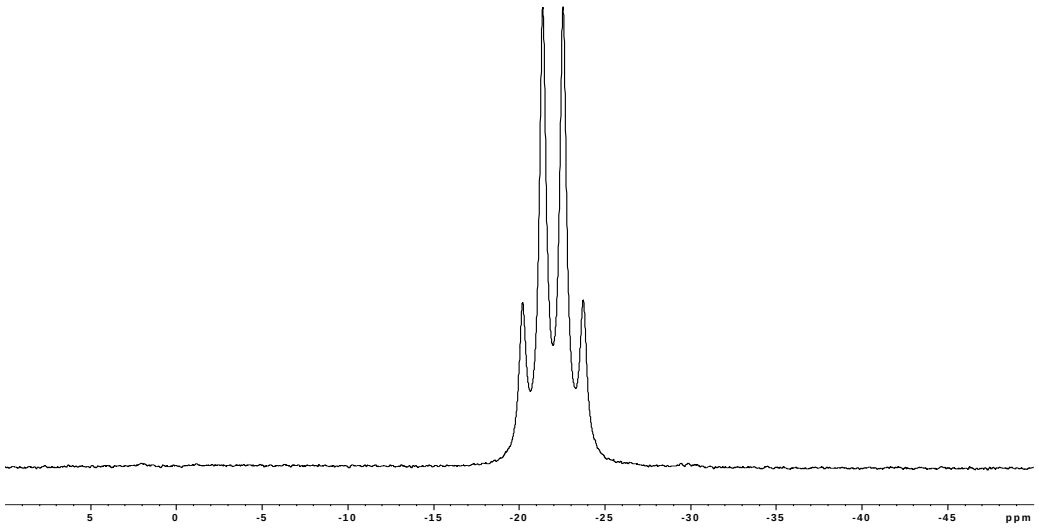


Figure S8. ^{11}B NMR spectrum of the product from the reaction of $THF{\cdot}BH_3$ with large excess NH_3 at -78 °C

In the reaction of $THF{\cdot}BH_3$ with larger excess of NH_3, all $THF{\cdot}BH_3$ was reacted with NH_3 in the initial period to produce AB. Thus, no more $THF{\cdot}BH_3$ left for further reacting with the formed AB in step 2 in scheme 1. As a result, pure AB was produced as observed in the ^{11}B NMR spectrum. In contrast, when NH_3 was passed over a $THF{\cdot}BH_3$ solution, the initially formed AB further reacted with a large amount of $THF{\cdot}BH_3$ existed in solution to form AaDB and then to form DADB; thus a mixture of AB and DADB was produced as observed in the corresponding ^{11}B NMR spectra (Figures 1 and S1).

Experimental evidence of the catalytic role of AB molecules leading to DADB

Two experiments directly support the argument that the presence of AB in the solution accelerates the formation of DADB.

In the first experiment, an equimolar of $THF{\cdot}BH_3$ and AB tetrahydrofuran solution (0.5 M) was used instead of 1.0 M $THF{\cdot}BH_3$ tetrahydrogen solution with the expectation that the intentional-addition of AB would make more dihydrogen bonds with AaDB, which would in turn result in a higher yield of DADB. At -78 °C, NH_3 gas was passed over a solution of 0.5 M $THF{\cdot}BH_3$ and 0.5 M AB. The reaction was monitored by boron NMR spectroscopy. The ^{11}B and $^{11}B\{1H\}$ NMR spectra were shown in Figures S9 and S10.

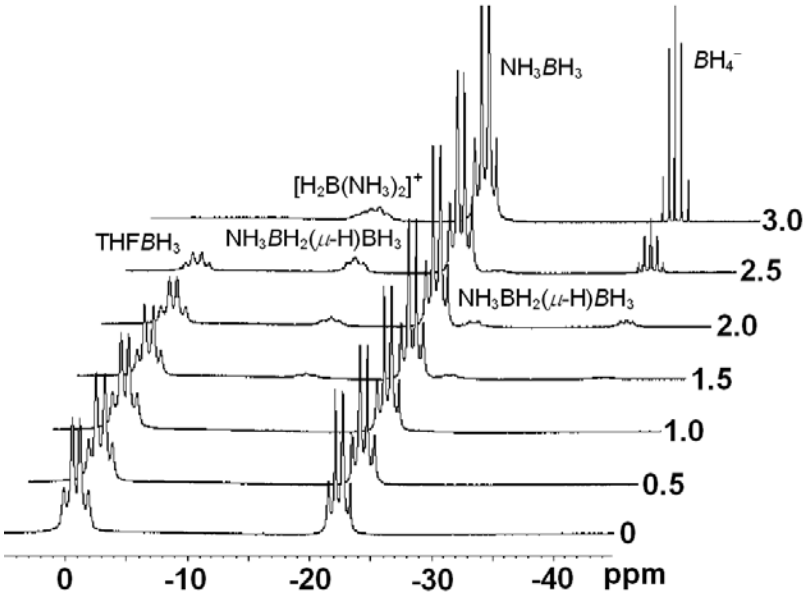


Figure S9. ^{11}B NMR spectra monitoring the progress (time shown on the right in minutes) of the reaction between $THF{\cdot}BH_3$ (0.5M) and NH_3 in the presence of AB (0.5M).

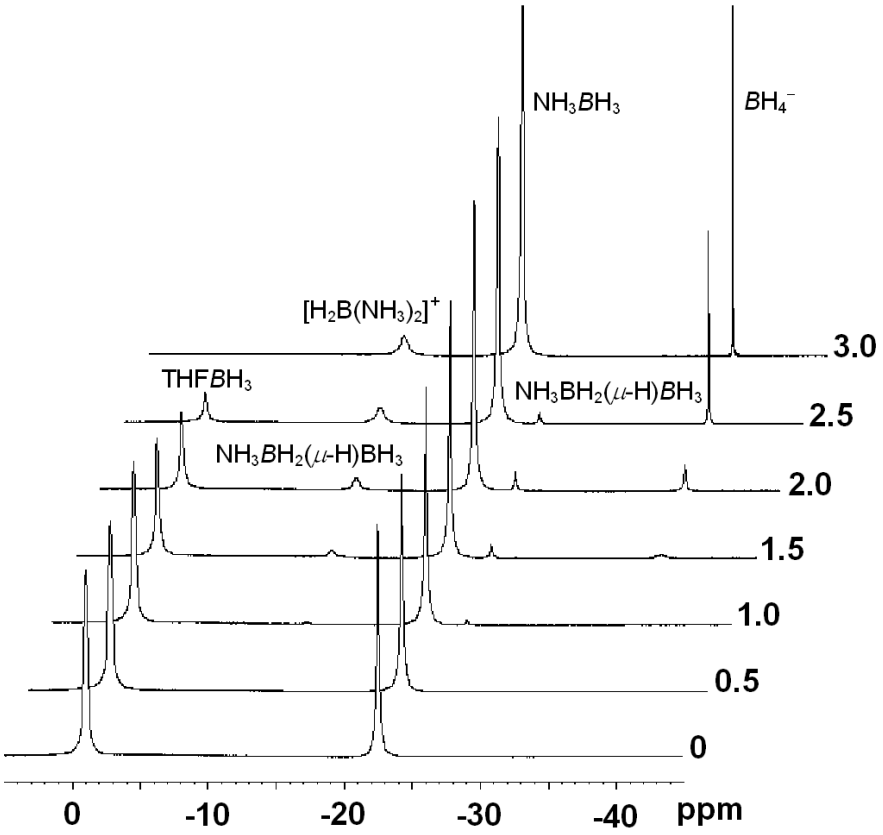


Figure S10. $^{11}B\{^{1}H\}$ NMR spectra monitoring the progression (time shown on the right in minutes) of the reaction between $THF{\cdot}BH_3$ (0.5M) and NH_3 in the presence of AB (0.5M).

In the second experiment, an equimolar of $THF{\cdot}BH_3$ and $(CH_3)_3NBH_3$ (TMAB) tetrahydrofuran solution (0.5 M) was used instead of an equimolar of $THF{\cdot}BH_3$ and AB tetrahydrofuran solution (0.5 M) in the first experiemnt with an expectation that the intentionally added TMAB would be less effective in forming dihydrogen bonds with AaDB (though a similar solvation effect was in effect). The less effective dihydrogen bonding would result in a lower yield of DADB. At -78 °C, NH_3 gas was passed over a solution of 0.5 M $THF{\cdot}BH_3$ and 0.5 M TMAB. The reaction was monitored by boron NMR spectroscopy. The ^{11}B and $^{11}B\{1H\}$ NMR spectra were shown in Figures S11 and S12.

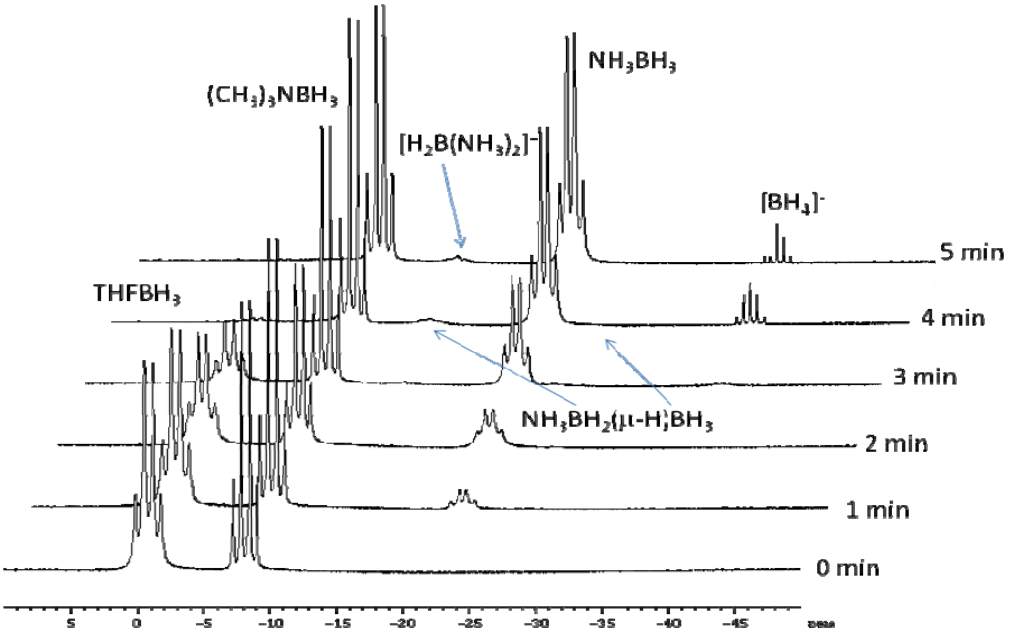


Figure S11. ^{11}B NMR spectra monitoring the progress (time shown on the right in minutes) of the reaction between $THF{\cdot}BH_3$ (0.5M) and NH_3 in the presence of TMAB (0.5M).

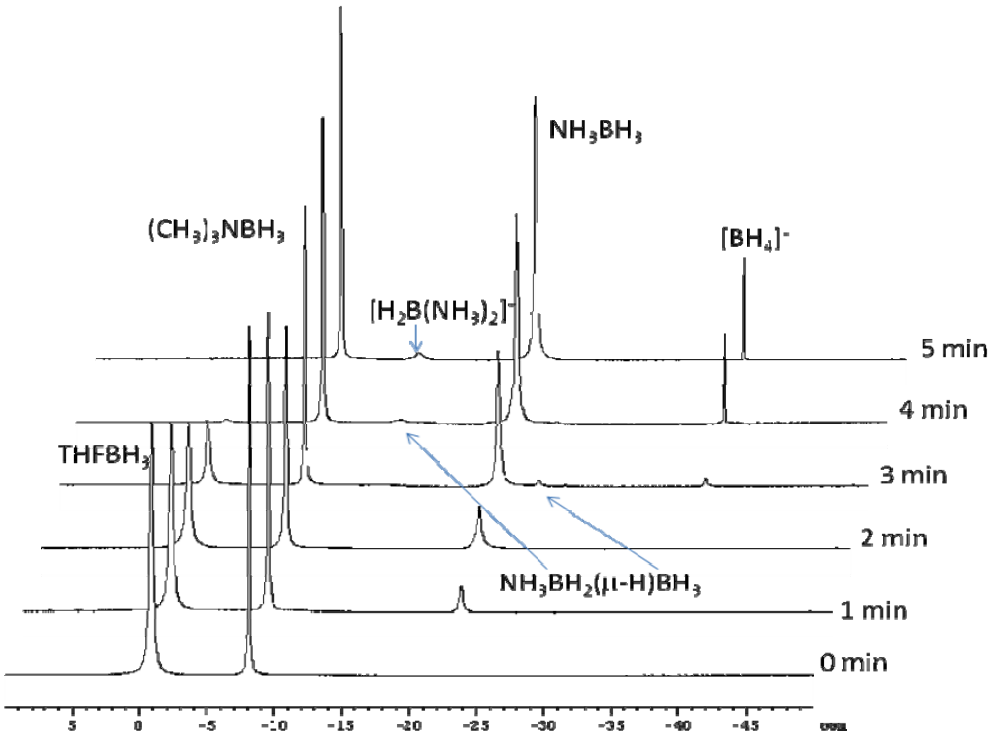


Figure S12. $^{11}B\{^{1}H\}$ NMR spectra monitoring the progression (time shown on the right in minutes) of the reaction between THF·BH_3 (0.5M) and NH_3 in the presence of TMAB (0.5M).

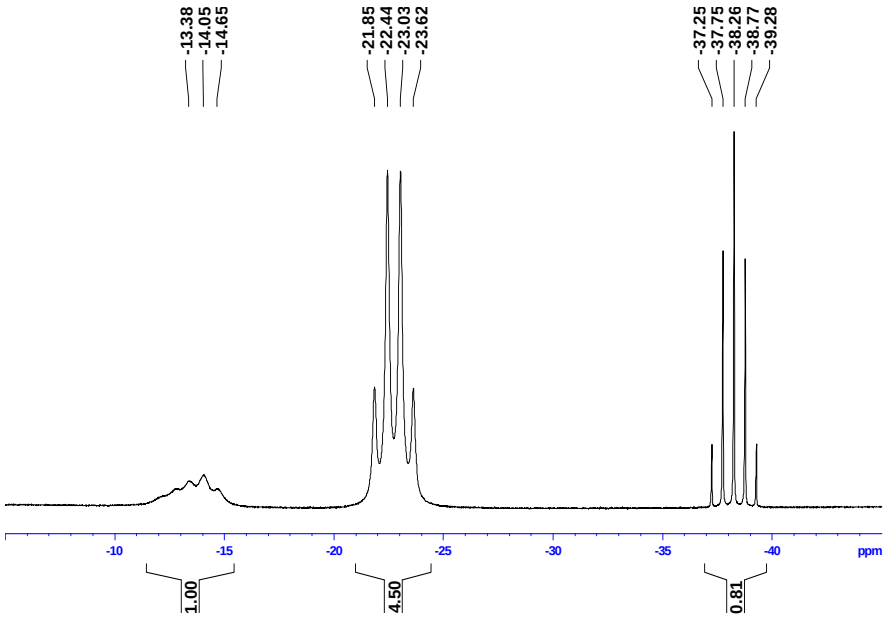


Figure S13. ^{11}B NMR spectrum of the reaction mixure (from Figure 1, THF·BH_3 (1M) + NH_3, 11-min spectrum when the reaction had just completed).

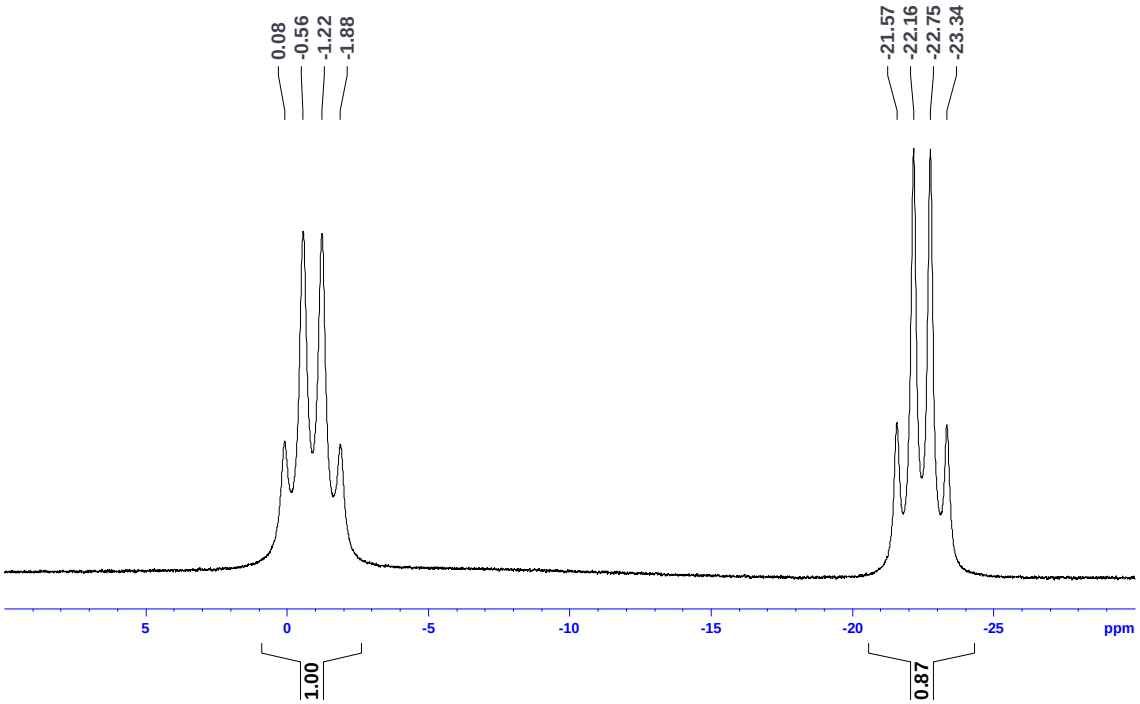


Figure S14. ^{11}B NMR spectrum of the starting solution (from Figure S9, THF·BH_3 (0.5M) + NH_3BH_3 (0.5M) + NH_3, 0-min spectrum).

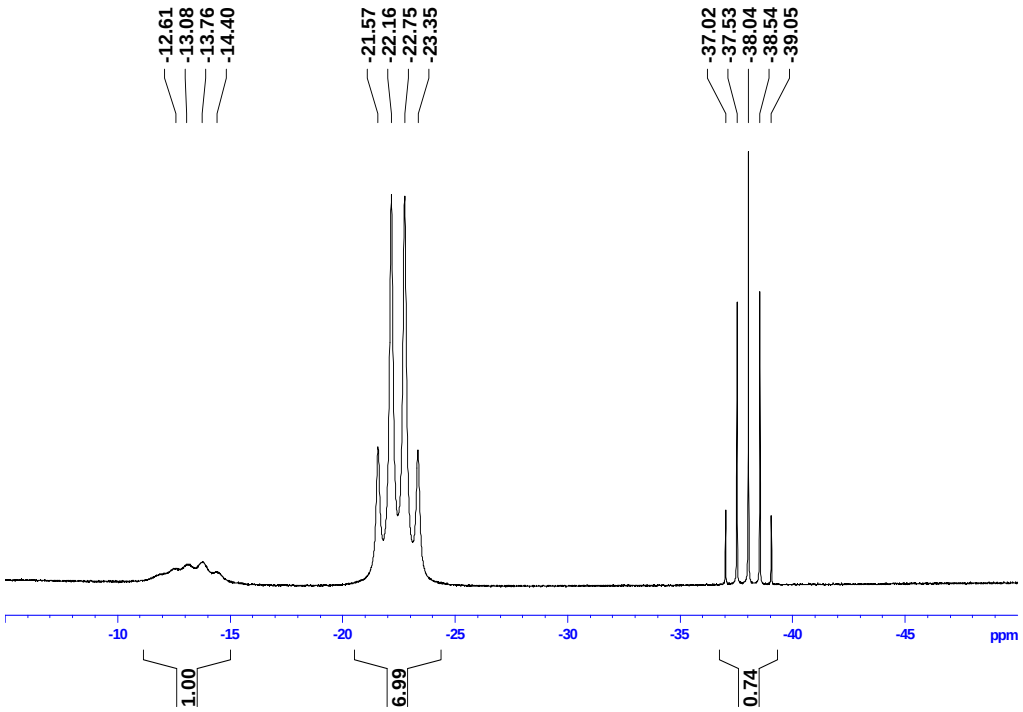


Figure S15. ^{11}B NMR spectrum of the reaction mixure (from Figure S9, THF·BH_3 (0.5M) + NH_3BH_3 (0.5M) + NH_3, 3-min spectrum when the reaction had just completed).

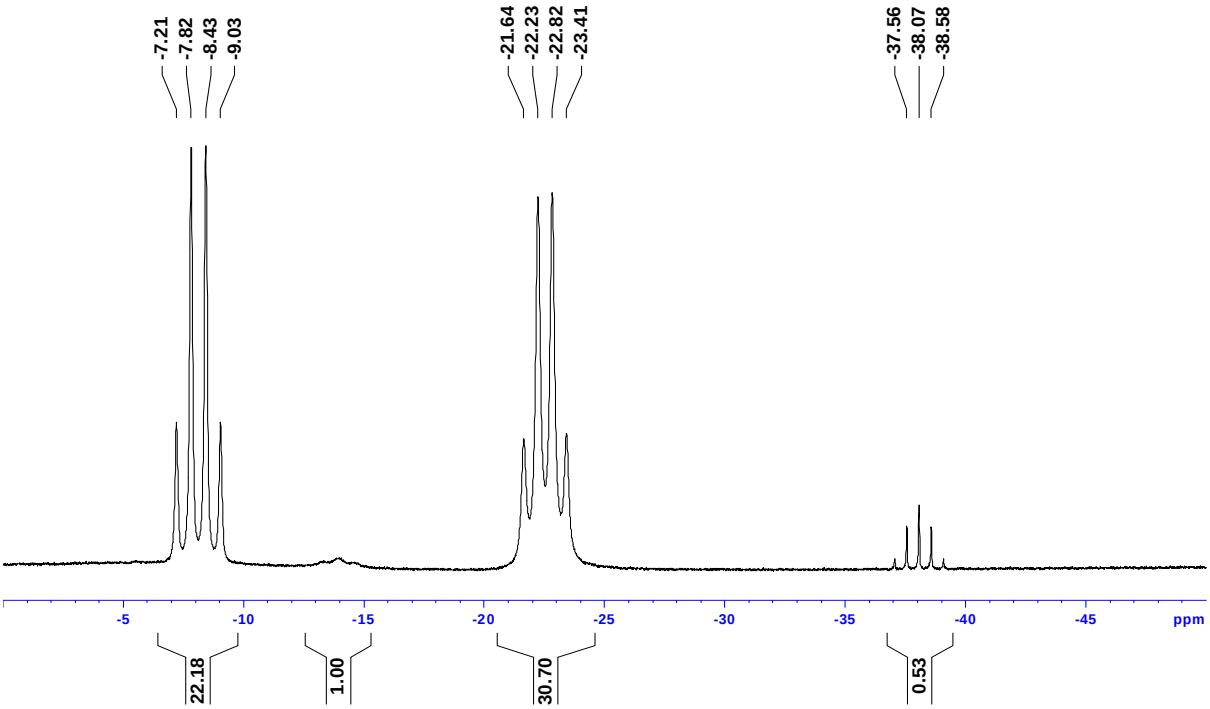


Figure S16. ^{11}B NMR spectrum of the reaction mixure (from Figure S11, THF·BH_3 (0.5M) + $(CH_3)_3NBH_3$ (0.5M) + NH_3, 5-min spectrum when the reaction had just completed).

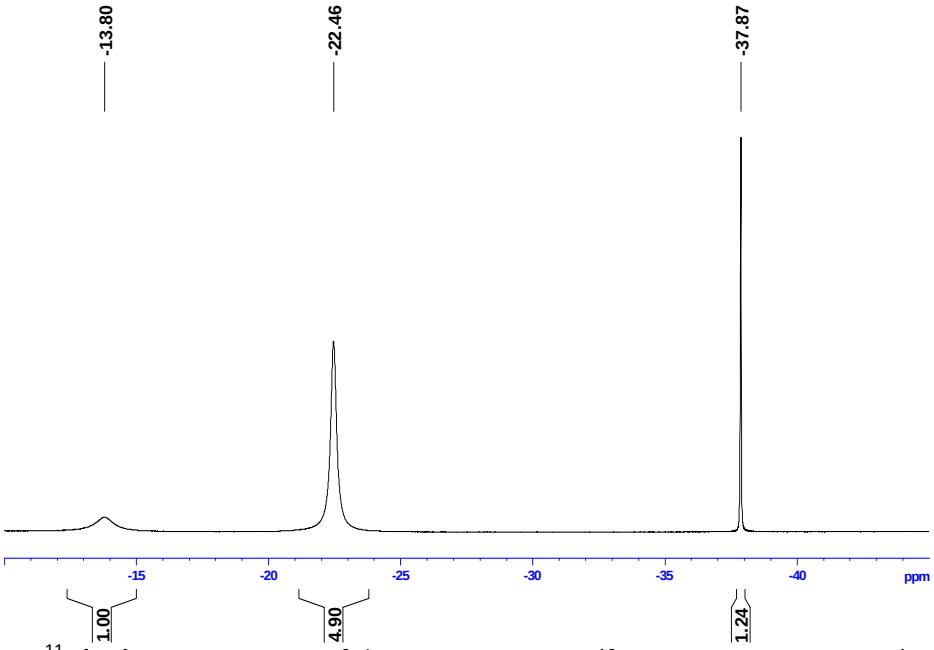


Figure S17. $^{11}B\{1H\}$ NMR spectrum of the reaction mixure (from Figure S1, THF·BH_3 (1M) + NH_3, 11-min spectrum when the reaction had just completed).

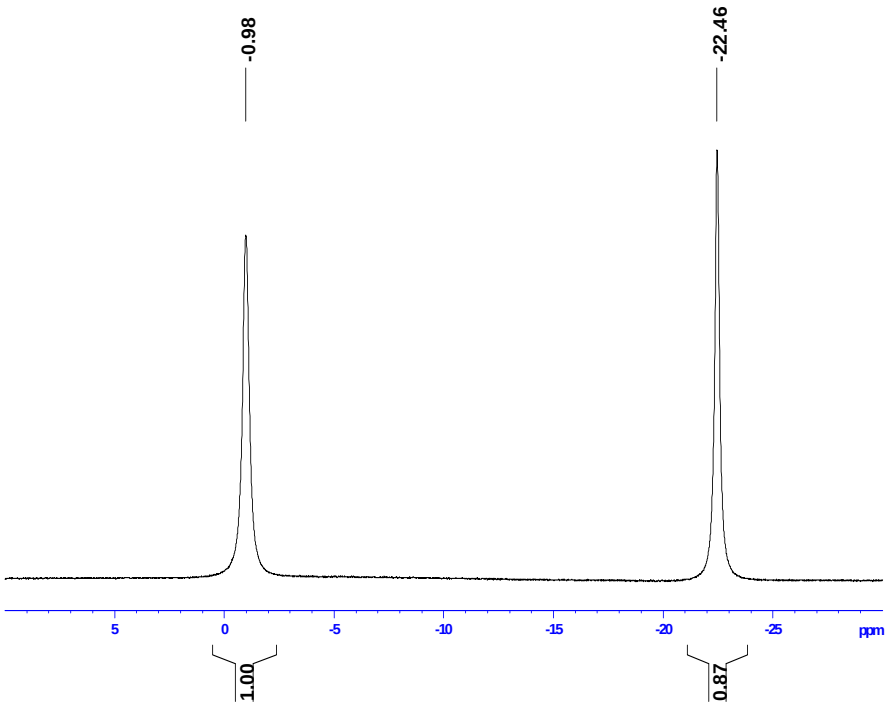


Figure S18. $^{11}B\{^1H\}$ NMR spectrum of the staring solution (from Figure S10, THF·BH_3 (0.5M) + NH_3BH_3 (0.5M) + NH_3, 0-min spectrum)

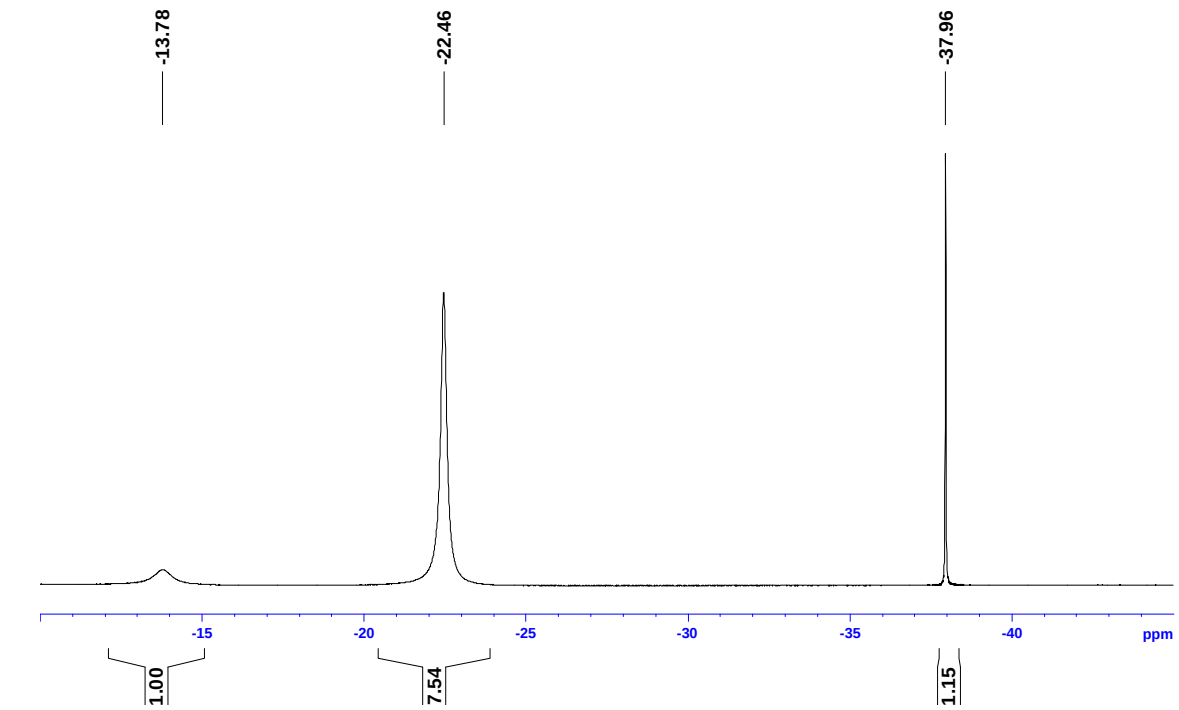


Figure S19. $^{11}B\{1H\}$ NMR spectrum of the reaction mixure (from Figure S10, THF·BH_3 (0.5M) + NH_3BH_3 (0.5M) + NH_3, 3-min spectrum when the reaction had just completed).

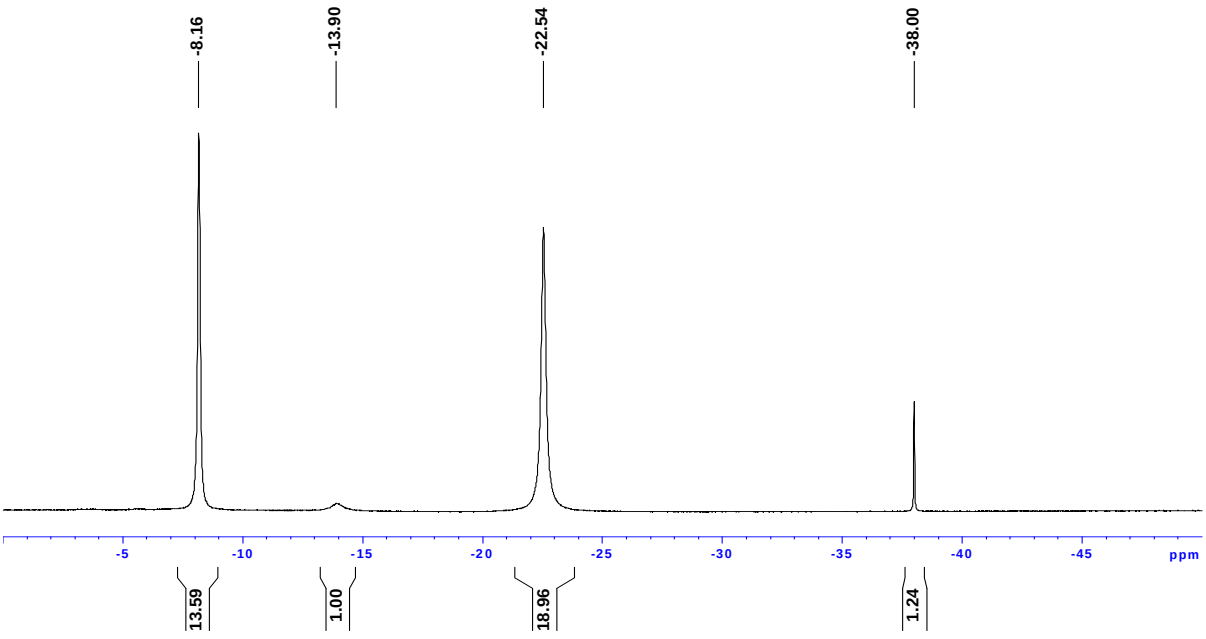


Figure S20. $^{11}B\{^1H\}$ NMR spectrum of the reaction mixure (from Figure S12, THF·BH_3 (0.5M) + $(CH_3)_3NBH_3$ (0.5M) + NH_3, 5-min spectrum when the reaction had just completed).

The ^{11}B and $^{11}B\{^1H\}$ spectra confirmed the catalytic role of AB through the dihydrogen bonding interaction with AaDB. The integrated values of AB and BH_4^- anion in ^{11}B and $^{11}B\{^1H\}$ NMR spectra were used to calculate the ratios of DADB to AB.

The molar ratios of DADB to AB in product in the original experiment based on the ^{11}B (Figures S13) or $^{11}B\{^1H\}$ NMR spectra (Figure S17) are:

DADB : AB = 0.81 : 4.50 = 1.0 : 5.6 (the ^{11}B NMR spectra, Figure S13)

DADB : AB = 1.24 : 4.90 = 1.0 : 4.0 (the $^{11}B\{^1H\}$ NMR spectra, Figure S17)

The molar ratios of DADB to AB in the first experiment with the presence of the intentionally-added AB, based on the ^{11}B (Figures S14 and S15) or $^{11}B\{^1H\}$ NMR spectra (Figures S18 and S19) are:

Formed AB in the final products (including intentionally-added AB and formed AB) in the first experiement based on the integrated values in ^{11}B NMR spectra (Figures S14 and S15):

$6.99 - [(1.00 + 6.99 + 0.74) \times 0.87]/(1.00 + 0.87) = 2.93$

DADB : AB = 0.74 : 2.93 = 1.0 : 4.0 (^{11}B spectra, Figures S14 and S15)

Formed AB in the final products (including intentionally-added AB and formed AB) in the first experiement based on the integrated values in $^{11}B\{^1H\}$ NMR spectra (Figures S18, S19):

$7.54 - [(1.00 + 7.54 + 1.15) \times 0.87]/(1.00 + 0.87) = 3.03$

DADB : AB = 1.15 : 3.03 = 1.0 : 2.6 (^{11}B spectra, Figures S18 and S19)

The ratios of DADB to AB in the second experiment with the presence of the intentionally-added TMAB, based on the ^{11}B (Figures S16) or $^{11}B\{^1H\}$ NMR spectra (Figures S20) are:

DADB : AB = 0.53 : 30.7 = 1.0 : 58 (the ^{11}B NMR spectra, Figure S16)

DADB : AB = 1.24 : 19.0 = 1.0 : 15 (the $^{11}B\{^1H\}$ NMR spectra, Figure S20)

In summary, in the first experiment, the intentionally-added AB clearly causes a higher yield of DADB (Figures S15, S19). In contrast, the addition of 0.5 M TMAB in the second experiment (instead of 0.5 M AB in the first experiment) significantly decreased the DADB yield since TMAB, after methyl group

sustitution, cannot effectively form the dihydorgen bond with the AaDB intermediate (Figures S16 and S20). Therefore, these experiment results support the positive catalytic effect of AB in the formation of DADB via dihydorgen bond interactions with the AaDB intermediate.

It is worth noting that the ratios of DADB to AB based on the integrated values from ^{11}B NMR spectra are always lower than those from the $^{11}B\{^{1}H\}$ NMR spectra. The ratio of DADB to AB based on integrated values from the ^{11}B NMR spectra in the second experiment may not be trustworthy because the very small peaks of DADB in the spectra can lead to large variations of the integrated values. Though equimolar of $THF{\cdot}BH_3$ to TMAB were added in the second experiment, the integrated values did not demostrate 1:1 ratios in ^{11}B and $^{11}B[^{1}H]$ NMR spectra because of the low solubility of TMAB at relatively low temperature. According to the integrated values, the saturated concentration of TMAB in 0.5 M $THF{\cdot}BH_3$ tetrahydrofuran solution at -78 °C is about 0.3 M.

The isotope effect for the reaction

The difference between the D–H interaction in D···H dihydrogen bonds and the H–H interaction in the regular H···H dihydrogen bonds is expected to be reflected on the ratios of DADB to AB, so deuterium ammonia, ND_3, was used instead of NH_3 to react with $THF{\cdot}BH_3$ in the reaction. At -78 °C, ND_3 gas was passed over a solution of 1.0 M $THF{\cdot}BH_3$ tetrahydrofuran solution. The reaction was monitored by boron NMR spectroscopy. The ^{11}B and $^{11}B\{1H\}$ NMR spectra were shown in Figures S21 and S22.

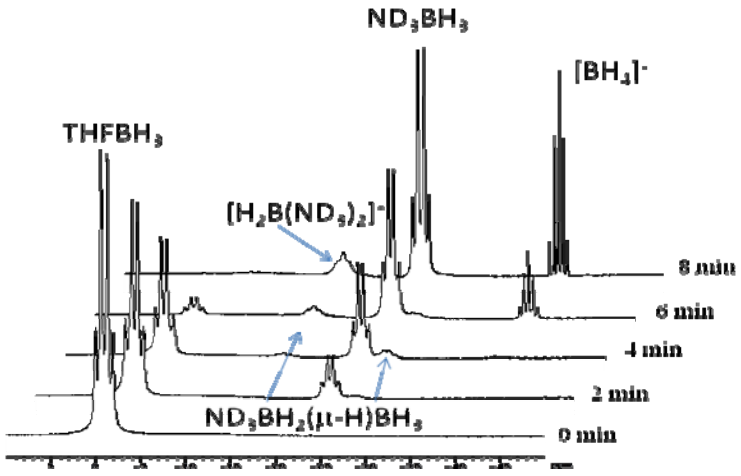


Figure S21. ^{11}B NMR spectra of the reaction of ND_3 with a $THF{\cdot}BH_3$ solution at – 78 °C (Samples were extracted at two-minute intervals and stored at –78 °C. After the reaction was complete, spectra were rapidly recorded individually as each sample was warmed to ambient temperature.)

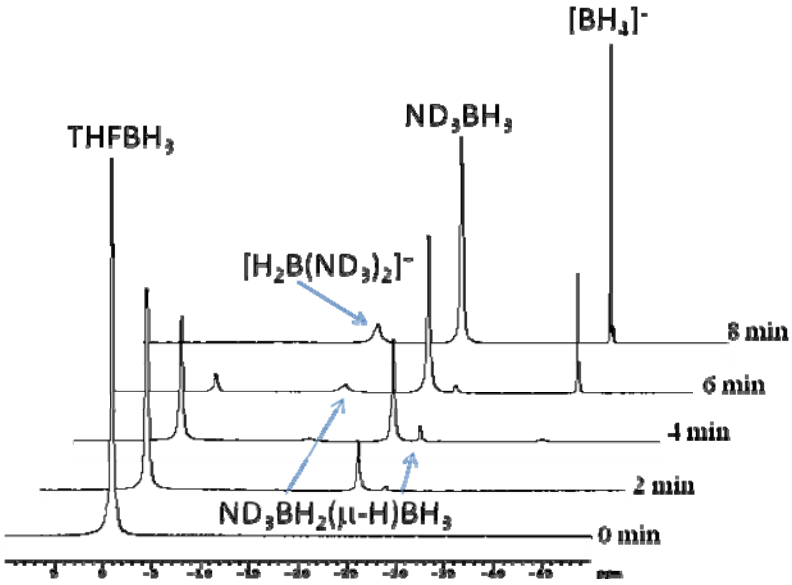


Figure S22. $^{11}B\{^{1}H\}$ NMR spectra of the reaction of ND_3 with a THF·BH_3 solution at – 78 °C (Samples were extracted at two-minute intervals and stored at –78 °C. After the reaction was complete, spectra were rapidly recorded individually as each sample was warmed to ambient temperature).

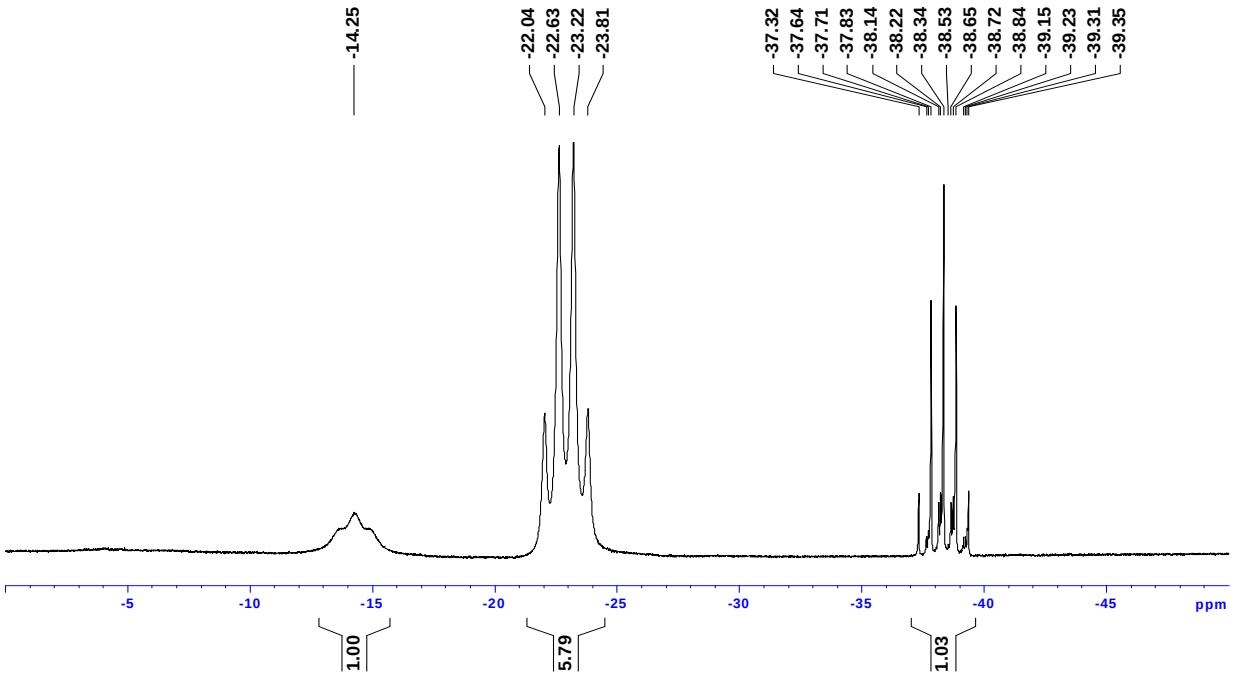


Figure S23. ^{11}B NMR spectrum of the reaction mixure (from Figure 21, 8-min spectrum when the reaction had just completed).

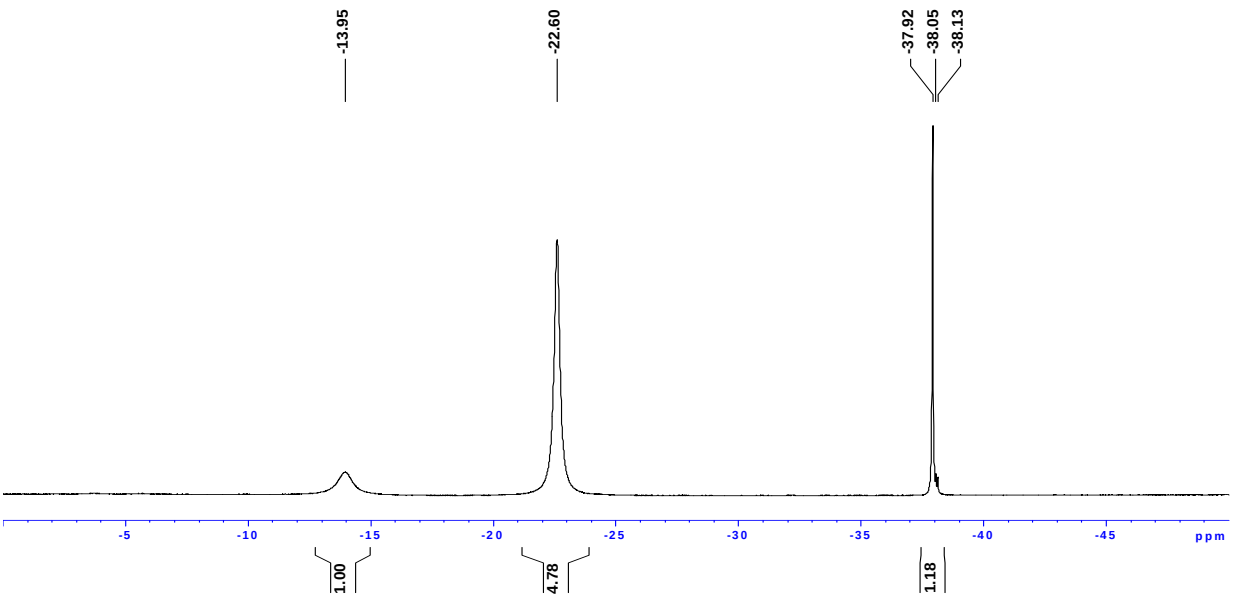


Figure S24. $^{11}B\{1H\}$ NMR spectrum of the reaction mixure (from Figure S22, 8-min spectrum when the reaction had just completed).

The molar ratios of the analogue of DADB* to ND_3BH_3 in reaction, based on the ^{11}B (Figures S23) or $^{11}B\{^1H\}$ NMR spectra (Figure S24) are:

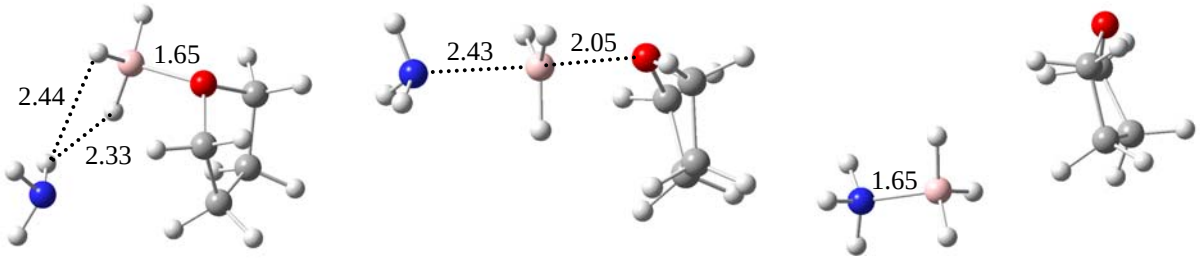
DADB* : ND_3BH_3 = 1.03 : 5.79 = 1.0 : 5.6 (the ^{11}B NMR spectra, Figure S23)

DADB* : ND_3BH_3 = 1.18 : 4.78 = 1.0 : 4.1 (the $^{11}B\{^1H\}$ NMR spectra, Figure S24)

In general, when ND_3 was used instead of NH_3 in reaction, the deuterium isotope effect was not detected. The possible reasons are either that the difference between the interaction of D···H and H···H in dihydrogen bonds is not sensitive enough to be reflected in the integrated values of boron signals or that the deuterium substitution affected on both pathway I and pathway II in the same way so that the product ratio was unaffected (Figures S23, S24, and S13, S17).

Computational methods and results

Quantum mechanical computations were performed using second-order perturbation theory (MP2). All of the structures were fully optimized with the 6-31++G(d,p) basis set. Vibrational frequency analyses were computed to ensure that the optimized structures corresponded to minima, and these analyses yielded the zero-point vibrational energy (ZPVE) corrections. Transition states (TS) were characterized as having only one imaginary vibrational frequency. The corresponding normal mode for the imaginary vibrational frequency then suggested the related reactant and product for that transition state. Natural population analysis (NPA)[S5] was used to evaluate the atomic charge of the models. The self-consistent reaction field (SCRF) polarizable continuum model (PCM)[S6] was employed to study the THF solvation effect. The UFF[S7] radii were used to generate cavity. Single point energy calculation with PCM approach was carried out using the fully optimized geometries in vacuum. The Gaussian 03 suite of programs[S4] was used for these calculations.



Reactant complex (NH_3 and $THF{\cdot}BH_3$) TS Product complex (AB and THF)

Figure S25. Optimized reaction complex, TS and product complex for the displacement reaction between NH_3 and $THF{\cdot}BH_3$. Colors: C, gray ; H, white; N, blue; B, pink; O, red. Bond lengths are shown in Å.

Table S1. Energy properties (in kcal/mol) at 0 K and 195 K for the reaction between NH_3 and $THF{\cdot}BH_3$ to produce the AB and THF complex calculated at MP2/6-31++G(d,p) level of theory. The THF solvation effect was considered by using PCM[a] approach.

	ΔE_0	ΔH_0	ΔH_{195}	ΔG_{195}	ΔH_0 (PCM)	ΔG_{195} (PCM)
RC	0.0	0.0	0.0	0.0	0.0	0.0
TS	9.6	8.4	8.4	8.4	9.2	9.2
PC	-6.4	-5.6	-5.4	-6.9	-11.5	-12.8

[a] The single point energies using optimized geometries in vacuum with ε = 7.4257.

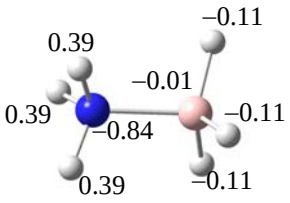
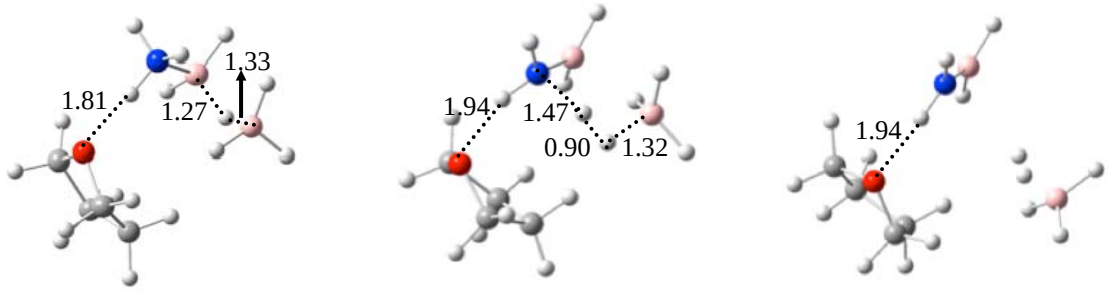


Figure S26. The NPA atomic charge distribution of the AB molecule. Colors: H, white; N, blue; B, pink.



Reactant complex (AaDB and THF) | TS | Product complex (NH_2BH_2, BH_3, H_2 and THF)

Figure S27. Optimized reaction complex, TS and product complex for the decomposition reaction of AaDB with one THF molecule. Colors: C, gray ; H, white; N, blue; B, pink; O, red. Bond lengths are shown in Å.

Table S2. Energy properties (in kcal/mol) at 0 K and 195 K for the AaDB decomposition reaction in the presence of one THF molecule calculated at MP2/6-31++G(d,p) level of theory. The THF solvation effect was considered by using PCM[a] approach.

	ΔE_0	ΔH_0	ΔH_{195}	ΔG_{195}	ΔH_0 (PCM)	ΔG_{195} (PCM)
RC	0.0	0.0	0.0	0.0	0.0	0.0
TS	32.8	28.0	28.1	27.9	31.9	31.7
PC	18.1	12.8	14.0	10.9	17.2	15.3

[a] The single point energies using optimized geometries in vacuum with ε = 7.4257.

Decomposition of AaDB in vacuum has been well investigated by Dixon *et al*.[S8] The most favourable reaction pathway is the elimination of both a protonic and a hydridic hydrogen, leading to the formation of NH_2BH_2, BH_3 and H_2. The calculated energy barrier for this reaction is 23.9 kcal/mol.[S8] In order to study the effect of solvation on this reaction, we constructed a microsolvation model in which one THF is H-bonded to AaDB. The predicted energy barrier for the dihydrogen elimination reaction of AaDB increases to 28.0 kcal/mol, implying that the decomposition of AaDB may become more difficult in the THF solution than in vacuum (Figure S27 and Table S2).

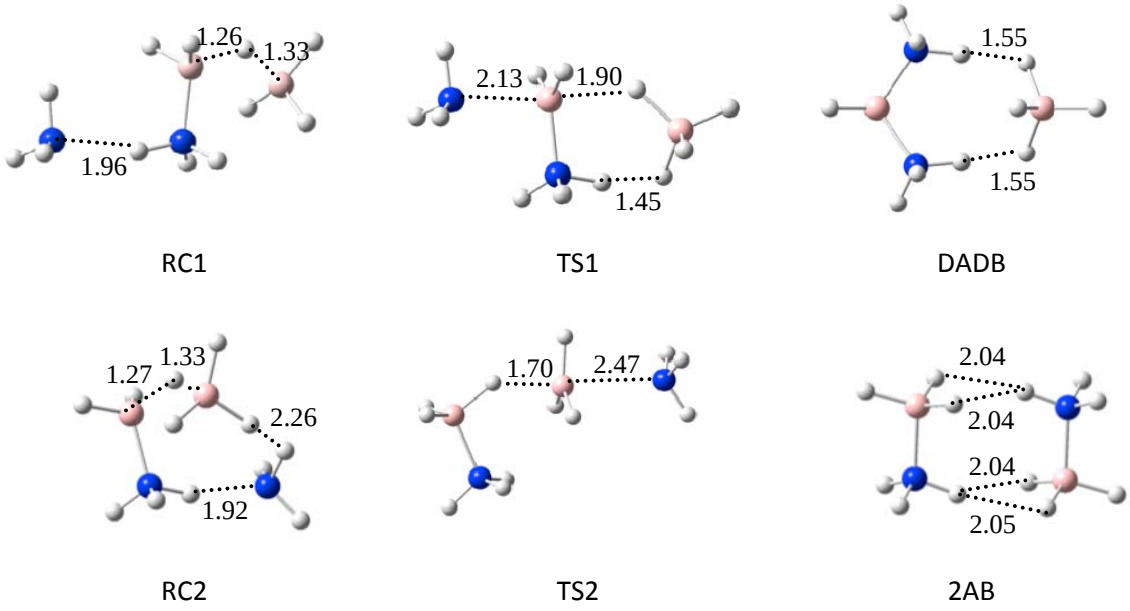


Figure S28. Optimized reactant complex (RC), TS, and corresponding product for both reaction pathways of NH_3 attacking the AaDB intermediate in vacuum. Colors: C, gray ; H, white; N, blue; B, pink. Bond lengths are shown in Å.

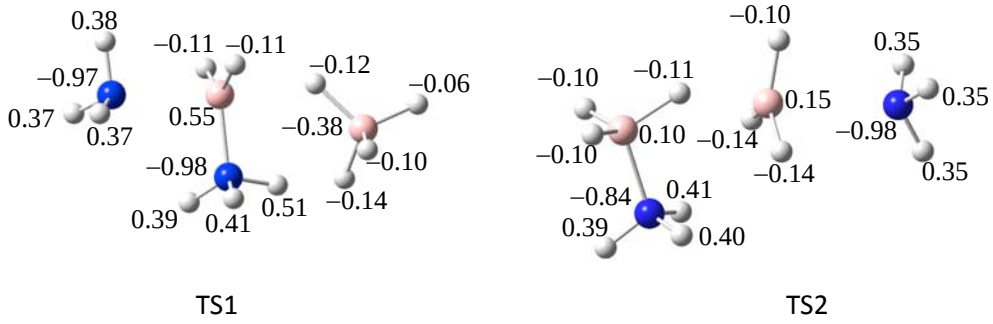


Figure S29. The NPA atomic charge distribution for the two TS structures of NH_3 attacking the AaDB intermediate in vacuum. Colors: C, gray ; H, white; N, blue; B, pink.

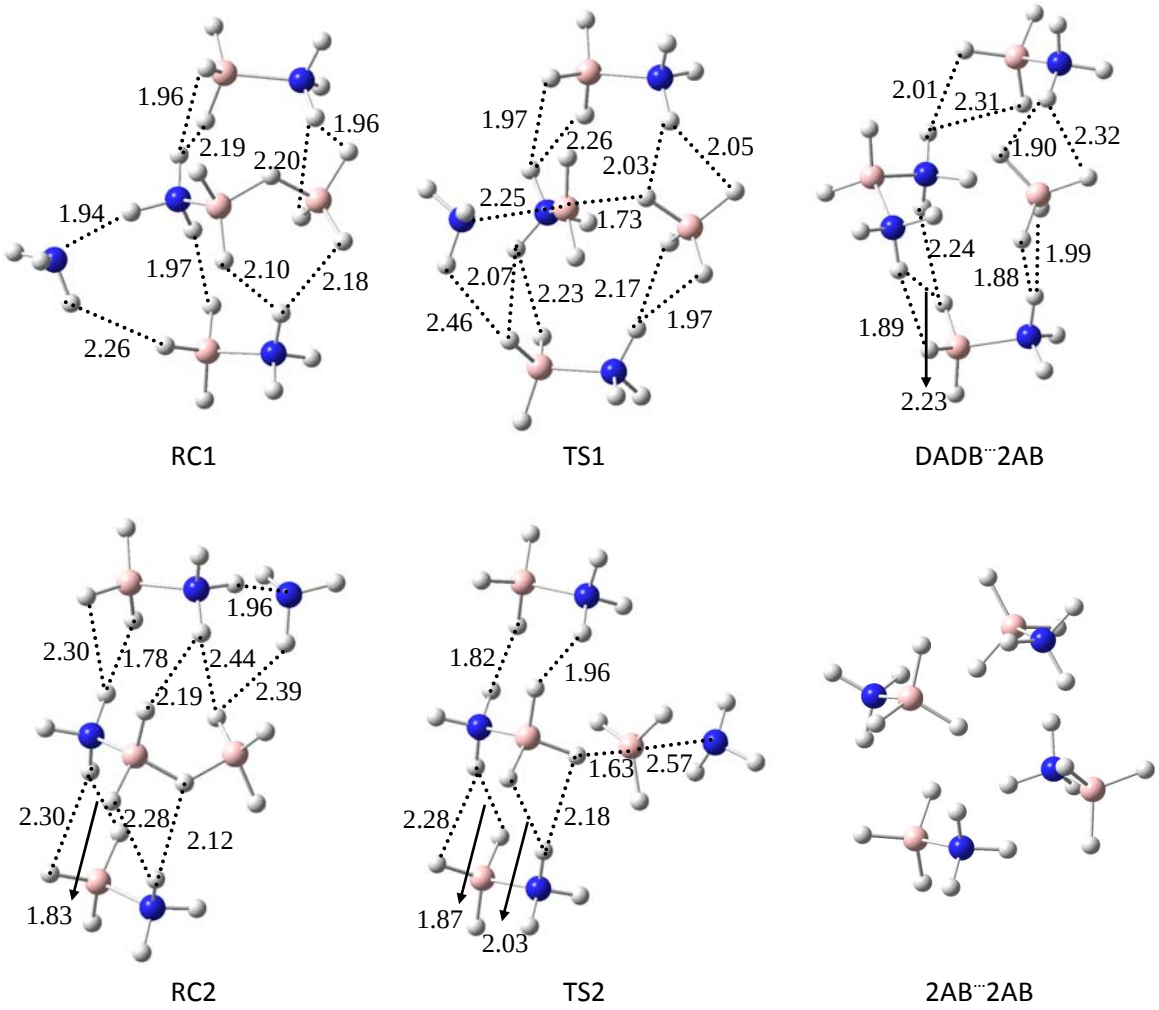


Figure S30. Optimized reactant complex (RC), TS, and corresponding product for both reaction pathways of NH_3 attacking the AaDB intermediate in the presence of two AB molecules. Colors: C, gray ; H, white; N, blue; B, pink. Bond lengths are shown in Å.

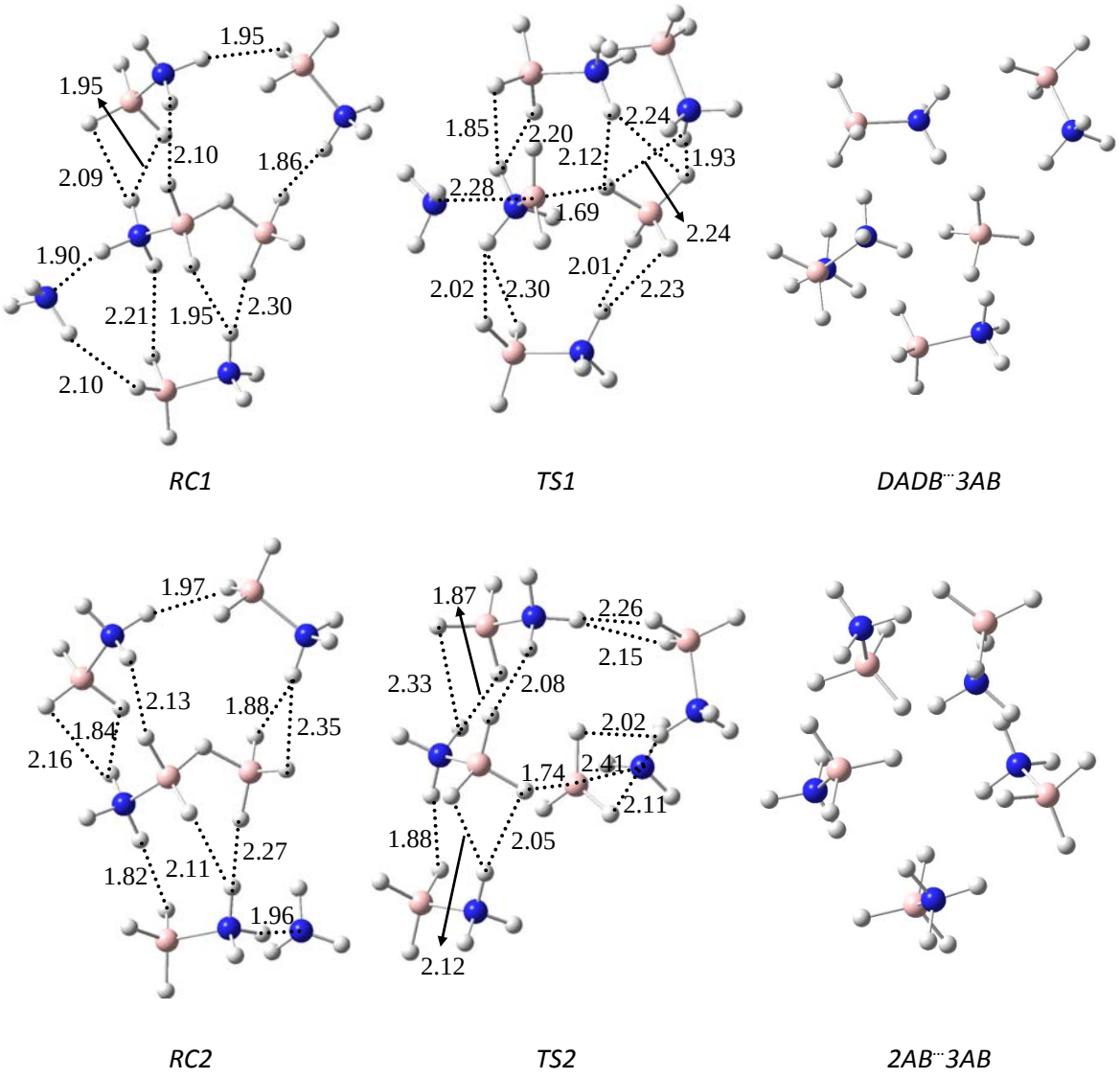


Figure S31. Optimized reactant complex (RC), TS, and corresponding product for both reaction pathways of NH_3 attacking the AaDB intermediate in the presence of three AB molecules. Colors: C, gray ; H, white; N, blue; B, pink. Bond lengths are shown in Å.

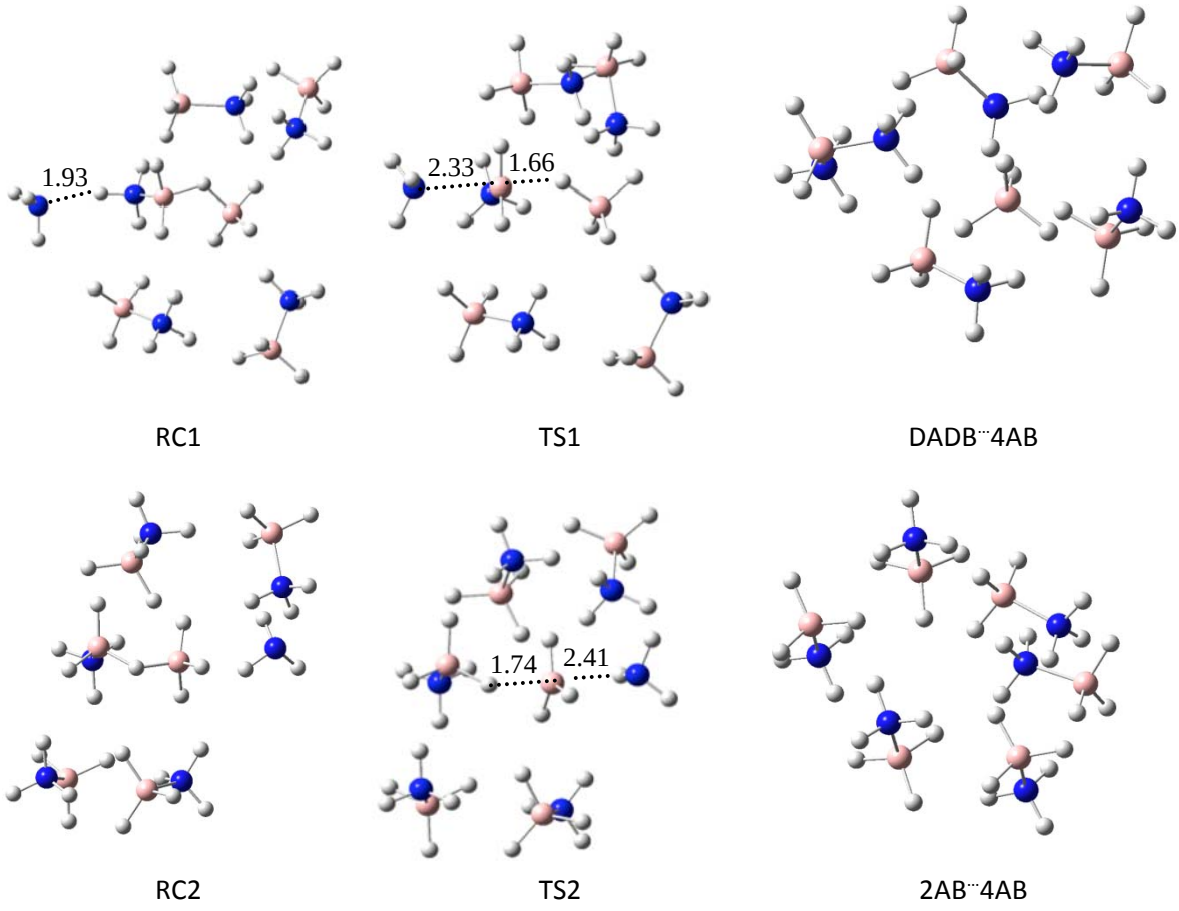


Figure S32. Optimized reactant complex (RC), TS, and corresponding product for both reaction pathways of NH_3 attacking the AaDB intermediate in the presence of four AB molecules. Colors: C, gray ; H, white; N, blue; B, pink. Bond lengths are shown in Å.

Cartesian coordinates, absolute energies (in Hartrees) and vibrational frequencies of the studied models

The displacement reaction between NH_3 and $THF{\cdot}BH_3$

Reactant

MP2/6-31++G(d,p) energy	Zero-point energy correction
-314.6723833	0.191144

Cartesian coordinates

1	5	0	-0.310414	1.774065	-0.446742
2	1	0	-0.577466	1.050578	-1.380071
3	1	0	0.421159	2.684855	-0.722313
4	1	0	-1.253031	2.066406	0.238085
5	1	0	-2.691940	0.336454	-0.698631
6	1	0	-3.924077	0.231283	0.366041
7	1	0	-3.767535	-0.897524	-0.801490
8	8	0	0.609808	0.848418	0.563724
9	6	0	-0.023655	-0.398881	1.004388
10	6	0	1.896659	0.436912	0.012149
11	6	0	0.381917	-1.450648	-0.031496
12	1	0	0.384751	-0.608303	1.994149
13	1	0	-1.091431	-0.217342	1.057608
14	6	0	1.595819	-0.837588	-0.767975
15	1	0	2.263515	1.271421	-0.576366
16	1	0	2.553748	0.255780	0.865027
17	1	0	-0.440158	-1.636813	-0.719076
18	1	0	0.632449	-2.390735	0.459359
19	1	0	1.335699	-0.592088	-1.795265
20	1	0	2.458952	-1.502772	-0.781105
21	7	0	-3.247923	-0.315378	-0.154919

Vibrational frequencies

27.2722	60.1865	74.7907
104.7535	114.2397	160.7777
180.2776	233.9627	296.9494
332.6213	348.6234	547.8405
626.5751	663.4375	815.6238
864.7939	909.0648	930.4835
940.9919	975.1375	994.0617
998.3481	1083.9658	1096.2378
1118.2690	1175.8588	1231.8889
1237.9472	1249.4531	1253.0083
1259.3674	1283.8459	1312.1130
1344.9105	1356.8627	1402.3472
1420.4289	1523.7390	1542.6893
1547.7535	1568.3480	1698.4125
1705.9235	2518.1109	2598.1442
2638.7766	3142.1063	3147.5757
3155.2055	3163.0006	3215.9620
3231.3120	3259.2221	3269.8895
3539.7837	3700.0344	3709.2430

TS

MP2/6-31++G(d,p) energy	Zero-point energy correction
-314.6571358	0.189292

Cartesian coordinates

1	5	0	1.491109	0.007464	-0.326727
2	1	0	1.197819	0.150283	0.824868
3	1	0	1.754004	0.965277	-0.987710
4	1	0	1.672871	-1.090918	-0.757459
5	1	0	4.400996	-0.197544	-0.441682
6	1	0	4.026242	-0.711159	1.066724
7	1	0	4.110515	0.891616	0.745138
8	8	0	-0.458357	0.021628	-0.966326
9	6	0	-1.226087	-1.124004	-0.551911
10	6	0	-1.190479	1.162175	-0.474241
11	6	0	-1.667427	-0.803674	0.875273
12	1	0	-2.082139	-1.231222	-1.227096
13	1	0	-0.577255	-1.991191	-0.644122
14	6	0	-1.765403	0.738769	0.887073
15	1	0	-0.486675	1.989387	-0.428100
16	1	0	-1.982740	1.396694	-1.192005
17	1	0	-0.909897	-1.142211	1.579586
18	1	0	-2.611581	-1.287422	1.126541
19	1	0	-1.178125	1.157582	1.702168
20	1	0	-2.793598	1.083655	0.998678
21	7	0	3.823892	-0.004681	0.368792

Vibrational frequencies

-267.7936	40.7404	63.6933
76.0819	88.5758	128.6949
142.9114	163.9345	205.6431
293.9676	355.7127	360.9411
630.4262	667.9629	812.2740
879.2777	907.6023	915.3708
931.8112	940.1810	974.7414
991.6276	1088.9099	1091.2991
1112.2045	1156.4262	1167.5498
1204.5580	1213.0605	1243.2935
1251.9954	1279.1096	1299.8632
1338.1539	1348.9712	1395.8440
1419.1766	1521.4969	1540.6355
1545.8258	1564.8418	1686.6487
1688.4752	2586.9320	2691.3618
2713.9491	3098.0715	3107.7502
3147.2949	3156.0499	3204.7992
3218.9749	3227.9404	3232.5095
3545.1490	3713.8638	3714.3569

Product complex

MP2/6-31++G(d,p) energy	Zero-point energy correction
-314.6825522	0.19242

Cartesian coordinates

1	5	0	2.450719	-0.233387	0.215428
2	1	0	2.575625	-1.167979	0.967036
3	1	0	2.040381	0.767054	0.750121
4	1	0	1.872848	-0.506833	-0.806766
5	1	0	3.991166	0.925832	-0.906543
6	1	0	4.431326	-0.644864	-0.727171
7	1	0	4.570167	0.395081	0.534847
8	8	0	-2.056446	0.320342	-1.044195
9	6	0	-1.615700	-1.006182	-0.696344
10	6	0	-1.345346	1.214052	-0.177981
11	6	0	-1.161334	-0.954864	0.778931
12	1	0	-2.460593	-1.671661	-0.870003
13	1	0	-0.789825	-1.299639	-1.351126
14	6	0	-1.373175	0.516071	1.174664
15	1	0	-0.315247	1.347572	-0.527283
16	1	0	-1.867108	2.169504	-0.205953

17	1	0	-0.110483	-1.226907	0.866049
18	1	0	-1.739493	-1.633188	1.406372
19	1	0	-0.605923	0.880988	1.857511
20	1	0	-2.352419	0.660022	1.633690
21	7	0	3.990125	0.142108	-0.259998

Vibrational frequencies

23.7342	35.3535	41.2289
48.7461	60.4130	68.0998
86.1450	279.5120	284.0429
606.5811	664.0337	665.9079
684.7340	691.7145	823.3226
902.5044	941.0492	943.6949
961.5570	991.6611	1074.9216
1095.9141	1098.5869	1120.6520
1177.0168	1229.3921	1232.4763
1234.7586	1236.8553	1248.0778
1259.8709	1296.6389	1335.8063
1359.0739	1379.1487	1392.8410
1418.8124	1524.7242	1542.6470
1554.5131	1571.1017	1698.7209
1699.9797	2526.6439	2591.6681
2594.7391	3096.1561	3106.9523
3136.8101	3151.5471	3185.5430
3197.6271	3204.6101	3219.9180
3526.9830	3668.4623	3668.5858

The reaction between AB and THF·BH_3 to produce the AaDB intermediate

Reactant complex

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.2194572	0.227398

Cartesian coordinates

1	5	0	0.044220	2.029568	0.150570
2	1	0	0.664252	1.596238	-0.799914
3	1	0	0.676778	2.057560	1.175901
4	1	0	-0.558733	3.035487	-0.100485
5	1	0	2.436853	-1.415200	1.028710
6	1	0	3.796848	-1.836072	-0.395248
7	8	0	-1.100094	0.911756	0.421209
8	6	0	-1.907982	0.549798	-0.756658
9	6	0	-0.635469	-0.317352	1.096767
10	6	0	-1.670129	-0.937247	-0.937455
11	1	0	-2.941582	0.785580	-0.503710
12	1	0	-1.567340	1.175784	-1.576441
13	6	0	-1.494379	-1.416347	0.505025
14	1	0	0.414205	-0.457146	0.853763
15	1	0	-0.763768	-0.141169	2.161660
16	1	0	-0.751688	-1.107512	-1.500404
17	1	0	-2.498448	-1.419402	-1.455709
18	1	0	-0.994257	-2.381470	0.573636
19	1	0	-2.458500	-1.479847	1.012938
20	1	0	1.888916	-1.444779	-0.913359
21	5	0	2.780367	-1.250637	-0.118282
22	7	0	3.133762	0.348827	-0.243502
23	1	0	3.496670	0.567637	-1.167091
24	1	0	2.310610	0.936376	-0.101410
25	1	0	3.838428	0.624340	0.434485

Vibrational frequencies

28.0863	38.2546	64.0956
94.7361	109.8263	141.3388
157.8516	262.0108	271.0160
282.4649	306.1768	337.6754
500.2913	574.0101	677.3523
710.0726	712.6892	714.3933
866.9634	883.3102	893.0565
929.9396	959.4475	963.3318
975.3482	1008.7716	1081.6547
1093.1726	1098.6331	1107.8341
1189.2322	1215.9870	1223.2768
1227.6769	1234.3840	1237.2084
1239.2772	1245.7792	1277.1395
1286.9384	1301.7761	1352.0247
1391.5613	1411.5890	1422.9909
1432.5393	1526.3547	1534.4700
1555.7088	1566.4284	1692.4287
1702.9654	2493.0746	2509.4838
2559.5031	2576.0502	2585.2294
2634.9830	3140.3651	3148.7736
3158.0446	3182.9764	3211.5381
3219.5935	3247.7323	3265.5739
3486.7485	3618.4466	3666.3893

TS

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.1925909	0.225192

Cartesian coordinates

1	5	0	1.008620	-0.129412	-0.273792
2	1	0	0.411321	-0.698103	-1.130797
3	1	0	1.266523	-0.691236	0.748645
4	1	0	1.299741	1.021260	-0.412825
5	1	0	4.005073	-1.740666	-0.284905
6	1	0	4.378269	-0.276649	-1.646132
7	8	0	-0.910605	0.548520	0.666209
8	6	0	-1.755031	1.237734	-0.272624
9	6	0	-1.713045	-0.538897	1.156330
10	6	0	-2.533862	0.141327	-1.014272
11	1	0	-2.426930	1.903103	0.280962
12	1	0	-1.103052	1.832384	-0.908656
13	6	0	-2.439241	-1.083604	-0.075494
14	1	0	-1.037231	-1.247099	1.630566
15	1	0	-2.417759	-0.152106	1.901825
16	1	0	-2.071392	-0.073800	-1.975904
17	1	0	-3.565027	0.445466	-1.195146
18	1	0	-1.848604	-1.873101	-0.536678
19	1	0	-3.416653	-1.493229	0.180220
20	1	0	2.508743	-0.661551	-1.069951
21	5	0	3.686240	-0.677861	-0.747468
22	7	0	3.839683	0.409045	0.462557
23	1	0	3.598669	1.345175	0.148033
24	1	0	3.207661	0.178804	1.226142
25	1	0	4.790484	0.426881	0.819694

Vibrational frequencies

-312.8542	16.6149	48.6401
63.3274	76.7726	93.3576
114.0595	168.0831	214.3615
243.1556	291.8283	324.0960
345.6718	637.6177	659.1430
678.2394	683.0846	723.8228
815.7332	860.9132	881.5893
896.1155	933.4898	939.7515
973.9547	990.7353	1058.9559
1090.3891	1097.8544	1115.4797
1149.8544	1166.5475	1193.1268
1214.6415	1222.1345	1232.0163
1243.0288	1249.5535	1273.6335
1281.6462	1294.2183	1337.5367

1346.6369	1392.1083	1395.0676
1419.5194	1522.4412	1541.7127
1546.3010	1565.1420	1680.6827
1693.7003	2436.5575	2568.4309
2598.4573	2625.0982	2699.5319
2738.9761	3087.5614	3093.4926
3147.0818	3155.7598	3202.6137
3212.8024	3218.6496	3227.0861
3517.8977	3651.3513	3668.5774

Product complex

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.2174849	0.227563

Cartesian coordinates

1	5	0	-2.097425	1.755653	-0.211942
2	1	0	-2.147989	2.771587	0.420433
3	1	0	-1.030158	1.513710	-0.715917
4	1	0	-3.050041	1.541098	-0.909755
5	1	0	-1.907489	-0.701941	1.730798
6	1	0	-3.714398	-0.267260	0.911002
7	8	0	0.775792	-1.011251	-0.489684
8	6	0	1.488116	0.009626	-1.235061
9	6	0	1.305184	-0.986112	0.853347
10	6	0	2.003969	1.030625	-0.203184
11	1	0	2.303240	-0.468404	-1.784133
12	1	0	0.778108	0.433907	-1.942688
13	6	0	1.490769	0.493383	1.142878
14	1	0	0.582244	-1.488199	1.493696
15	1	0	2.256090	-1.530410	0.878362
16	1	0	1.627623	2.031312	-0.407929
17	1	0	3.093844	1.065657	-0.216732
18	1	0	0.527995	0.937671	1.392576
19	1	0	2.185318	0.678484	1.962428
20	1	0	-2.098337	0.953802	0.852171
21	5	0	-2.526916	-0.238492	0.812351
22	7	0	-2.054118	-0.975116	-0.519877
23	1	0	-2.437669	-0.503470	-1.336748
24	1	0	-1.022697	-0.983915	-0.597778
25	1	0	-2.379719	-1.938742	-0.523100

Vibrational frequencies

40.7738	62.0052	81.3235
91.5845	108.4392	126.9921
189.2335	234.8395	245.3519
301.3865	310.5306	362.4172
454.8723	603.2813	690.9924
741.2710	777.4660	809.2851
823.3891	879.6370	896.2843
924.1629	937.9733	946.0753
967.0601	990.8122	1065.2282
1083.6864	1100.3935	1132.7845
1147.8988	1177.0815	1179.5502
1231.0334	1232.8227	1240.3937
1250.2753	1254.4590	1266.0983
1302.9209	1343.3129	1362.7874
1400.1393	1422.0325	1467.9891
1525.0321	1540.0318	1552.0921
1567.9617	1645.9198	1685.7131
1745.1688	2384.5163	2554.6485
2598.3398	2626.8045	2662.4403
2694.9117	3093.6906	3119.7621
3146.9617	3153.7141	3200.7438
3208.7160	3215.3156	3226.0074
3273.9275	3561.9908	3645.8968

AaDB decomposition with one THF molecule

Reactant

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.2167677	0.227479

Cartesian coordinates

1	7	0	1.948094	-1.100407	-0.465816
2	5	0	2.242131	-0.474116	0.970810
3	5	0	2.540742	1.548359	-0.040726
4	1	0	2.578407	-0.704195	-1.160629
5	1	0	3.573858	1.118835	-0.473270
6	1	0	1.333256	-0.773648	1.697018
7	1	0	0.973653	-0.913192	-0.754300
8	1	0	2.085408	-2.108016	-0.446336
9	1	0	3.333533	-0.771943	1.345571
10	1	0	1.618464	1.534425	-0.816423
11	1	0	2.089554	0.783995	0.955723
12	1	0	2.637266	2.539624	0.624499
13	8	0	-0.819921	-0.666910	-0.874712
14	6	0	-1.571548	-1.167356	0.256281
15	6	0	-1.314785	0.667559	-1.118260
16	6	0	-1.953791	0.060091	1.105850
17	1	0	-2.453493	-1.694766	-0.117818
18	1	0	-0.928243	-1.875506	0.776614
19	6	0	-1.462416	1.260304	0.273864
20	1	0	-0.586175	1.171776	-1.749002
21	1	0	-2.275786	0.603066	-1.641448
22	1	0	-1.479264	0.031366	2.085323
23	1	0	-3.033129	0.097277	1.254617
24	1	0	-0.488651	1.602760	0.621391
25	1	0	-2.155070	2.101471	0.300046

Vibrational frequencies

26.9755	41.8542	78.2179
83.6960	94.9948	127.9302
194.0407	242.4632	257.2408
307.3814	311.4425	365.5591
457.7373	609.6499	687.5524
737.2658	773.8507	808.0094
818.1110	875.9660	893.6253
928.4595	938.4284	944.0063
969.8647	990.0039	1067.1088
1083.7282	1101.8266	1133.1923
1145.1073	1173.3651	1179.7439
1231.2976	1237.6747	1242.5512
1249.8929	1254.3395	1268.6931
1305.2649	1340.2348	1355.7624
1400.1949	1421.1008	1457.7289
1526.7672	1542.5107	1549.1938
1568.2123	1646.3162	1684.8792
1743.0146	2378.3913	2552.4168
2595.4127	2626.1081	2664.3597
2694.9807	3092.9946	3113.0523
3148.3118	3156.0814	3194.4821
3211.1661	3220.1098	3227.1282
3294.4941	3562.8870	3645.2972

TS

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.164516	0.219913

Cartesian coordinates

1	7	0	1.783637	-1.073515	-0.526647
2	5	0	2.048586	-0.974854	0.919003

3	5	0	3.097990	1.312085	0.121306
4	1	0	2.152901	0.332107	-0.751555
5	1	0	4.117393	0.801253	-0.235619
6	1	0	1.121716	-0.723442	1.620608
7	1	0	0.805700	-1.144916	-0.812963
8	1	0	2.397805	-1.660751	-1.077069
9	1	0	3.052523	-1.430219	1.353506
10	1	0	2.231558	1.223511	-0.871026
11	1	0	2.546741	0.719162	1.045119
12	1	0	3.089951	2.501178	0.250339
13	8	0	-1.080629	-0.689931	-0.895148
14	6	0	-1.837004	-1.029795	0.289579
15	6	0	-1.278196	0.717605	-1.115136
16	6	0	-1.968902	0.265531	1.117005
17	1	0	-2.812412	-1.419718	-0.013577
18	1	0	-1.284399	-1.817539	0.799317
19	6	0	-1.221061	1.317979	0.281058
20	1	0	-0.491032	1.052228	-1.789709
21	1	0	-2.252162	0.886602	-1.589597
22	1	0	-1.539260	0.156364	2.111617
23	1	0	-3.018356	0.538072	1.232211
24	1	0	-0.182347	1.400471	0.601522
25	1	0	-1.678649	2.305615	0.338000

Vibrational frequencies

-988.4470	34.5005	43.1325
51.6046	76.2483	81.9831
112.9838	162.9505	229.7606
257.0555	273.8633	301.4314
562.8714	602.0105	605.8957
690.3410	735.0961	773.0046
814.8495	822.1265	897.3657
925.6651	935.7076	943.7622
963.9287	989.2912	1035.6648
1064.5804	1079.1587	1106.9570
1111.8198	1117.1215	1175.2510
1179.7805	1202.7888	1208.9072
1230.7707	1249.8804	1262.0971
1293.7189	1297.9327	1324.9532
1339.2767	1352.2180	1360.9747
1397.8333	1420.3489	1526.3456
1541.9585	1555.4157	1571.8119
1654.4273	1929.5416	2331.2140
2438.0153	2625.6908	2682.3107
2697.0164	2779.9645	3087.9890
3115.5919	3146.3290	3150.7433
3194.2025	3197.9669	3209.3225
3221.2741	3486.5803	3687.6639

Product

MP2/6-31++G(d,p) energy	Zero-point energy correction
-341.1879687	0.21904

Cartesian coordinates

1	7	0	-1.680582	1.532025	-0.482106
2	5	0	-1.701167	2.083422	0.801360
3	5	0	-2.923441	-1.990872	0.076461
4	1	0	-2.917801	-0.578810	0.274469
5	1	0	-2.033344	-2.208014	0.837282
6	1	0	-0.836044	1.782285	1.564149
7	1	0	-0.914544	0.950445	-0.814803
8	1	0	-2.350458	1.789291	-1.191216
9	1	0	-2.586933	2.814251	1.115763
10	1	0	-3.613216	-0.860772	0.521507
11	1	0	-2.686442	-1.882543	-1.085874
12	1	0	-3.969279	-2.507572	0.341601
13	8	0	0.783747	0.055371	-1.085570
14	6	0	1.855085	0.826332	-0.503001
15	6	0	0.944227	-1.279600	-0.574868
16	6	0	2.152414	0.191058	0.871451
17	1	0	2.725564	0.779655	-1.164516
18	1	0	1.508253	1.856822	-0.446953
19	6	0	1.262928	-1.067014	0.898093
20	1	0	0.017598	-1.814724	-0.767101
21	1	0	1.770344	-1.775741	-1.099171
22	1	0	1.913097	0.870429	1.688204
23	1	0	3.207841	-0.070464	0.951493
24	1	0	0.337887	-0.873807	1.441272
25	1	0	1.756697	-1.925271	1.354041

Vibrational frequencies

28.9633	32.9260	44.8927
46.9813	63.1223	70.4278
81.7199	93.5666	105.1719
113.1397	174.9593	192.3448
238.0131	306.7031	324.7043
610.0780	686.9229	759.2730
787.8557	816.7847	853.1684
896.3815	937.3012	941.3919
965.7704	983.9563	991.3943
1020.1045	1038.3640	1071.4532
1079.3652	1111.8807	1172.7097
1175.3831	1192.3400	1222.9459
1234.9080	1237.8719	1246.9422
1251.3994	1266.3665	1302.7969
1336.2742	1351.7942	1388.9323
1396.2005	1420.5318	1525.7438
1542.9306	1553.2548	1570.0014
1692.4358	1791.7466	2607.2716
2657.2018	2705.8857	2738.4093
2739.9245	3082.5632	3105.8552
3144.9223	3151.0626	3195.2185
3207.2000	3219.2022	3229.0188
3529.4441	3733.0649	3758.4584

A NH_3 molecule attacking the AaDB intermediate without AB molecule

Reactant complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-165.8580327	0.143712

Cartesian coordinates

1	5	0	-2.738911	-0.062392	0.145427
2	5	0	-0.650852	0.815961	-0.124955
3	1	0	-3.702562	0.646981	0.115316
4	1	0	-1.903184	0.882813	-0.284581
5	1	0	-2.687165	-0.899433	-0.719857
6	1	0	-2.411699	-0.428874	1.241681
7	1	0	-0.274301	1.345068	-1.134409
8	1	0	-0.354761	1.358575	0.897709
9	7	0	-0.086993	-0.671841	-0.112341
10	1	0	0.943624	-0.632039	-0.054703
11	1	0	-0.460870	-1.185405	0.682566
12	1	0	-0.361682	-1.180566	-0.948590
13	1	0	2.587949	1.037741	0.108510
14	7	0	2.781710	0.041317	0.080260
15	1	0	3.407284	-0.116450	-0.702518
16	1	0	3.303162	-0.182595	0.921086

Vibrational frequencies

25.5488	41.9205	53.9490

170.3183	195.8976	271.0548
276.6570	320.2890	356.2174
420.2482	444.7778	722.3051
762.6123	835.0937	910.1400
945.1398	1076.7230	1137.4888
1147.5852	1176.1402	1184.5865
1232.3558	1241.0843	1249.9056
1465.4198	1649.5017	1689.9036
1692.9649	1705.9800	1729.0394
2398.8475	2545.5979	2598.1839
2616.9330	2665.3566	2677.1034
3291.6317	3540.0244	3576.2683
3649.8691	3692.1911	3699.4290

TS1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-165.8068908	0.141345

Cartesian coordinates

1	5	0	-2.610666	-0.376510	0.052386
2	5	0	0.211487	-0.554549	-0.094883
3	1	0	-3.614579	-1.004399	-0.160772
4	1	0	-1.615439	-1.059200	-0.244090
5	1	0	-2.502248	-0.005451	1.208422
6	1	0	-2.577688	0.613658	-0.701585
7	1	0	0.236371	-1.168238	0.912375
8	1	0	0.324128	-0.993649	-1.187043
9	7	0	-0.205277	0.950609	-0.015732
10	1	0	0.323860	1.550131	-0.641297
11	1	0	-1.227253	0.947766	-0.302890
12	1	0	-0.166251	1.327913	0.927007
13	1	0	2.600296	-1.181655	0.011766
14	7	0	2.311798	-0.208118	0.042322
15	1	0	2.664625	0.169718	0.917560
16	1	0	2.804430	0.261260	-0.713100

Vibrational frequencies

-530.2813	90.1768	131.0104
182.3211	192.1867	229.1846
312.0854	358.4018	450.6333
492.6722	501.7822	539.9940
738.2711	889.2060	964.0384
964.8784	1060.7450	1119.5482
1151.7846	1167.7908	1202.5838
1230.0683	1240.6269	1250.8356
1300.1707	1467.1498	1647.7894
1683.8603	1686.2531	1697.0943
2248.2071	2309.8754	2462.2648
2592.7058	2709.9375	2817.1992
2835.7075	3519.7318	3576.8914
3673.9916	3675.3897	3678.1419

Product (DADB)

MP2/6-31++G(d,p) energy	Zero-point energy correction
-165.8628236	0.145561

Cartesian coordinates

1	5	0	-1.396482	0.000056	-0.274654
2	5	0	2.262686	-0.000098	-0.070591
3	1	0	1.908633	0.993206	-0.711673
4	1	0	1.906999	-0.992311	-0.712497
5	1	0	-1.514078	0.000118	-1.465321
6	1	0	3.459619	-0.001245	0.049738
7	1	0	1.713519	-0.000154	1.028675
8	1	0	-2.427317	0.000141	0.338321
9	7	0	-0.531411	1.279229	0.134248
10	1	0	-0.505087	1.454711	1.136325
11	1	0	0.465332	1.189466	-0.169278
12	7	0	-0.531661	-1.279182	0.134248
13	1	0	-0.928486	-2.105280	-0.307426
14	1	0	0.465167	-1.189343	-0.169190
15	1	0	-0.928306	2.105397	-0.307228
16	1	0	-0.505515	-1.454825	1.136300

Vibrational frequencies

133.5544	137.1813	215.8098
277.6746	290.6106	294.5387
407.7316	420.5242	428.8893
715.0430	749.7307	803.6226
849.2179	873.8460	1069.5018
1133.8719	1138.8633	1153.2085
1158.4686	1233.5459	1245.0751
1255.1787	1272.0988	1327.8284
1506.9524	1527.1982	1670.3680
1680.2704	1690.7822	1698.0114
2346.2164	2361.5786	2386.6100
2590.7661	2603.2896	2666.8822
3047.9095	3101.7282	3564.7609
3565.3363	3649.4943	3650.0674

Reactant complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-165.8592706	0.143998

Cartesian coordinates

1	5	0	1.425190	1.410715	-0.213287
2	5	0	1.160039	-0.653661	0.731478
3	1	0	1.997497	2.266054	0.397741
4	1	0	1.251839	0.606811	0.833150
5	1	0	2.073766	0.873412	-1.067957
6	1	0	0.290616	1.672527	-0.526216
7	1	0	2.240658	-1.151012	0.653232
8	1	0	0.537523	-0.886400	1.731157
9	7	0	0.256906	-1.071295	-0.513834
10	1	0	0.187524	-2.084363	-0.566714
11	1	0	-0.699760	-0.681997	-0.425648
12	1	0	0.668940	-0.729600	-1.379781
13	1	0	-2.670582	0.027495	0.980315
14	7	0	-2.258517	0.303340	0.095270
15	1	0	-3.023964	0.497590	-0.541230
16	1	0	-1.768928	1.179901	0.250938

Vibrational frequencies

61.9126	78.0202	104.7142
195.9354	223.2963	249.9818
291.4570	309.8168	359.7133
404.0701	492.1711	743.7948
782.4764	811.6499	883.1128
941.3165	1067.7948	1137.2139
1151.1186	1174.2048	1182.2774
1227.8202	1242.5430	1249.9257
1476.4493	1644.3835	1683.7568
1696.0261	1699.2046	1749.7002
2390.7425	2550.6175	2601.1123
2622.5276	2667.8538	2695.7422
3228.1408	3535.3106	3563.0222
3649.7391	3687.2935	3700.0005

TS2

MP2/6-31++G(d,p) energy	Zero-point energy correction

-165.8336276	0.141128

Cartesian coordinates

1	5	0	-0.630341	0.528620	-0.060744
2	5	0	2.060757	0.799107	0.037179
3	1	0	-1.079757	1.625106	-0.152345
4	1	0	0.923318	1.203669	-0.159980
5	1	0	-0.482205	-0.141656	-1.040352
6	1	0	-0.470919	0.036669	1.017297
7	1	0	2.779202	1.125857	-0.869796
8	1	0	2.443034	1.090670	1.137842
9	7	0	1.979990	-0.828652	-0.005851
10	1	0	2.886188	-1.245807	0.185251
11	1	0	1.311434	-1.163063	0.684478
12	1	0	1.660746	-1.154168	-0.914430
13	1	0	-3.253948	-1.186855	0.077394
14	7	0	-2.988556	-0.209911	0.023912
15	1	0	-3.424066	0.180946	-0.803599
16	1	0	-3.385143	0.259941	0.829642

Vibrational frequencies

-311.3296	55.8372	75.7723
95.3210	155.7722	161.1636
210.0406	236.0127	263.1259
341.1862	372.1497	682.7914
685.6581	730.5145	853.4627
885.9844	1046.5965	1099.0881
1099.6838	1145.1336	1185.3443
1208.7624	1221.9345	1232.5866
1286.9078	1392.2950	1678.6396
1685.7309	1691.7628	1695.2960
2427.7444	2573.7804	2596.5435
2634.6362	2689.4406	2742.7689
3518.1068	3544.3920	3652.0823
3669.6191	3710.3482	3713.8145

Product (AB)

MP2/6-31++G(d,p) energy	Zero-point energy correction
-165.8825219	0.146408

Cartesian coordinates

1	5	0	-1.625097	0.928983	0.001134
2	5	0	1.625463	-0.928945	0.001189
3	1	0	-1.024973	1.226978	1.009772
4	1	0	1.029573	-1.227690	1.012031
5	1	0	-2.761151	1.322658	0.003558
6	1	0	-1.028440	1.229925	-1.008700
7	1	0	2.761858	-1.321765	-0.001016
8	1	0	1.025517	-1.230259	-1.006658
9	7	0	1.683837	0.705397	-0.000918
10	1	0	2.169315	1.054189	-0.822510
11	1	0	0.744930	1.110358	0.001112
12	1	0	2.173487	1.055649	0.817574
13	1	0	-2.174124	-1.053787	-0.820061
14	7	0	-1.684242	-0.705401	-0.000912
15	1	0	-2.169590	-1.055892	0.820036
16	1	0	-0.745396	-1.110524	-0.003944

Vibrational frequencies

92.9384	104.8378	154.1264
184.9002	186.2091	215.9119
294.1920	330.4332	690.4610
691.4361	723.1373	726.2217
732.4731	742.0073	1097.0248
1106.0913	1109.6497	1125.0477
1223.3376	1232.3974	1243.9420
1247.7002	1273.1013	1273.3196
1423.1340	1439.0398	1690.1133
1694.2120	1694.5505	1703.8006
2501.6977	2508.2666	2543.6556
2554.6772	2603.7264	2606.4992
3466.0284	3477.3371	3611.5225
3612.9047	3666.8768	3666.8974

A NH_3 molecule attacking the AaDB intermediate (in the presence of one AB)

Reactant complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.809125	0.218125

Cartesian coordinates

1	5	0	-1.035994	2.206323	-0.137172
2	5	0	1.003481	1.413254	0.328026
3	1	0	-1.949191	1.994918	0.628973
4	1	0	-0.153530	1.766914	0.730069
5	1	0	-0.828085	3.364993	-0.328162
6	1	0	-1.066975	1.514712	-1.123422
7	1	0	1.525396	2.129794	-0.466746
8	1	0	1.518978	1.373493	1.412018
9	7	0	0.895757	-0.062238	-0.245295
10	1	0	0.255629	-0.662390	0.279195
11	1	0	0.547207	-0.065083	-1.200767
12	1	0	1.835551	-0.491230	-0.233981
13	1	0	4.147301	0.007425	0.201308
14	7	0	3.742524	-0.900143	-0.005491
15	1	0	4.265561	-1.290456	-0.781871
16	1	0	3.921628	-1.493495	0.797626
17	7	0	-3.041203	-0.539536	0.011072
18	1	0	-3.662576	-0.644518	-0.786051
19	1	0	-2.573443	0.366441	-0.074930
20	1	0	-3.621349	-0.495869	0.844462
21	5	0	-1.980250	-1.776956	0.095003
22	1	0	-1.384983	-1.769499	-0.957468
23	1	0	-1.268338	-1.526617	1.045886
24	1	0	-2.624501	-2.779218	0.262570

Vibrational frequencies

24.5508	29.2352	40.3154
65.4610	81.2619	93.0383
149.9893	168.5704	192.9978
212.9380	253.6250	272.7613
286.2158	317.8599	347.0882
352.5175	433.5382	588.9664
658.3910	693.6138	726.0952
740.6583	766.7000	843.1352
898.6061	976.4464	1104.9530
1111.1582	1115.1751	1131.0668
1153.4495	1166.6899	1186.3665
1225.2323	1229.8987	1244.3426
1245.4937	1270.4012	1270.5791
1441.0504	1502.2306	1688.8438
1691.8611	1698.0427	1700.8042
1704.4578	1708.1143	1743.9541
2366.1966	2492.3248	2522.5834
2545.9023	2585.1888	2597.5522
2600.2038	2684.7939	2704.5399
3291.8105	3461.7582	3514.5995
3541.8880	3605.3129	3622.3668
3663.6397	3696.0540	3700.5379

TS1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.7668429	0.215553

Cartesian coordinates

1	5	0	0.948847	2.338505	-0.030185
2	5	0	-1.308465	0.590316	-0.429675
3	1	0	2.034344	2.338633	-0.579583
4	1	0	0.239279	1.511237	-0.639454
5	1	0	0.413767	3.416289	-0.064446
6	1	0	1.076760	1.936593	1.129444
7	1	0	-1.978306	1.563058	-0.452114
8	1	0	-0.939513	-0.014085	-1.375351
9	7	0	-0.786702	0.142890	0.977247
10	1	0	-0.234953	-0.719915	0.920858
11	1	0	-0.127903	0.878419	1.287741
12	1	0	-1.526145	0.033736	1.663901
13	1	0	-3.409389	-0.498632	-1.275451
14	7	0	-3.038536	-0.732882	-0.359562
15	1	0	-3.806977	-0.627400	0.297835
16	1	0	-2.793705	-1.719160	-0.388272
17	7	0	2.534854	-0.493962	-0.473431
18	1	0	3.446419	-0.329397	-0.053767
19	1	0	2.045884	0.408638	-0.448302
20	1	0	2.694791	-0.712256	-1.453361
21	5	0	1.773733	-1.719068	0.280948
22	1	0	1.636931	-1.372437	1.433086
23	1	0	0.714331	-1.864443	-0.293531
24	1	0	2.476500	-2.689959	0.175545

Vibrational frequencies

-513.9093	22.5638	65.0774
95.8409	108.2203	121.8238
139.9746	174.4932	192.0159
198.3250	213.4773	248.3908
279.5817	305.6797	334.8005
368.6206	476.6852	488.1819
570.2237	696.0297	725.1146
750.9240	753.4982	896.6293
936.3463	962.6346	1052.3913
1097.6903	1105.7375	1117.2550
1154.1418	1173.5194	1189.8495
1224.5171	1226.5512	1237.3866
1249.0502	1250.5430	1285.0235
1296.8581	1459.9197	1462.0426
1651.6075	1684.9681	1693.0653
1697.2695	1702.7860	1721.5393
2258.3500	2350.4668	2480.7276
2495.7447	2538.1991	2589.2140
2596.3552	2713.2118	2832.0549
3260.3934	3420.2747	3456.0921
3519.5576	3588.1360	3648.0249
3657.0814	3672.9900	3681.2119

Product complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.8254564	0.220177

Cartesian coordinates

1	5	0	-0.162823	2.297892	-0.191164
2	5	0	2.221588	-0.658115	-0.050208
3	1	0	-0.517395	3.447532	-0.240697
4	1	0	-0.520945	1.782333	0.867291
5	1	0	1.057236	2.218241	-0.278056
6	1	0	-0.656979	1.659463	-1.122191
7	1	0	2.425313	-1.827499	0.108930
8	1	0	3.189165	0.004662	-0.287207
9	7	0	1.159925	-0.453048	-1.222619
10	1	0	0.311007	-1.014927	-1.104356
11	1	0	0.849621	0.528134	-1.276949
12	1	0	1.574616	-0.704780	-2.116584
13	1	0	2.160653	-0.005154	2.020070
14	7	0	1.503163	-0.060869	1.246364
15	1	0	0.708241	-0.628521	1.543141
16	1	0	1.134135	0.884633	1.059420
17	7	0	-2.570572	0.036593	0.095750
18	1	0	-3.299014	0.088259	-0.611161
19	1	0	-1.893287	0.786484	-0.094321
20	1	0	-3.003439	0.248848	0.990643
21	5	0	-1.867064	-1.424674	0.113677
22	1	0	-1.429751	-1.600950	-1.005197
23	1	0	-0.989251	-1.364622	0.950097
24	1	0	-2.706048	-2.236375	0.399146

Vibrational frequencies

64.0920	87.1672	107.2984
134.2461	151.0893	183.0456
204.0654	225.8939	233.6069
260.4434	292.9122	299.1609
330.2557	346.3348	349.2186
384.6502	697.3764	718.0727
744.8958	749.1720	765.5216
805.5546	806.7115	860.3940
1070.2872	1100.9827	1118.1675
1131.6031	1150.4151	1163.8483
1175.5622	1190.6231	1221.1286
1236.5035	1246.7785	1264.7037
1273.3578	1307.2200	1318.1039
1464.3780	1465.6826	1493.1251
1672.2661	1685.0753	1693.5407
1697.2852	1704.0149	1720.1886
2373.4666	2387.9506	2422.9557
2490.8853	2522.5574	2582.7842
2605.8466	2612.0435	2671.9077
3328.8628	3362.7422	3386.5608
3478.0488	3536.6595	3588.7358
3628.4330	3639.3703	3660.8463

Reactant complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.8083649	0.217864

Cartesian coordinates

1	5	0	-1.154313	1.967844	0.001274
2	5	0	-2.281530	0.138831	0.746647
3	1	0	-1.024009	2.924610	0.710678
4	1	0	-2.056976	1.385927	0.771036
5	1	0	-0.177681	1.279809	-0.102255
6	1	0	-1.748354	2.162190	-1.027416
7	1	0	-1.576814	-0.409135	1.541871
8	1	0	-3.448793	0.147929	1.013222
9	7	0	-2.095486	-0.518671	-0.691329
10	1	0	-2.569196	-1.419035	-0.721697
11	1	0	-2.491354	0.077555	-1.415260
12	1	0	-1.112860	-0.697202	-0.932144
13	1	0	2.024274	1.875762	-0.311960
14	7	0	2.807272	1.230886	-0.261037
15	1	0	3.010758	0.933579	-1.209690
16	1	0	3.610994	1.754120	0.068285
17	7	0	1.280520	-1.042865	0.835979
18	1	0	1.959950	-0.303227	0.595035
19	1	0	1.687204	-1.643815	1.547000

20	1	0	0.475526	-0.580100	1.254040
21	5	0	0.867234	-1.899583	-0.480084
22	1	0	0.556410	-1.077925	-1.322196
23	1	0	1.839088	-2.522218	-0.821251
24	1	0	-0.061259	-2.609733	-0.161777

Vibrational frequencies

38.4942	55.8102	68.2850
80.3906	102.6702	110.7331
123.4867	158.9806	212.7952
225.2245	237.6767	244.7484
263.4329	294.1451	339.8343
348.5572	423.5284	440.8377
725.4109	737.5467	759.7043
771.0694	782.8678	820.9822
905.3666	928.8668	1060.0638
1110.0382	1127.6931	1133.4262
1143.7804	1159.8507	1180.6509
1224.8369	1232.2317	1239.8862
1243.8244	1254.8299	1281.1995
1472.5928	1485.6761	1660.7830
1675.9675	1687.6019	1695.3588
1700.5564	1701.2588	1741.9275
2412.7191	2473.2102	2524.9673
2557.8314	2593.2003	2612.7214
2638.4591	2666.0854	2679.3627
3293.7973	3400.4835	3536.1751
3565.4031	3573.1406	3646.3411
3650.4112	3690.2134	3701.3003

TS2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.7857256	0.2152

Cartesian coordinates

1	5	0	1.487298	0.309764	0.516175
2	5	0	-0.747819	1.756393	0.824213
3	1	0	1.831691	-0.023310	1.606472
4	1	0	0.111022	0.942271	1.162533
5	1	0	0.904480	-0.460383	-0.187599
6	1	0	1.895974	1.328338	0.046619
7	1	0	-1.814244	1.403049	1.263705
8	1	0	-0.421790	2.865597	1.136209
9	7	0	-0.852159	1.683386	-0.783668
10	1	0	-1.511205	2.374637	-1.132064
11	1	0	0.056371	1.866405	-1.204561
12	1	0	-1.167471	0.765617	-1.114508
13	1	0	3.739606	-1.720048	-0.065458
14	7	0	3.648741	-0.738846	-0.303096
15	1	0	4.373417	-0.236182	0.196449
16	1	0	3.840730	-0.647554	-1.294272
17	7	0	-1.675190	-1.476908	0.691031
18	1	0	-0.834236	-2.048090	0.693097
19	1	0	-2.350502	-1.910529	1.314386
20	1	0	-1.425088	-0.572747	1.092983
21	5	0	-2.302554	-1.328244	-0.814830
22	1	0	-1.380556	-0.980322	-1.520567
23	1	0	-2.711475	-2.416011	-1.125868
24	1	0	-3.171087	-0.493728	-0.725224

Vibrational frequencies

-274.6808	44.0174	52.0915
67.8338	96.2374	108.8642
120.2544	144.7557	153.4666
158.0559	181.2874	198.1590
218.1467	240.1274	282.6853
312.1796	321.2334	385.6150
693.4149	700.4515	719.2174
726.6318	745.0184	775.7107
851.1509	894.6027	1048.9888
1095.3805	1097.8592	1103.1312
1124.3789	1143.4902	1189.1543
1206.4574	1221.0785	1227.4375
1238.4685	1242.8268	1274.1996
1311.1729	1424.8565	1454.1171
1683.1962	1687.5700	1688.4865
1690.4368	1700.7745	1705.1785
2388.2428	2505.1398	2552.8522
2562.9269	2601.6696	2603.3088
2645.4253	2707.5100	2731.7401
3430.3087	3495.2485	3543.9304
3584.8342	3619.4383	3653.3881
3664.2581	3710.1065	3711.7562

Product complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-248.8306462	0.220333

Cartesian coordinates

1	5	0	0.739175	-1.876429	-0.283673
2	5	0	-2.742433	0.686545	0.013750
3	1	0	0.323716	-1.064706	-1.084489
4	1	0	-2.268679	0.961463	-1.064475
5	1	0	0.129295	-1.845488	0.762949
6	1	0	0.792851	-2.984350	-0.751701
7	1	0	-2.147379	1.192450	0.940323
8	1	0	-3.929493	0.878698	0.066805
9	7	0	-2.527348	-0.925278	0.188651
10	1	0	-2.932555	-1.255370	1.060165
11	1	0	-2.975826	-1.436340	-0.566660
12	1	0	-1.541450	-1.192351	0.193044
13	1	0	2.270269	-0.469160	0.466588
14	7	0	2.250287	-1.421026	0.086857
15	1	0	2.856111	-1.427625	-0.729313
16	1	0	2.660996	-2.044171	0.776630
17	7	0	0.410689	1.846741	-0.372629
18	1	0	0.197046	0.952398	-0.811770
19	1	0	0.388848	2.550332	-1.105925
20	1	0	-0.380340	2.031192	0.242706
21	5	0	1.842351	1.830299	0.393137
22	1	0	1.716560	1.042663	1.308539
23	1	0	2.652714	1.460943	-0.429857
24	1	0	2.056447	2.944285	0.790217

Vibrational frequencies

25.5374	59.1995	62.6584
88.9866	112.7102	119.2480
154.5274	162.4816	179.5466
199.5971	206.5004	226.1463
314.1060	345.2562	348.7924
689.2621	697.8987	700.9077
712.7951	720.2591	732.1861
739.2538	762.5708	773.4746
1099.5773	1103.7586	1106.6538
1108.6602	1121.1903	1126.6983
1224.3933	1231.4047	1234.6620
1245.0407	1245.9133	1248.5505
1264.2893	1274.4913	1283.4974
1433.2702	1445.8338	1455.7478
1694.1792	1696.2817	1697.1897
1705.6432	1706.6653	1709.1439
2485.6379	2497.8758	2502.9008
2525.0646	2534.0295	2552.1717

2592.2494	2596.7983	2606.7797
3432.7965	3484.7845	3507.0347
3597.1077	3611.6122	3615.8381
3649.6637	3662.3697	3663.6510

A NH_3 molecule attacking the AaDB intermediate (in the presence of two AB molecules)

Reactant complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.7603831	0.292023

Cartesian coordinates

1	5	0	0.961203	-1.620191	1.239434
2	5	0	-0.248934	0.248930	1.613297
3	1	0	2.120341	-1.707038	1.562843
4	1	0	0.817555	-0.449829	1.795856
5	1	0	0.266002	-2.424287	1.792231
6	1	0	0.802126	-1.535804	0.047726
7	1	0	-1.272111	-0.356691	1.706040
8	1	0	-0.040852	1.022921	2.503581
9	7	0	-0.143886	0.974289	0.219859
10	1	0	0.787385	1.355884	0.041685
11	1	0	-0.369758	0.353512	-0.558808
12	1	0	-0.840647	1.739295	0.181744
13	1	0	-2.899106	3.045623	0.912648
14	7	0	-2.498447	2.737588	0.033201
15	1	0	-3.086250	1.989474	-0.323465
16	1	0	-2.570103	3.514395	-0.614956
17	7	0	-2.056171	-2.312690	-0.287527
18	1	0	-1.400087	-2.026688	0.439257
19	1	0	-1.641829	-3.114761	-0.754658
20	1	0	-2.904236	-2.631590	0.172779
21	7	0	3.613401	-0.302708	-0.484795
22	1	0	3.912359	-0.784743	-1.327869
23	1	0	2.896198	-0.874050	-0.034634
24	1	0	4.408622	-0.271490	0.147410
25	5	0	-2.381036	-1.115877	-1.353626
26	1	0	-3.139087	-1.581238	-2.165190
27	1	0	-2.874000	-0.224999	-0.701435
28	1	0	-1.314074	-0.813322	-1.839560
29	5	0	3.076788	1.203495	-0.831379
30	1	0	2.176096	1.051269	-1.622251
31	1	0	2.709544	1.662783	0.228238
32	1	0	4.011537	1.804228	-1.293007

Vibrational frequencies

30.4927	41.6643	53.2930
59.3150	72.0874	91.2781
93.4848	100.8888	114.6181
117.3694	150.6312	164.3107
175.3919	179.0266	186.2562
203.5308	250.1836	282.8361
306.2660	319.3081	320.8138
331.9039	358.1669	476.0501
591.3303	653.1672	686.0690
688.5687	700.6530	716.4857
730.6747	731.1562	783.1882
867.2774	899.2905	985.1090
1097.8973	1102.3176	1104.3831
1109.5553	1124.0035	1150.6891
1154.2833	1158.3814	1187.6277
1226.6324	1229.3838	1238.4902
1243.5992	1250.1895	1250.7705
1257.7136	1266.5194	1275.1869
1426.0884	1428.2411	1535.6737
1674.3253	1687.6832	1690.2047
1692.6241	1696.6596	1698.0301
1702.4027	1703.9676	1743.0350
2353.0914	2504.8886	2509.0564
2533.4315	2555.5854	2558.9845
2592.8670	2597.0201	2600.7758
2616.9026	2642.8370	2691.6259
3259.4083	3483.7625	3498.2165
3505.8012	3534.0213	3567.6060
3615.1965	3627.2850	3662.9545
3663.9680	3687.5601	3701.6495

TS1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.7251604	0.289769

Cartesian coordinates

1	5	0	-0.395743	-1.915953	-1.083368
2	5	0	0.079451	0.830436	-0.949185
3	1	0	-1.374807	-2.545116	-1.418079
4	1	0	-0.644027	-0.709036	-1.289685
5	1	0	0.572868	-2.215838	-1.744709
6	1	0	-0.186466	-2.051881	0.118132
7	1	0	1.093856	0.544820	-1.481872
8	1	0	-0.853850	1.319975	-1.485526
9	7	0	-0.013721	0.582062	0.592248
10	1	0	-0.831716	1.036974	1.001520
11	1	0	-0.131179	-0.422918	0.755651
12	1	0	0.846331	0.852506	1.068046
13	1	0	0.982429	3.219485	-1.521813
14	7	0	0.955213	2.865687	-0.570724
15	1	0	1.917930	2.800952	-0.249662
16	1	0	0.488350	3.573166	-0.009826
17	7	0	2.833722	-1.566808	-0.002352
18	1	0	1.888113	-1.648687	-0.388027
19	1	0	3.049067	-2.471914	0.408607
20	1	0	3.461294	-1.443418	-0.792709
21	7	0	-3.380366	-0.773107	-0.109474
22	1	0	-3.822146	-1.619011	0.241555
23	1	0	-2.499233	-1.068921	-0.538686
24	1	0	-3.970134	-0.415966	-0.856434
25	5	0	3.047760	-0.385711	1.106388
26	1	0	4.189284	-0.473442	1.476810
27	1	0	2.834357	0.660866	0.531697
28	1	0	2.251445	-0.607990	1.988844
29	5	0	-3.222862	0.325304	1.089824
30	1	0	-2.498778	-0.185427	1.912725
31	1	0	-2.738107	1.312845	0.578571
32	1	0	-4.331848	0.532757	1.508688

Vibrational frequencies

-500.5107	27.3275	50.0234
67.2296	75.6285	88.4137
116.0111	126.5529	137.8073
144.1936	151.5209	173.6116
189.2073	196.2723	205.1184
213.1640	220.0259	244.8402
255.6087	323.5857	334.9739
337.3977	348.2829	448.6393
476.2769	553.5740	687.7883
690.1594	714.4079	718.5177
737.9636	739.5168	757.7136
880.3519	932.0093	940.1903
1038.7673	1093.5861	1097.8770
1103.0417	1105.7261	1123.7642
1169.9016	1173.3150	1195.9195
1201.3708	1225.8413	1227.0675

1235.9305	1247.3050	1247.9313
1254.9782	1271.7442	1276.0862
1300.7679	1447.6476	1457.3368
1460.5845	1634.1304	1686.6418
1689.2097	1694.4021	1695.8300
1702.0408	1703.0055	1715.8374
2260.9250	2401.8038	2497.6459
2503.1532	2513.7534	2546.9209
2548.7529	2551.4225	2595.4841
2597.7444	2709.8175	2825.1261
3426.7422	3454.0025	3463.1677
3518.4868	3529.4374	3593.6815
3599.4095	3602.0205	3655.3779
3658.5283	3673.9200	3685.2142

Product complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.7806449	0.294326

Cartesian coordinates

1	5	0	0.171336	-1.293783	1.343742
2	5	0	-0.117293	2.333237	0.149568
3	1	0	0.725672	-2.264472	1.804774
4	1	0	0.806726	-0.276590	1.596791
5	1	0	-0.948956	-1.174613	1.820545
6	1	0	0.087616	-1.407668	0.122435
7	1	0	0.790943	2.637308	0.866244
8	1	0	-0.611370	3.236228	-0.463142
9	7	0	0.374603	1.199499	-0.856658
10	1	0	1.332145	1.367636	-1.171587
11	1	0	0.410548	0.276254	-0.406088
12	1	0	-0.223286	1.103717	-1.674766
13	1	0	-1.593793	2.297487	1.735782
14	7	0	-1.241828	1.633683	1.050064
15	1	0	-0.858116	0.828212	1.558210
16	1	0	-2.045191	1.284585	0.518175
17	7	0	-2.673243	-1.822114	-0.350818
18	1	0	-1.872501	-1.738094	0.284565
19	1	0	-2.374899	-2.404080	-1.129081
20	1	0	-3.409491	-2.324310	0.137800
21	7	0	3.286612	-1.063382	0.322319
22	1	0	3.405923	-2.044587	0.085432
23	1	0	2.382028	-0.985317	0.794671
24	1	0	4.003426	-0.828610	1.003449
25	5	0	-3.192246	-0.370616	-0.868621
26	1	0	-4.094008	-0.560462	-1.639963
27	1	0	-3.557983	0.223114	0.124409
28	1	0	-2.236164	0.154455	-1.397738
29	5	0	3.409951	-0.121150	-1.005276
30	1	0	2.550272	-0.505512	-1.764945
31	1	0	3.227274	1.014127	-0.618474
32	1	0	4.521433	-0.281051	-1.438914

Vibrational frequencies

36.9125	58.7827	75.2573
89.3763	92.9742	102.7781
132.6360	137.7938	162.9094
177.9973	182.8856	197.8293
216.0693	218.5395	225.5500
249.3686	269.2306	316.4180
321.9544	341.9451	346.7274
348.8152	385.7206	690.5607
696.8693	711.9003	715.1294
737.6517	739.1613	747.1402
755.5716	802.7613	813.2305
869.6640	1053.6155	1102.9207
1103.9546	1106.9244	1116.9703
1129.0146	1146.0379	1165.5988
1183.6516	1191.4294	1222.2821
1227.6262	1239.2420	1245.0445
1246.8026	1271.3885	1272.4741
1273.7888	1311.9928	1318.9375
1443.2759	1452.2693	1473.6925
1501.8558	1668.5860	1690.4590
1692.5008	1696.5836	1697.4551
1703.1255	1706.8836	1725.1689
2391.9426	2418.9008	2439.3967
2495.7486	2496.9112	2536.4822
2544.2883	2545.3335	2594.3331
2606.9136	2610.9212	2671.0131
3389.7276	3412.3548	3424.9547
3462.1988	3499.7067	3530.0624
3594.3213	3603.1987	3623.7824
3629.0107	3660.5811	3662.3112

Reactant complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.7562605	0.291229

Cartesian coordinates

1	5	0	0.181165	1.188358	1.045687
2	5	0	0.849719	-1.029841	1.123858
3	1	0	-0.460345	1.223222	2.055980
4	1	0	1.075106	0.218345	1.183708
5	1	0	1.025535	2.042872	0.949911
6	1	0	-0.428054	0.990242	0.031819
7	1	0	1.901103	-1.417280	1.561232
8	1	0	-0.107026	-1.391790	1.732139
9	7	0	0.737782	-1.410885	-0.409697
10	1	0	0.877728	-2.412289	-0.528504
11	1	0	-0.189664	-1.200849	-0.795872
12	1	0	1.448893	-0.931245	-0.970070
13	1	0	-2.342888	2.267112	-0.597088
14	7	0	-3.323679	2.004666	-0.612479
15	1	0	-3.861479	2.827342	-0.363656
16	1	0	-3.555416	1.769907	-1.571968
17	7	0	3.760755	0.829517	0.259599
18	1	0	3.495369	1.811141	0.244502
19	1	0	4.722874	0.769151	0.581257
20	1	0	3.175046	0.374909	0.956701
21	7	0	-2.845670	-0.628820	0.622237
22	1	0	-2.009387	-0.466664	1.180112
23	1	0	-3.531131	-1.077360	1.222897
24	1	0	-3.200482	0.299138	0.344063
25	5	0	3.599348	0.140784	-1.221371
26	1	0	2.487625	0.440887	-1.593689
27	1	0	4.452320	0.625911	-1.915218
28	1	0	3.740731	-1.045905	-1.041891
29	5	0	-2.547193	-1.529270	-0.695143
30	1	0	-1.830116	-0.846610	-1.402689
31	1	0	-1.998706	-2.541498	-0.319498
32	1	0	-3.607147	-1.740189	-1.226960

Vibrational frequencies

28.4717	32.1232	51.5740
58.3908	64.7124	72.7482
90.1190	97.6720	101.4705
118.1975	141.3210	153.0074
164.9978	172.2270	195.5058
222.1253	235.6130	247.1093
265.7417	298.8207	323.2006
331.1386	342.8220	432.9935
556.4927	640.7452	690.8244
696.8161	719.1255	722.8116

756.2700	780.2201	791.3665
831.1698	894.6378	942.8971
1085.5088	1096.5598	1100.2214
1110.2711	1126.6402	1144.5212
1152.2058	1154.1040	1180.3741
1218.7239	1223.5347	1225.3346
1236.8781	1241.0164	1243.1969
1246.8742	1278.6841	1279.4006
1413.0774	1470.1682	1506.2822
1614.0302	1686.6625	1688.1526
1690.3523	1692.0760	1697.6570
1698.3951	1699.0722	1741.8073
2404.6252	2473.0670	2513.1334
2527.5061	2553.8702	2561.5333
2584.8427	2587.7971	2611.3550
2630.1118	2667.0445	2703.4016
3314.3436	3400.6247	3495.4240
3519.0855	3537.7210	3569.3331
3615.3899	3646.0180	3652.6874
3662.3780	3692.7977	3703.3356

TS2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.735718	0.288984

Cartesian coordinates

1	5	0	-0.221640	1.335782	0.568738
2	5	0	0.343425	-1.304479	1.149508
3	1	0	-0.983500	1.471136	1.475355
4	1	0	0.383421	-0.073093	1.126540
5	1	0	0.857670	1.842097	0.639574
6	1	0	-0.595650	0.902266	-0.476332
7	1	0	1.361115	-1.705831	1.656351
8	1	0	-0.643419	-1.690637	1.718205
9	7	0	0.307718	-1.796236	-0.373220
10	1	0	0.389549	-2.809211	-0.423335
11	1	0	-0.564492	-1.549834	-0.850531
12	1	0	1.086920	-1.400494	-0.906928
13	1	0	-0.752987	4.372945	0.271779
14	7	0	-0.950992	3.614967	-0.371893
15	1	0	-1.874447	3.781109	-0.756811
16	1	0	-0.290431	3.684956	-1.137779
17	7	0	3.306010	0.191254	0.462798
18	1	0	3.168936	1.196795	0.407123
19	1	0	4.183870	0.019706	0.944923
20	1	0	2.554750	-0.181304	1.043198
21	7	0	-3.009526	-0.568390	0.463236
22	1	0	-2.163380	-0.676626	1.022112
23	1	0	-3.799011	-0.801752	1.059106
24	1	0	-3.074528	0.418411	0.227890
25	5	0	3.316703	-0.494912	-1.024651
26	1	0	2.294550	-0.124000	-1.557261
27	1	0	4.296409	-0.081382	-1.586941
28	1	0	3.345143	-1.687820	-0.829097
29	5	0	-2.996463	-1.515351	-0.872443
30	1	0	-2.147250	-1.043371	-1.596876
31	1	0	-2.722437	-2.625693	-0.482015
32	1	0	-4.093397	-1.434735	-1.360458

Vibrational frequencies

-253.5701	32.8939	46.7756
53.9118	57.4359	78.6044
80.4998	96.6934	116.2995
122.4679	124.0865	145.0595
152.5631	167.3272	178.5749
195.1247	202.9397	217.4574
233.9729	256.2805	292.2596
311.5434	318.5845	321.7356
393.7897	681.2366	692.2841
695.6375	710.8697	713.3898
725.6131	728.1052	779.0374
804.4096	853.4283	883.5822
1057.2624	1097.4715	1100.4787
1101.9711	1105.9531	1107.5339
1121.4977	1143.4277	1190.6814
1203.6088	1221.5042	1227.4731
1227.7421	1237.2071	1242.3272
1243.4535	1270.0448	1273.6486
1287.4764	1420.4800	1426.8035
1496.8666	1682.8836	1687.5720
1688.4558	1689.9230	1691.5212
1697.4973	1702.0171	1705.2999
2387.2388	2503.8604	2508.6669
2550.7096	2553.9658	2560.7436
2599.0791	2602.1597	2606.0982
2609.5171	2714.5826	2735.3541
3423.8606	3500.3914	3503.7476
3518.3575	3540.8695	3622.6717
3623.8958	3626.9213	3664.1840
3665.6968	3703.6342	3708.3882

Product complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-331.7901167	0.29524

Cartesian coordinates

1	5	0	0.371503	-2.506783	-0.791500
2	5	0	-0.372179	2.505968	-0.792052
3	1	0	-0.673191	-3.085858	-0.991513
4	1	0	-0.331003	1.373780	-1.223972
5	1	0	1.330540	-3.119554	-1.183766
6	1	0	0.333038	-1.375110	-1.225162
7	1	0	0.671083	3.087273	-0.992935
8	1	0	-1.332805	3.115794	-1.185026
9	7	0	-0.515316	2.361336	0.820638
10	1	0	-0.560384	3.273308	1.266669
11	1	0	-1.353214	1.838478	1.078743
12	1	0	0.276591	1.852535	1.216202
13	1	0	0.557859	-3.271793	1.268145
14	7	0	0.514943	-2.360282	0.820948
15	1	0	-0.275835	-1.849214	1.215897
16	1	0	1.354033	-1.839050	1.078462
17	7	0	2.362192	0.514657	-0.820824
18	1	0	1.850517	-0.275896	-1.215464
19	1	0	3.273592	0.556979	-1.268288
20	1	0	1.841247	1.353882	-1.078392
21	7	0	-2.361772	-0.515064	-0.820685
22	1	0	-1.850565	0.275528	-1.215850
23	1	0	-3.273278	-0.558012	-1.267884
24	1	0	-1.840647	-1.354325	-1.077898
25	5	0	2.508927	0.371543	0.791676
26	1	0	1.377274	0.334443	1.225538
27	1	0	3.086985	-0.673664	0.991874
28	1	0	3.122730	1.330112	1.183441
29	5	0	-2.508266	-0.371477	0.791763
30	1	0	-1.376553	-0.332752	1.225343
31	1	0	-3.087559	0.673046	0.991837
32	1	0	-3.120708	-1.330713	1.184028

Vibrational frequencies

56.8483	62.9066	93.6825
93.9241	94.5433	101.9669
114.4479	114.5400	142.8120
147.8247	164.9453	176.6054

176.7688	180.3767	226.4813
241.6733	248.7883	248.9241
343.0214	351.3870	354.5213
354.7554	709.4517	713.2497
713.3203	719.4909	737.8550
740.9223	740.9569	744.3157
756.8004	757.4738	757.4800
759.3356	1100.7395	1107.4845
1107.5071	1107.5129	1121.2191
1121.7261	1121.7775	1133.2909
1216.6213	1221.1584	1221.1642
1230.6528	1243.1701	1243.1778
1244.1654	1245.7318	1288.5094
1289.0814	1289.2365	1290.3024
1442.5484	1447.6393	1447.7159
1462.0541	1684.7506	1692.1316
1692.1586	1694.4077	1701.4884
1701.5086	1702.6312	1707.4415
2498.3956	2499.8851	2499.9998
2512.0910	2535.1275	2535.1860
2541.8355	2543.3838	2594.5518
2594.6309	2595.9102	2596.1633
3467.5920	3471.9461	3471.9983
3479.0010	3574.4401	3574.4820
3581.4640	3581.5238	3645.4282
3645.4540	3645.7306	3646.2708

A NH_3 molecule attacking the AaDB intermediate (in the presence of three AB molecules)

Reactant complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.7074937	0.365748

Cartesian coordinates

1	5	0	-0.275728	-1.642923	0.614853
2	5	0	0.407940	0.089835	-0.613036
3	1	0	-1.223021	-1.532464	1.353135
4	1	0	-0.543961	-0.528089	-0.018282
5	1	0	-0.358868	-2.523931	-0.199476
6	1	0	0.759773	-1.594219	1.216342
7	1	0	1.222794	-0.589230	-1.156935
8	1	0	-0.272044	0.718357	-1.378573
9	7	0	1.057181	1.044189	0.454223
10	1	0	0.352692	1.644773	0.891120
11	1	0	1.530761	0.513517	1.183742
12	1	0	1.784639	1.636523	0.006598
13	1	0	3.337587	2.550740	-1.783671
14	7	0	3.379874	2.278854	-0.807367
15	1	0	3.932451	1.426587	-0.752061
16	1	0	3.894141	3.005716	-0.321274
17	7	0	3.159814	-2.365655	0.008418
18	1	0	2.298980	-2.041056	-0.429444
19	1	0	2.883409	-2.863428	0.850422
20	1	0	3.601116	-3.034354	-0.616498
21	7	0	-2.673470	2.107777	-0.168457
22	1	0	-3.407159	1.457583	0.114108
23	1	0	-2.097322	1.592514	-0.831041
24	1	0	-3.116874	2.865659	-0.680160
25	5	0	4.168884	-1.124003	0.347737
26	1	0	5.136304	-1.607399	0.877036
27	1	0	4.420542	-0.615586	-0.721313
28	1	0	3.548869	-0.392465	1.085491
29	5	0	-1.802261	2.674926	1.084475
30	1	0	-1.422947	1.696832	1.689685
31	1	0	-0.888878	3.303302	0.591977
32	1	0	-2.535281	3.363389	1.744541
33	7	0	-3.581038	-2.266398	-0.100873
34	1	0	-4.187273	-2.720826	0.576417
35	1	0	-2.682378	-2.094045	0.353184
36	1	0	-3.412875	-2.929206	-0.852765
37	5	0	-4.255423	-0.891099	-0.667491
38	1	0	-5.291998	-1.206406	-1.192850
39	1	0	-4.425993	-0.195155	0.310567
40	1	0	-3.450783	-0.432689	-1.444318

Vibrational frequencies

25.1631	31.2627	35.7200
44.2792	53.7783	63.7991
67.5348	76.2696	86.0218
95.8155	106.2597	119.9288
129.7292	131.3855	142.4338
151.8107	161.9726	174.7737
177.1128	190.6263	200.0954
238.7298	255.7419	306.7793
307.4419	319.0890	326.8990
337.4459	346.8796	360.0601
489.3253	594.8176	676.4318
685.1625	694.9830	695.4464
697.7969	705.9068	712.9313
729.9816	738.4896	751.6584
785.7347	868.4107	884.1582
991.1752	1100.3812	1101.9091
1104.5733	1105.1373	1108.5527
1113.0971	1113.8413	1141.9777
1154.1258	1175.5920	1182.3788
1224.9757	1228.7115	1230.7630
1239.0767	1240.6434	1241.3174
1243.4492	1250.6019	1254.2325
1266.9291	1270.7986	1279.5728
1414.9375	1430.7566	1444.6746
1529.3878	1685.8129	1690.0007
1691.6170	1694.2657	1696.0167
1697.8093	1701.6125	1702.6574
1708.5215	1717.0896	1735.3333
2347.3079	2494.3193	2501.3241
2510.4741	2538.5645	2540.6121
2552.1194	2554.4999	2592.7178
2593.9465	2598.0305	2599.2121
2610.1934	2645.6007	2685.4038
3187.0873	3479.6524	3482.1586
3500.0238	3512.0089	3526.2274
3598.4608	3609.2156	3613.3535
3636.3128	3652.0972	3663.2176
3665.1255	3676.1288	3699.0201

TS1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.676339	0.363302

Cartesian coordinates

1	5	0	0.151286	-1.615169	-1.008586
2	5	0	-0.559807	0.270260	0.899124
3	1	0	1.226079	-1.738603	-1.560276
4	1	0	0.312889	-0.764882	-0.109017
5	1	0	-0.212559	-2.642859	-0.479532
6	1	0	-0.671797	-1.181242	-1.795820
7	1	0	-1.237666	-0.590680	1.343965
8	1	0	0.480075	0.610784	1.345694
9	7	0	-1.140881	1.082564	-0.305413
10	1	0	-0.621052	1.954949	-0.448004
11	1	0	-1.056942	0.541546	-1.168097
12	1	0	-2.137702	1.255747	-0.176522
13	1	0	-1.205986	1.398597	3.195878

14	7	0	-1.577110	1.737857	2.313982
15	1	0	-2.589909	1.669355	2.373273
16	1	0	-1.336017	2.724029	2.259661
17	7	0	-3.267862	-1.839516	-0.571260
18	1	0	-2.255522	-1.773092	-0.700744
19	1	0	-3.621259	-2.374873	-1.360522
20	1	0	-3.426864	-2.397179	0.263664
21	7	0	2.276823	1.245159	-1.293222
22	1	0	2.804600	1.122329	-2.153701
23	1	0	1.670299	0.428887	-1.211839
24	1	0	2.942109	1.160989	-0.524492
25	5	0	-4.041987	-0.399371	-0.482953
26	1	0	-5.217423	-0.651803	-0.447739
27	1	0	-3.656971	0.126171	0.539337
28	1	0	-3.718623	0.208079	-1.476994
29	5	0	1.471742	2.659238	-1.312647
30	1	0	0.618983	2.544044	-2.166390
31	1	0	1.000592	2.801490	-0.201679
32	1	0	2.270706	3.520589	-1.566324
33	7	0	2.911132	-2.122495	0.791262
34	1	0	3.410430	-2.972719	0.544446
35	1	0	2.167296	-1.999946	0.101261
36	1	0	2.462650	-2.284537	1.688668
37	5	0	3.933936	-0.846110	0.854439
38	1	0	4.794394	-1.139512	1.644266
39	1	0	4.352016	-0.714887	-0.273195
40	1	0	3.262617	0.090018	1.226450

Vibrational frequencies

-471.3387	20.0200	30.8264
44.6033	53.7160	60.1057
70.0144	80.0589	94.8312
104.3506	109.6754	121.8830
125.9125	147.9817	149.6514
162.6847	174.4263	184.1269
191.3887	198.1170	206.6834
222.3751	244.1566	247.9089
267.5152	301.4208	318.7006
325.6867	339.5265	348.0855
437.8905	464.6279	546.5239
684.7556	687.0069	697.9073
705.6697	712.8599	721.0130
729.7877	730.7207	755.6990
764.6008	879.5434	933.0601
939.8017	1035.9315	1091.1604
1095.9216	1100.8589	1102.6836
1104.0716	1105.9152	1125.8938
1163.8737	1175.5694	1194.4298
1210.8190	1225.5504	1226.9290
1228.7848	1238.3646	1242.1807
1245.9124	1247.7662	1258.4260
1266.5772	1271.4577	1281.2438
1304.4514	1430.2649	1444.8310
1460.8383	1468.4475	1645.7253
1685.7369	1686.0432	1690.5535
1692.4190	1693.7752	1699.4679
1701.1988	1704.8356	1716.0070
2279.4821	2451.3293	2483.8622
2501.7617	2505.9510	2508.3134
2525.1812	2537.1611	2553.1552
2555.0182	2591.6894	2601.7086
2604.9952	2707.3401	2820.5336
3424.4678	3474.3825	3479.3761
3495.4587	3518.4530	3534.9074
3585.2688	3595.4760	3603.5905
3611.1107	3640.9420	3657.3195
3662.3886	3673.5045	3684.0444

Product complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.7329802	0.36811

Cartesian coordinates

1	5	0	-0.434597	0.996180	0.896677
2	5	0	2.735175	-1.707674	1.049948
3	1	0	-1.022756	2.048492	0.712353
4	1	0	-1.208537	0.119596	1.240809
5	1	0	0.411744	1.158300	1.762759
6	1	0	0.118502	0.653682	-0.142554
7	1	0	3.503910	-1.090570	1.728425
8	1	0	2.972845	-2.877207	0.941745
9	7	0	1.262939	-1.545202	1.641060
10	1	0	0.562746	-2.031420	1.069638
11	1	0	1.226182	-1.953028	2.572627
12	1	0	0.947216	-0.570148	1.721589
13	1	0	3.550303	-1.278838	-0.898873
14	7	0	2.685669	-1.060835	-0.407177
15	1	0	2.614535	-0.036982	-0.409989
16	1	0	1.917905	-1.437448	-0.972948
17	7	0	1.595940	3.153050	-0.401197
18	1	0	0.828616	2.554666	-0.084408
19	1	0	1.243992	3.730352	-1.159874
20	1	0	1.831208	3.773089	0.368943
21	7	0	-1.547433	-1.283973	-1.401729
22	1	0	-1.682829	-1.013385	-2.372223
23	1	0	-1.172822	-0.471680	-0.907077
24	1	0	-2.479103	-1.434913	-1.013448
25	5	0	2.881429	2.276044	-0.870948
26	1	0	3.728746	3.046482	-1.241175
27	1	0	3.223967	1.659062	0.114613
28	1	0	2.480851	1.558376	-1.760535
29	5	0	-0.567401	-2.555484	-1.262793
30	1	0	0.505562	-2.204283	-1.717254
31	1	0	-0.507618	-2.815330	-0.077577
32	1	0	-1.032507	-3.468233	-1.890158
33	7	0	-3.841695	1.123307	0.928363
34	1	0	-4.094860	2.091982	0.755184
35	1	0	-2.821864	1.085016	1.009015
36	1	0	-4.230866	0.864852	1.830713
37	5	0	-4.405693	0.149505	-0.255714
38	1	0	-5.601632	0.288691	-0.277668
39	1	0	-3.866519	0.526481	-1.271074
40	1	0	-4.079427	-0.972948	0.067340

Vibrational frequencies

25.0872	26.8864	43.9499
55.8966	59.6168	69.5551
84.3494	88.0774	98.7833
112.3470	131.5507	135.0102
155.1941	172.4043	175.2626
184.2385	204.3284	209.5790
220.9166	238.6004	242.7973
267.8604	294.2473	308.2116
329.9794	344.4935	349.2336
362.8729	372.8286	397.1946
690.5395	703.4013	703.8583
706.7370	724.5635	727.3706
730.2223	737.7537	746.9695
756.3048	791.4845	800.8696
820.6132	867.2799	1062.6024
1098.9707	1104.0917	1104.5041
1113.0137	1113.6037	1113.7718
1140.6063	1150.9137	1159.8171
1191.3882	1208.4379	1217.0724
1226.6546	1228.6230	1241.5500
1241.9600	1244.4984	1250.7545

1256.2522	1266.0403	1273.3352
1289.4313	1292.8450	1327.7416
1424.3930	1437.7516	1472.3811
1486.0100	1506.0250	1688.5456
1690.3555	1692.5694	1695.0540
1696.1589	1702.8710	1706.7509
1712.0397	1713.2468	1719.3117
2411.7666	2440.9530	2463.1082
2478.2040	2481.1808	2497.4851
2500.0232	2503.9902	2543.0648
2544.6995	2591.0963	2594.8757
2606.1410	2610.1432	2668.9040
3378.8380	3408.1389	3452.5227
3459.3399	3463.5784	3474.2960
3496.8421	3569.2237	3603.3384
3606.9319	3613.8297	3620.8592
3639.1868	3662.8356	3664.7619

Reactant complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.7064516	0.365709

Cartesian coordinates

1	5	0	-0.163549	1.108169	0.003534
2	5	0	0.025030	-0.777710	-1.163816
3	1	0	0.590334	1.333432	0.919214
4	1	0	0.573770	0.116001	-0.435047
5	1	0	-0.175257	1.934453	-0.868074
6	1	0	-1.237301	0.746910	0.387988
7	1	0	-0.820989	-0.422111	-1.921936
8	1	0	1.024165	-1.174240	-1.699997
9	7	0	-0.513399	-1.873291	-0.156211
10	1	0	0.180717	-2.069942	0.572635
11	1	0	-1.404541	-1.605923	0.273197
12	1	0	-0.690501	-2.747173	-0.647782
13	1	0	-3.064425	1.864497	1.672646
14	7	0	-4.038232	1.791593	1.395080
15	1	0	-4.458486	1.068694	1.970357
16	1	0	-4.488106	2.668531	1.632737
17	7	0	-3.639648	0.145366	-1.008056
18	1	0	-2.688499	0.338470	-1.315187
19	1	0	-3.900991	0.886714	-0.340292
20	1	0	-4.243943	0.203646	-1.822427
21	7	0	3.367166	-1.618900	0.212814
22	1	0	3.749699	-0.755276	0.598190
23	1	0	2.858113	-1.335905	-0.622267
24	1	0	4.151365	-2.188545	-0.093340
25	5	0	-3.765241	-1.305823	-0.287914
26	1	0	-4.933646	-1.478765	-0.051085
27	1	0	-3.311953	-2.124499	-1.055997
28	1	0	-3.116465	-1.218396	0.737786
29	5	0	2.427653	-2.433157	1.261642
30	1	0	1.606210	-1.633036	1.656324
31	1	0	1.931458	-3.339086	0.626517
32	1	0	3.137930	-2.821869	2.150337
33	7	0	2.805184	2.804417	-0.176644
34	1	0	3.044314	3.493617	0.530808
35	1	0	1.918462	2.375453	0.093895
36	1	0	2.643658	3.303674	-1.047051
37	5	0	3.991129	1.694826	-0.344230
38	1	0	4.984147	2.295845	-0.664322
39	1	0	4.095659	1.175224	0.746460
40	1	0	3.602495	0.933787	-1.199255

Vibrational frequencies

21.5152	26.4328	35.1783
44.4627	49.3685	57.3000
66.8795	67.6572	73.8965
86.3751	95.7987	109.0290
120.5815	141.9102	151.8150
153.9431	168.4490	179.6905
192.2466	209.0329	234.3456
238.5579	250.1874	260.5826
307.1815	333.1164	334.4501
336.7014	344.6788	348.2963
425.9861	574.1474	671.9149
695.2810	698.8681	706.5497
713.4077	720.1092	739.6481
752.5691	755.1520	777.9217
788.4407	830.0627	890.6702
953.9750	1093.6146	1100.5304
1105.0033	1109.2017	1110.1047
1114.0301	1127.4490	1141.1732
1152.3363	1154.6126	1176.5552
1222.7823	1224.5266	1230.7947
1234.7673	1240.6361	1242.4082
1243.3523	1253.3904	1268.1149
1270.2458	1275.1097	1284.6063
1429.2446	1448.0382	1458.5335
1497.9097	1683.6123	1685.7252
1689.1475	1695.4598	1695.9662
1697.6827	1699.4864	1701.8024
1707.6117	1722.6818	1739.2820
2356.1157	2472.6289	2492.9202
2500.2056	2528.9757	2532.4588
2540.4189	2551.1981	2585.4530
2593.9082	2598.3307	2603.8939
2616.4779	2668.1189	2698.5237
3317.8773	3409.8226	3481.7980
3499.9264	3505.9065	3537.5047
3571.4531	3610.2334	3613.8388
3614.7267	3650.5628	3654.0408
3663.3868	3692.6433	3702.6078

TS2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.6847303	0.364045

Cartesian coordinates

1	5	0	0.098323	-1.052187	0.161466
2	5	0	1.381777	0.811495	-1.412095
3	1	0	-0.762915	-0.246712	0.024311
4	1	0	1.067414	-0.334655	-1.086271
5	1	0	0.066630	-2.069414	-0.466640
6	1	0	0.948585	-0.889304	0.977055
7	1	0	2.360882	0.760007	-2.115399
8	1	0	0.451892	1.370165	-1.936485
9	7	0	1.776567	1.594131	-0.069131
10	1	0	2.106486	2.531745	-0.287203
11	1	0	0.986999	1.713584	0.571973
12	1	0	2.529089	1.120640	0.438323
13	1	0	-1.324894	-2.742996	2.374610
14	7	0	-1.317099	-1.821111	1.948897
15	1	0	-2.279094	-1.496425	1.894154
16	1	0	-0.846578	-1.200429	2.600114
17	7	0	3.751609	-1.419956	-0.543385
18	1	0	3.347556	-2.234960	-0.089867
19	1	0	4.455672	-1.745943	-1.199736
20	1	0	3.010706	-0.973193	-1.084431
21	7	0	-1.910513	2.241409	-0.207059
22	1	0	-1.286396	1.828168	-0.898954
23	1	0	-2.455348	2.953689	-0.686317
24	1	0	-2.562688	1.505641	0.064345
25	5	0	4.416304	-0.393847	0.551615
26	1	0	3.538911	-0.171000	1.355517

27	1	0	5.344304	-0.979199	1.044911
28	1	0	4.742849	0.582371	-0.080035
29	5	0	-1.092933	2.883660	1.047634
30	1	0	-0.552752	1.949715	1.604149
31	1	0	-0.298843	3.657413	0.559930
32	1	0	-1.901711	3.422209	1.756781
33	7	0	-2.942495	-1.868071	-0.991928
34	1	0	-3.152287	-2.689538	-0.431777
35	1	0	-1.962916	-1.636414	-0.823383
36	1	0	-3.038554	-2.137149	-1.967298
37	5	0	-3.934461	-0.618249	-0.630270
38	1	0	-3.654368	-0.296591	0.505015
39	1	0	-3.670354	0.240632	-1.438293
40	1	0	-5.059812	-1.031238	-0.732609

Vibrational frequencies

-360.8189	31.3240	36.8394
42.7878	48.8661	62.6731
70.7979	79.1346	94.0784
98.9228	102.4392	112.0275
125.5587	137.1757	140.4810
144.7436	172.9203	174.0190
181.8388	194.5046	209.1318
226.6302	231.8024	239.8271
268.0271	275.7007	308.3800
309.8410	346.4470	363.7955
412.5369	461.1156	686.7989
687.3244	696.0261	703.2866
708.3968	714.3239	715.3893
718.5314	730.2077	748.0237
779.5371	800.4096	847.5579
927.5460	1057.3196	1096.9419
1098.5591	1101.1684	1104.4193
1105.5194	1109.4036	1139.8737
1142.9115	1177.4287	1202.3425
1218.9456	1225.1553	1227.4426
1230.4808	1235.6146	1238.7504
1240.2482	1243.7407	1244.0514
1263.6946	1269.1374	1269.8174
1301.8387	1417.2642	1419.7981
1445.6072	1499.2776	1685.7726
1689.1230	1689.9157	1693.9238
1696.1957	1699.4829	1700.1376
1702.5921	1709.4554	1712.1696
2361.9449	2489.9666	2501.6878
2511.7996	2532.3480	2544.5709
2554.1704	2564.3798	2590.3189
2598.9475	2601.6841	2603.8521
2610.7271	2724.5173	2769.7450
3430.6821	3493.4128	3495.6641
3496.8773	3520.4754	3524.9774
3604.7572	3621.2179	3622.2175
3623.1408	3642.0245	3662.7130
3664.0484	3673.5340	3687.4312

Product complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-414.74015	0.368979

Cartesian coordinates

1	5	0	-1.007666	2.576759	0.722574
2	5	0	-0.258013	-1.323063	-1.550249
3	1	0	-1.002197	2.135038	-0.404915
4	1	0	-0.059862	-0.338474	-0.871184
5	1	0	-0.280676	3.533172	0.834560
6	1	0	-2.131244	2.794446	1.109347
7	1	0	-1.133785	-1.144918	-2.367189
8	1	0	0.757216	-1.725488	-2.076973
9	7	0	-0.767908	-2.473469	-0.537609
10	1	0	-0.918664	-3.355309	-1.020549
11	1	0	-0.093560	-2.641153	0.213814
12	1	0	-1.650871	-2.211222	-0.094058
13	1	0	-0.399130	1.691204	2.643137
14	7	0	-0.403047	1.402572	1.667709
15	1	0	0.558932	1.160731	1.426647
16	1	0	-0.951432	0.543237	1.610604
17	7	0	-3.169466	0.405290	-0.664161
18	1	0	-2.900211	1.322169	-0.306160
19	1	0	-4.032851	0.511135	-1.189850
20	1	0	-2.438300	0.121299	-1.316780
21	7	0	2.709311	-1.569846	0.216647
22	1	0	2.181636	-1.604012	-0.655650
23	1	0	3.557471	-2.114074	0.084233
24	1	0	2.982629	-0.593866	0.337079
25	5	0	-3.355481	-0.678563	0.534557
26	1	0	-2.297869	-0.701314	1.130431
27	1	0	-4.261428	-0.300926	1.226328
28	1	0	-3.583281	-1.738693	-0.006516
29	5	0	1.836729	-2.128380	1.470633
30	1	0	0.899834	-1.368792	1.587683
31	1	0	1.483409	-3.246408	1.153113
32	1	0	2.553548	-2.132936	2.435408
33	7	0	1.598334	2.057972	-1.352626
34	1	0	0.887519	2.660173	-0.936215
35	1	0	1.117361	1.198660	-1.617347
36	1	0	1.932628	2.505732	-2.201599
37	5	0	2.828170	1.781916	-0.323329
38	1	0	2.329393	1.251075	0.649554
39	1	0	3.590739	1.041216	-0.901266
40	1	0	3.313786	2.847322	-0.056341

Vibrational frequencies

39.5675	51.4712	54.0016
59.6571	77.1900	92.5161
102.8679	106.2355	116.0076
117.0176	123.5064	131.9718
135.0333	155.4444	168.8209
169.8447	196.8932	197.4468
210.1366	216.3858	226.1829
228.7138	236.3713	249.0592
326.9986	336.6799	339.1211
341.2907	362.6172	705.4526
706.3802	709.7155	715.6604
720.0556	724.0093	727.4157
732.0692	735.5932	751.9003
753.8034	755.1301	761.0306
769.3423	786.5672	1099.8698
1101.3843	1106.3619	1107.3896
1109.0202	1110.1085	1116.9866
1121.6566	1127.2702	1139.0546
1218.3196	1222.8231	1223.7651
1227.3984	1233.6705	1238.4637
1239.5722	1244.1480	1252.3068
1254.0065	1263.5304	1270.4802
1277.0509	1279.6714	1306.7013
1439.6226	1442.3968	1446.4730
1453.3550	1478.5700	1685.4224
1687.5682	1691.2125	1693.0602
1696.0849	1698.8492	1700.9506
1705.7036	1707.3544	1720.1448
2484.7821	2490.0595	2492.2222
2496.0647	2511.6392	2526.1322
2530.7949	2534.2883	2541.2185
2547.3634	2559.4370	2580.7209
2606.3360	2615.7619	2616.9386
3442.8596	3473.3497	3481.3027

3483.6621	3488.3326	3538.7080
3580.8613	3586.9787	3589.4108
3598.3479	3633.0206	3633.7256
3644.4073	3645.6424	3647.9016

A NH_3 molecule attacking the AaDB intermediate (in the presence of four AB molecules)

Reactant complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.6544108	0.439104

Cartesian coordinates

1	5	0	0.412489	0.807469	-0.428270
2	5	0	-0.263163	-1.156419	-1.217627
3	1	0	1.448152	0.948912	0.185557
4	1	0	0.706290	-0.371972	-0.850607
5	1	0	0.323914	1.532312	-1.383365
6	1	0	-0.538306	0.818834	0.304601
7	1	0	-1.177185	-0.626437	-1.769192
8	1	0	0.420050	-1.847116	-1.917846
9	7	0	-0.705304	-1.923175	0.076576
10	1	0	0.102427	-2.185943	0.647715
11	1	0	-1.345593	-1.369178	0.649708
12	1	0	-1.225252	-2.783276	-0.179147
13	1	0	-3.371314	-3.569440	-0.556261
14	7	0	-2.525637	-4.125831	-0.642428
15	1	0	-2.622777	-4.924015	-0.023990
16	1	0	-2.493189	-4.487124	-1.589698
17	7	0	-3.449210	0.850409	-0.511783
18	1	0	-2.575082	0.735567	-1.021622
19	1	0	-3.400904	1.762480	-0.053309
20	1	0	-4.194114	0.902784	-1.201423
21	7	0	3.078800	-0.867156	1.847399
22	1	0	3.403838	-0.697334	2.795020
23	1	0	2.507100	-0.071824	1.569812
24	1	0	3.889078	-0.844382	1.227744
25	5	0	-3.702886	-0.369326	0.533096
26	1	0	-4.769383	-0.173339	1.054347
27	1	0	-3.682952	-1.382489	-0.131771
28	1	0	-2.789668	-0.320804	1.331019
29	5	0	2.251783	-2.265080	1.740839
30	1	0	1.229780	-2.092200	2.371591
31	1	0	2.049752	-2.431900	0.559027
32	1	0	2.946657	-3.126404	2.212528
33	7	0	3.591597	1.027044	-1.831090
34	1	0	3.695496	1.973745	-2.186146
35	1	0	2.660516	0.963060	-1.420319
36	1	0	3.622648	0.398475	-2.629366
37	5	0	4.769001	0.676281	-0.745385
38	1	0	5.812958	0.934983	-1.284315
39	1	0	4.539368	1.374067	0.215472
40	1	0	4.647888	-0.506451	-0.519846
41	7	0	-0.842501	3.647238	0.888853
42	1	0	-0.758114	3.875007	1.875718
43	1	0	-0.139924	4.184255	0.387948
44	1	0	-0.606269	2.661842	0.772319
45	5	0	-2.347544	3.979986	0.333713
46	1	0	-2.341543	3.655493	-0.829963
47	1	0	-3.088132	3.306428	1.015413
48	1	0	-2.518835	5.159126	0.498123

Vibrational frequencies

-7.0485	17.7689	21.5485
30.2025	38.0305	42.7960
54.2473	62.5311	67.3376
76.1349	79.4220	85.1795
88.6198	95.3029	100.6464
109.4248	114.1621	133.7404
139.3112	155.7784	159.1512
167.2108	169.4102	189.0719
195.2664	202.7766	224.1182
228.2937	251.8055	265.3894
317.7779	324.7388	327.3742
328.0554	334.8677	344.6622
348.8992	488.1125	591.8164
683.1356	683.9032	686.6799
695.6705	696.8959	697.2867
702.9612	710.4915	713.8639
723.1241	724.3135	752.7917
755.2222	788.5012	875.4925
908.4013	1008.4678	1097.7388
1099.7157	1101.6947	1103.1987
1103.5375	1105.8850	1108.2519
1112.1044	1115.7534	1153.1183
1157.0845	1162.7971	1195.0417
1223.7424	1226.4475	1228.7322
1229.5170	1237.2115	1238.5755
1239.4613	1240.9619	1243.0779
1250.3952	1261.2989	1264.8062
1268.8703	1273.4722	1285.9119
1411.5722	1413.8255	1436.9678
1442.1909	1536.4842	1688.7589
1690.2502	1691.3042	1693.9302
1695.1367	1696.0500	1700.5835
1702.5637	1705.4262	1707.6213
1717.3943	1726.0589	1745.4717
2350.8968	2491.2672	2495.7528
2508.5503	2510.2629	2517.1520
2532.1439	2543.0787	2556.9909
2559.8026	2590.6708	2596.5770
2599.1278	2602.5801	2604.4351
2621.4686	2634.2279	2695.1685
3229.4349	3469.7877	3478.0410
3497.3656	3498.0946	3503.5784
3533.8356	3544.9505	3595.1303
3607.9520	3624.0682	3628.9147
3647.1933	3654.0884	3661.2817
3663.6268	3688.3020	3700.2565

TS1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.6265974	0.436697

Cartesian coordinates

1	5	0	0.230184	-1.240173	0.020433
2	5	0	-0.675357	1.243502	-0.705047
3	1	0	-0.421684	-2.190213	0.408421
4	1	0	-0.594234	-0.361163	-0.289694
5	1	0	0.882951	-1.508780	-0.964752
6	1	0	0.921411	-0.797416	0.920735
7	1	0	0.167836	1.197224	-1.533381
8	1	0	-1.826711	1.076057	-0.914770
9	7	0	-0.249199	1.726598	0.717978
10	1	0	-1.070510	1.957847	1.286719
11	1	0	0.257620	0.992238	1.213561
12	1	0	0.398015	2.512981	0.650744
13	1	0	-0.129367	4.012086	-1.369417
14	7	0	-0.989066	3.476688	-1.277865
15	1	0	-1.654553	4.047675	-0.763610
16	1	0	-1.369028	3.364005	-2.212411
17	7	0	3.065859	1.073889	-0.708011
18	1	0	2.217540	0.519372	-0.817418
19	1	0	3.734280	0.459262	-0.238516

20	1	0	3.430003	1.239194	-1.642843
21	7	0	-2.870451	-0.607605	1.752324
22	1	0	-3.044751	-1.330808	2.445630
23	1	0	-1.998690	-0.861092	1.287687
24	1	0	-3.591629	-0.703261	1.037221
25	5	0	2.835946	2.470508	0.093297
26	1	0	3.880703	3.064127	0.070975
27	1	0	1.961675	3.066556	-0.507740
28	1	0	2.498841	2.163443	1.214242
29	5	0	-2.836336	0.860112	2.456939
30	1	0	-1.809441	0.896576	3.099310
31	1	0	-2.853218	1.672977	1.554705
32	1	0	-3.819395	0.946061	3.143093
33	7	0	-2.328380	-2.254407	-1.913227
34	1	0	-2.192917	-3.217948	-2.207228
35	1	0	-1.556534	-2.019712	-1.287816
36	1	0	-2.237935	-1.669707	-2.739628
37	5	0	-3.792436	-2.065404	-1.202137
38	1	0	-4.607107	-2.452873	-1.999013
39	1	0	-3.750157	-2.740217	-0.199212
40	1	0	-3.890429	-0.880105	-0.977009
41	7	0	3.145983	-2.733188	0.755650
42	1	0	3.266318	-2.960495	1.738880
43	1	0	3.012694	-3.607031	0.254244
44	1	0	2.280695	-2.198886	0.665004
45	5	0	4.437854	-1.914307	0.175702
46	1	0	4.183172	-1.687207	-0.984149
47	1	0	4.509695	-0.913098	0.854704
48	1	0	5.392351	-2.632678	0.318865

Vibrational frequencies

-447.5832	12.9052	27.4064
28.1220	38.5982	45.4511
49.3947	57.5365	68.0336
74.0950	83.7951	89.2911
98.8687	108.7827	111.5314
121.0880	125.0088	136.4512
144.7316	148.8511	161.0154
174.9902	178.6132	191.0634
192.2688	199.4438	209.6767
219.8242	233.4486	239.8362
246.1561	297.8237	323.4033
334.8405	337.1291	341.0811
345.8198	420.8914	454.4548
561.2182	682.3870	686.8637
698.2501	698.6538	700.8255
706.6575	712.6008	717.2949
725.3680	730.7378	754.0285
755.0429	767.7878	889.8284
929.1061	933.1584	1038.0168
1091.9661	1096.6552	1099.5075
1101.3969	1103.0410	1104.4805
1105.7526	1108.2535	1128.6744
1166.1560	1176.2735	1187.4935
1216.3334	1224.8227	1226.3097
1228.1086	1228.7717	1241.4051
1242.5812	1244.2728	1246.1825
1246.7231	1255.8929	1267.2536
1272.4173	1273.7982	1283.3655
1311.1373	1421.3537	1423.0958
1459.1465	1462.1702	1469.5751
1644.9523	1684.3799	1686.8646
1691.2231	1692.1873	1693.5743
1695.2965	1696.9398	1699.5030
1702.6462	1708.2619	1716.2101
2305.2630	2452.4004	2479.5925
2487.2492	2501.1941	2503.7656
2508.5286	2528.6150	2534.4844
2537.4082	2553.8588	2555.8710
2596.3713	2600.1959	2604.4252
2606.6008	2706.8384	2817.1950
3426.5437	3478.6883	3490.0458
3494.0447	3497.1563	3518.3085
3549.1034	3579.9200	3585.7985
3598.6919	3617.4166	3620.7931
3641.0004	3641.5028	3661.6141
3663.5838	3673.2553	3684.6034

Product complex 1

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.6907251	0.442509

Cartesian coordinates

1	5	0	0.413911	0.169265	-2.051123
2	5	0	-3.799842	-0.856574	-0.752555
3	1	0	1.302725	0.848260	-2.531161
4	1	0	0.369752	-0.920189	-2.598709
5	1	0	-0.654387	0.745562	-2.234096
6	1	0	0.582712	0.027560	-0.845081
7	1	0	-4.314538	-0.224868	-1.628886
8	1	0	-4.355487	-1.878287	-0.463889
9	7	0	-2.295910	-1.187011	-1.152728
10	1	0	-1.761906	-1.628657	-0.396900
11	1	0	-2.292919	-1.841849	-1.932942
12	1	0	-1.728919	-0.389244	-1.473651
13	1	0	-3.217048	0.942175	0.397169
14	7	0	-3.715035	0.057419	0.556421
15	1	0	-3.236439	-0.414771	1.326601
16	1	0	-4.656073	0.285688	0.869392
17	7	0	-0.340322	2.939178	-0.423964
18	1	0	-0.253104	2.283435	-1.204143
19	1	0	0.562045	2.938292	0.058764
20	1	0	-0.477920	3.869785	-0.809055
21	7	0	0.378655	-0.624108	2.009259
22	1	0	0.368346	-0.232528	2.948451
23	1	0	0.176864	0.149486	1.374403
24	1	0	1.341146	-0.907416	1.815371
25	5	0	-1.543029	2.506978	0.546575
26	1	0	-1.608886	3.283593	1.463187
27	1	0	-2.555573	2.516038	-0.131545
28	1	0	-1.281907	1.381846	0.921303
29	5	0	-0.660820	-1.848652	1.865962
30	1	0	-1.771884	-1.391098	2.040659
31	1	0	-0.532115	-2.279950	0.735026
32	1	0	-0.380568	-2.678436	2.687848
33	7	0	1.940477	-2.584953	-0.750591
34	1	0	2.189683	-3.264976	-1.464088
35	1	0	1.486856	-1.797704	-1.223694
36	1	0	1.233132	-3.010134	-0.154242
37	5	0	3.257061	-2.159521	0.105774
38	1	0	3.679574	-3.158067	0.625208
39	1	0	4.029365	-1.668102	-0.683111
40	1	0	2.878199	-1.348537	0.927673
41	7	0	3.264228	1.242694	-0.432973
42	1	0	3.510728	0.325362	-0.060247
43	1	0	4.084168	1.601427	-0.914838
44	1	0	2.540489	1.073863	-1.135995
45	5	0	2.766844	2.267644	0.719821
46	1	0	2.504548	3.309105	0.154018
47	1	0	1.781596	1.762666	1.217572
48	1	0	3.662469	2.392433	1.513390

Vibrational frequencies

39.0942	45.0333	50.4484
54.6784	79.2878	87.0822
91.1834	94.6038	101.0453
106.4541	115.3576	121.5372
131.7264	134.3358	138.6086
147.8842	169.0961	180.3877
183.8197	187.6320	195.7884
199.7762	206.2861	217.9894
228.4507	237.2511	253.4079
266.4227	281.8247	301.5634
321.4282	331.3321	338.7978
346.5477	355.0667	362.2207
393.9852	706.4575	708.7047
711.1013	726.0344	726.9763
728.5975	736.2373	741.4643
744.5722	753.1002	764.8983
769.8541	788.1487	800.1193
812.2857	820.3765	868.7404
1061.2229	1097.2400	1103.0081
1107.0759	1107.7381	1114.9241
1117.7684	1121.0968	1137.5846
1139.4474	1152.3874	1158.0212
1186.0221	1190.7875	1215.4753
1223.4093	1225.9950	1226.7186
1231.7217	1236.1391	1236.8911
1242.9598	1248.9029	1270.8762
1272.0430	1273.6847	1275.7023
1277.7446	1301.8799	1317.1025
1449.9318	1457.7045	1465.1564
1471.8085	1488.8718	1520.0442
1680.0219	1682.2872	1689.2254
1689.9880	1691.4203	1693.2230
1694.3112	1705.2663	1707.2294
1715.0842	1720.6725	1727.2438
2394.2725	2427.0433	2458.7244
2464.7115	2476.6513	2486.2664
2492.7766	2500.4716	2511.4749
2516.8770	2529.1254	2549.3310
2595.5881	2596.8481	2606.2235
2607.1271	2612.7883	2669.4566
3362.8898	3395.7502	3444.2966
3448.2532	3457.6741	3465.1187
3473.4888	3524.1043	3535.8679
3563.5570	3575.0604	3584.2501
3608.6288	3627.1252	3628.6341
3635.2853	3640.0983	3647.0806

Reactant complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.656806	0.439582

Cartesian coordinates

1	5	0	-0.100618	-0.598693	-0.405869
2	5	0	0.717182	1.365949	-1.114917
3	1	0	-1.189067	-0.107244	-0.441424
4	1	0	0.803248	0.086553	-1.060407
5	1	0	0.012680	-1.592342	-1.079190
6	1	0	0.355914	-0.685722	0.705226
7	1	0	1.824525	1.556537	-1.537348
8	1	0	-0.156008	1.737551	-1.837403
9	7	0	0.596632	1.998246	0.327398
10	1	0	0.717621	3.008247	0.272315
11	1	0	-0.324288	1.850742	0.754277
12	1	0	1.332535	1.638798	0.940082
13	1	0	-2.649436	-2.118683	3.084640
14	7	0	-2.571097	-1.636205	2.196012
15	1	0	-3.221672	-0.856229	2.219106
16	1	0	-1.639538	-1.234873	2.151878
17	7	0	4.485961	1.016485	-0.228199
18	1	0	4.756447	0.051340	-0.432873
19	1	0	5.321646	1.594113	-0.261343
20	1	0	3.875206	1.305659	-0.989681
21	7	0	-3.061032	2.016456	-0.784258
22	1	0	-2.270783	1.716819	-1.351836
23	1	0	-3.603372	2.669376	-1.343792
24	1	0	-3.641275	1.185567	-0.633144
25	5	0	3.750737	1.145636	1.214167
26	1	0	2.796729	0.393792	1.168073
27	1	0	4.545639	0.813890	2.052431
28	1	0	3.399196	2.298794	1.320618
29	5	0	-2.584743	2.700276	0.610871
30	1	0	-2.056764	1.811236	1.252565
31	1	0	-1.806209	3.579269	0.308706
32	1	0	-3.569766	3.115677	1.160370
33	7	0	-3.238772	-2.155682	-0.627455
34	1	0	-3.066889	-2.314834	0.375576
35	1	0	-2.365837	-1.786356	-0.998239
36	1	0	-3.417684	-3.043280	-1.087242
37	5	0	-4.479550	-1.121383	-0.833589
38	1	0	-4.341841	-0.281173	0.032532
39	1	0	-4.378353	-0.662202	-1.949135
40	1	0	-5.494714	-1.747395	-0.668513
41	7	0	2.821269	-2.309543	0.212904
42	1	0	3.058369	-3.092885	0.815361
43	1	0	1.885634	-2.465852	-0.156564
44	1	0	2.762603	-1.473754	0.795099
45	5	0	3.914725	-2.130902	-0.986445
46	1	0	3.488899	-1.237381	-1.680284
47	1	0	4.956625	-1.843412	-0.432252
48	1	0	3.980587	-3.183067	-1.564093

Vibrational frequencies

-20.0761	23.2116	27.1193
30.5692	38.7203	53.2923
59.6794	64.9940	67.7789
79.9176	91.9457	93.5455
98.0881	105.9734	113.8902
121.2495	125.3765	146.4260
153.4985	173.7973	179.1031
192.8428	201.3389	213.9428
226.3966	228.7916	239.6313
245.7018	250.5918	256.7759
280.5999	307.9188	338.0215
347.0393	352.0326	358.3554
368.7343	390.3222	499.2124
700.8624	702.9481	708.5653
709.5843	723.3798	725.3598
734.6622	735.1311	740.7867
754.1794	758.2702	760.2795
784.7990	786.5571	833.2017
893.7197	944.1847	1066.5614
1100.4420	1102.1056	1102.4498
1103.1138	1109.8803	1111.7910
1117.8030	1120.3776	1134.7120
1155.3300	1165.6079	1182.6738
1220.2441	1222.1567	1226.8777
1228.2409	1236.7019	1239.7447
1243.8924	1245.1964	1245.6720
1255.6284	1258.3049	1274.2002
1276.4677	1286.5665	1290.6323
1426.3563	1448.5178	1451.8525
1461.7687	1494.0673	1680.5699
1681.5950	1682.5780	1688.8035

1690.3704	1691.3906	1693.8910
1695.7517	1700.4039	1701.3584
1702.4093	1717.3334	1732.4690
2350.5765	2471.0940	2484.8424
2490.5346	2496.9319	2517.6843
2535.0988	2535.9342	2542.0643
2548.3093	2590.2011	2602.8628
2605.7061	2606.6641	2607.6296
2609.8640	2672.0826	2688.4840
3351.0676	3417.0767	3441.0669
3462.5572	3493.2717	3529.6716
3532.7649	3574.9073	3583.1706
3590.3599	3610.3028	3612.5892
3647.4363	3651.2818	3654.3442
3657.6490	3683.7051	3696.8116

TS2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.6369768	0.438528

Cartesian coordinates

1	5	0	-0.285630	-0.590959	0.297144
2	5	0	0.322821	1.513891	-1.280345
3	1	0	-1.363284	-0.171552	0.036608
4	1	0	0.509006	0.345763	-0.935655
5	1	0	0.110110	-1.584133	-0.235083
6	1	0	0.351575	-0.089438	1.167733
7	1	0	1.210014	1.848589	-2.029362
8	1	0	-0.765938	1.668029	-1.774112
9	7	0	0.432210	2.412873	0.044214
10	1	0	0.375405	3.404682	-0.175378
11	1	0	-0.318855	2.224187	0.713649
12	1	0	1.329669	2.251529	0.506244
13	1	0	-1.265380	-2.484917	2.641137
14	7	0	-1.536888	-1.729541	2.018861
15	1	0	-2.479997	-1.928718	1.696030
16	1	0	-1.604433	-0.887847	2.583853
17	7	0	3.783532	0.881784	-1.105043
18	1	0	3.954183	-0.126498	-1.095754
19	1	0	4.535805	1.316332	-1.632716
20	1	0	2.914656	1.034695	-1.617409
21	7	0	-3.262641	1.752869	-0.087648
22	1	0	-2.536976	1.623411	-0.791889
23	1	0	-4.020025	2.265792	-0.531947
24	1	0	-3.621247	0.820595	0.117247
25	5	0	3.697437	1.512781	0.388644
26	1	0	2.759272	0.961513	0.930682
27	1	0	4.740106	1.280839	0.941965
28	1	0	3.483553	2.695491	0.252634
29	5	0	-2.712184	2.552206	1.220953
30	1	0	-1.881812	1.828740	1.731826
31	1	0	-2.232048	3.580748	0.797552
32	1	0	-3.655335	2.736300	1.944959
33	7	0	-2.616275	-2.293138	-1.415933
34	1	0	-2.521533	-3.201814	-0.970245
35	1	0	-1.812073	-1.735784	-1.126766
36	1	0	-2.548593	-2.442868	-2.419057
37	5	0	-4.028430	-1.566502	-1.024147
38	1	0	-3.958710	-1.330989	0.164201
39	1	0	-4.067865	-0.562450	-1.695343
40	1	0	-4.903470	-2.347798	-1.290411
41	7	0	2.858457	-1.861548	1.063018
42	1	0	3.336739	-2.285565	1.853015
43	1	0	1.873977	-2.112926	1.112465
44	1	0	2.903301	-0.847622	1.181893
45	5	0	3.522856	-2.340638	-0.352566
46	1	0	2.825347	-1.859560	-1.215306
47	1	0	4.647275	-1.889603	-0.350079
48	1	0	3.504456	-3.544144	-0.357884

Vibrational frequencies

-370.2182	23.8382	32.1345
35.7666	44.5572	53.7532
59.5590	69.2748	82.8527
86.1493	97.4329	98.9416
108.2732	112.3620	124.2364
129.2119	135.3090	141.9596
150.6576	161.1493	171.5252
177.5887	178.8549	190.6254
200.5893	217.3843	219.8513
243.1130	251.8301	270.5900
280.4821	307.7567	310.2832
318.8774	336.2609	348.8216
383.3862	417.3101	477.4398
687.3851	696.5188	700.0553
701.2279	708.9368	712.9144
713.2509	719.6551	730.6154
733.1269	744.3479	748.7387
759.9679	768.8280	797.1068
844.6020	926.1653	1055.7568
1097.3918	1100.4470	1100.5446
1103.2580	1104.0999	1105.4431
1111.0327	1125.0592	1135.8854
1138.1070	1180.0674	1199.4768
1219.7750	1224.9818	1227.7051
1228.2290	1233.8996	1237.9068
1240.5914	1243.8710	1245.1926
1246.1497	1254.1398	1259.7115
1267.7317	1271.9700	1296.9914
1300.6418	1418.9164	1430.1925
1447.5248	1455.6839	1478.4564
1685.3646	1686.5064	1687.9445
1692.5810	1694.6926	1695.5140
1698.6979	1701.5331	1702.8448
1705.1449	1707.9136	1711.5290
2360.6813	2487.4049	2490.6211
2499.5900	2506.6037	2530.5157
2535.9425	2539.8223	2552.4915
2553.6817	2578.0725	2595.8006
2597.1707	2601.4550	2602.8902
2619.0233	2732.0522	2778.9155
3444.1589	3460.1814	3478.2188
3495.9924	3498.8117	3518.1160
3548.5511	3570.4266	3603.8197
3605.5050	3623.1832	3626.9167
3641.1665	3641.5557	3658.9641
3659.9771	3671.1099	3681.5320

Product complex 2

MP2/6-31++G(d,p) energy	Zero-point energy correction
-497.6963693	0.443052

Cartesian coordinates

1	5	0	0.437932	-1.584399	-1.749980
2	5	0	0.190767	2.466052	0.956399
3	1	0	0.150003	-0.722598	-0.945892
4	1	0	0.260583	1.305100	1.297286
5	1	0	-0.081974	-2.648431	-1.477519
6	1	0	0.200776	-1.230589	-2.877159
7	1	0	-0.803973	3.015132	1.372525
8	1	0	1.176056	3.101465	1.261215
9	7	0	0.107179	2.468642	-0.659635
10	1	0	0.062038	3.414610	-1.030093
11	1	0	0.924072	2.014178	-1.072535

12	1	0	-0.722938	1.975388	-0.996122
13	1	0	2.374008	-2.449735	-2.340101
14	7	0	2.032163	-1.816404	-1.622466
15	1	0	2.283015	-2.211626	-0.713854
16	1	0	2.538011	-0.933212	-1.709622
17	7	0	-3.233831	1.572920	0.768584
18	1	0	-3.284812	0.610333	1.106450
19	1	0	-4.038504	2.078370	1.129190
20	1	0	-2.395417	1.993154	1.173017
21	7	0	3.400824	1.343255	0.709907
22	1	0	2.642192	1.924518	1.071517
23	1	0	4.274204	1.700526	1.087813
24	1	0	3.261134	0.402723	1.083070
25	5	0	-3.192240	1.620423	-0.854564
26	1	0	-2.218731	0.968092	-1.172064
27	1	0	-4.212309	1.109398	-1.249226
28	1	0	-3.083503	2.777815	-1.175863
29	5	0	3.427098	1.341329	-0.914852
30	1	0	2.346197	0.907091	-1.253950
31	1	0	3.583193	2.482301	-1.269417
32	1	0	4.323066	0.605912	-1.253512
33	7	0	0.485428	-1.717491	1.714018
34	1	0	-0.151390	-2.441738	2.039162
35	1	0	0.161447	-1.456494	0.781281
36	1	0	0.325348	-0.900429	2.298773
37	5	0	2.031091	-2.191814	1.719058
38	1	0	2.092499	-3.170623	1.008347
39	1	0	2.657784	-1.266253	1.242479
40	1	0	2.351303	-2.418990	2.855395
41	7	0	-2.798151	-1.769498	-0.850876
42	1	0	-3.468182	-2.419877	-1.252120
43	1	0	-1.869196	-2.040212	-1.177092
44	1	0	-2.989978	-0.843136	-1.234886
45	5	0	-2.882082	-1.761669	0.769932
46	1	0	-2.073236	-0.937551	1.136078
47	1	0	-4.012874	-1.443040	1.059294
48	1	0	-2.598029	-2.871147	1.151444

Vibrational frequencies

32.7425	41.6834	46.9179
48.6510	55.1087	66.6044
80.1504	97.0496	97.9462
100.9734	109.3293	115.3474
116.3217	120.1774	129.1864
130.4483	139.2921	147.6361
152.9175	162.5278	165.5553
174.8154	176.3163	189.2689
209.4645	239.3246	240.7767
247.5609	253.9818	268.7450
317.9108	333.5988	358.7505
365.4103	372.2432	379.8342
694.6255	709.5229	710.7341
715.1027	716.0569	719.7853
733.9787	742.0868	744.2909
749.0466	751.7415	758.5178
760.0743	761.4945	765.5253
775.5141	779.3683	787.7573
1096.4844	1101.8806	1103.8067
1105.1751	1110.8944	1112.1579
1115.5626	1119.6095	1122.2769
1129.4189	1134.6734	1136.6878
1214.1703	1217.9446	1219.7383
1223.6529	1227.3106	1234.8098
1236.8182	1238.8131	1241.4408
1242.6834	1248.4521	1251.9099
1263.0815	1275.7380	1278.5940
1296.4476	1308.3490	1311.0853
1443.3699	1448.5448	1449.1813
1453.7599	1465.4545	1470.2913
1686.4404	1688.5446	1689.5917
1690.8549	1695.4275	1696.8183
1699.0193	1701.9460	1704.8863
1710.4327	1711.2789	1712.8694
2482.9608	2491.2093	2497.1310
2503.6725	2506.3235	2508.3804
2520.3617	2533.5431	2540.0013
2544.6721	2548.1139	2552.5658
2558.4653	2571.4715	2583.0184
2585.3758	2591.9626	2604.9418
3448.1144	3457.3394	3461.1207
3463.8486	3473.1015	3489.3529
3549.0008	3558.3174	3564.7813
3569.7710	3576.9358	3601.3471
3631.7836	3639.0091	3641.1429
3641.3441	3642.9037	3645.8663

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