Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

Supporting Information

Reactivity and mechanisms of hydridic hydrogen of B-H in ammonia borane towards acetic acids: the ammonia B-monoacyloxy boranes

HuizhenLi,[*,ab] *Yunhui Li,*[⊥a] *Jiaxin Kang,*[⊥b] *Lin Fan,*[d] *Qiuyu Yang,*[*,b] *Shujun Li,*[b] *Abdul Rahman,*[a] *Daqi Chen*[*,c]

[a]School of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou 510006, P. R. China

[b]Henan Key Laboratory of Boron Chemistry and Advanced Energy Materials, School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 453007, P. R. China

[c]School of Mechanical and Electrical Engineering, Guangzhou University, Guangzhou, 510006, P. R. China

[d]Beijing Normal University Publishing Group, College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China

Table of Contents

1. Supporting Results

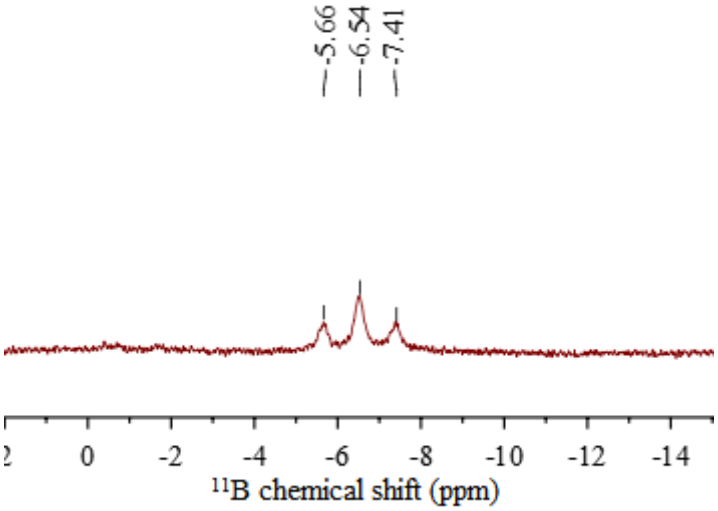

Figure S1a. ^{11}B NMR spectrum of $NH_3BH_2OOCCH_3$ in CD_3CN.

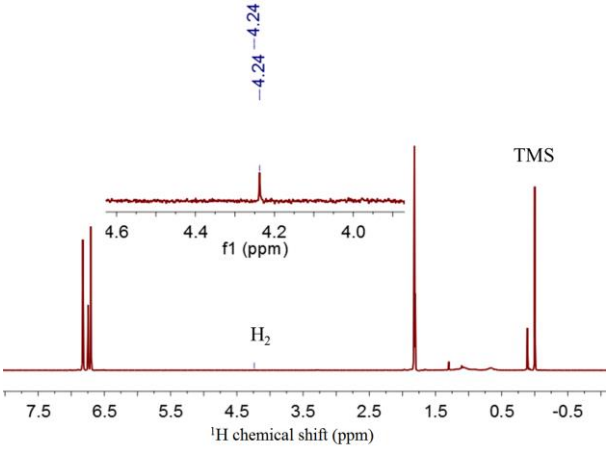

Figure S1b. ^1H NMR spectrum of the product H_2 in d_8-Toluene.

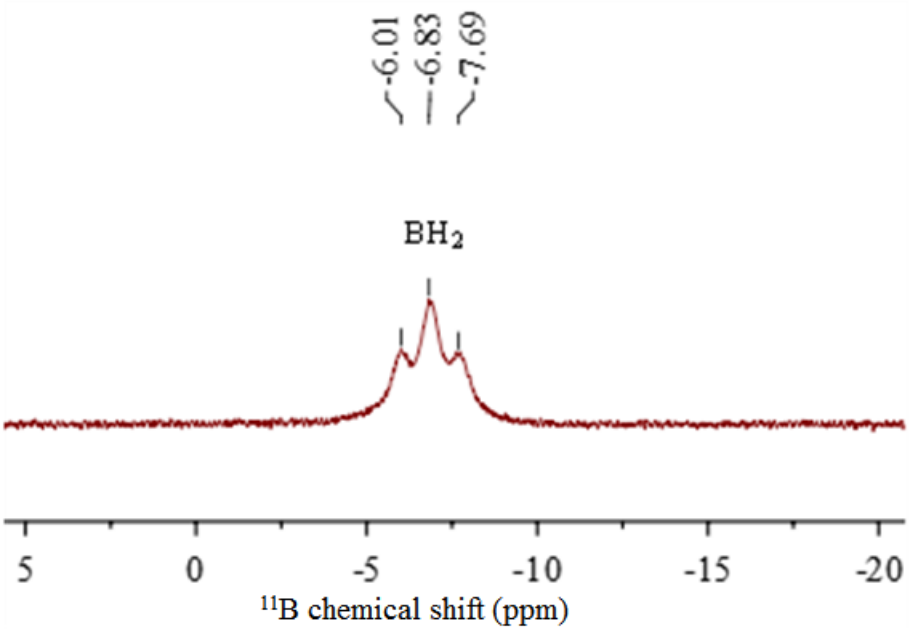

Figure S2a. ^{11}B NMR spectrum of $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**) in CD_3CN.

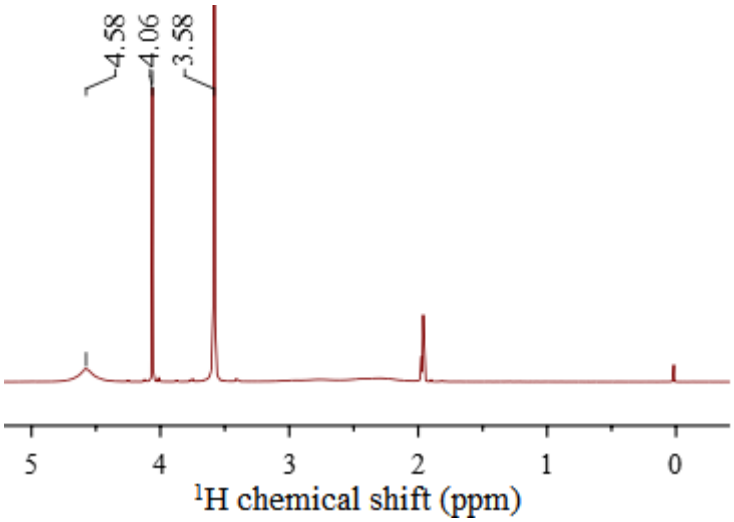

Figure S2b. ^{1}H NMR spectrum of $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**) in CD_3CN.

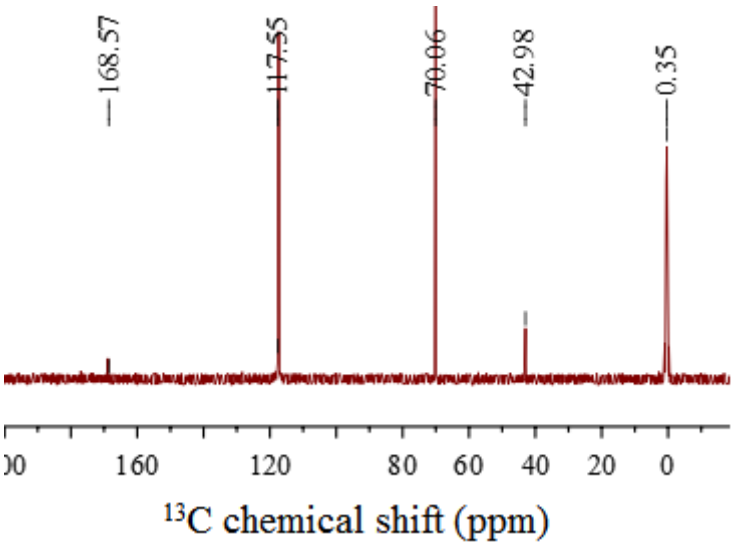

Figure S2c. ^{13}C NMR spectrum of $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**) in CD_3CN.

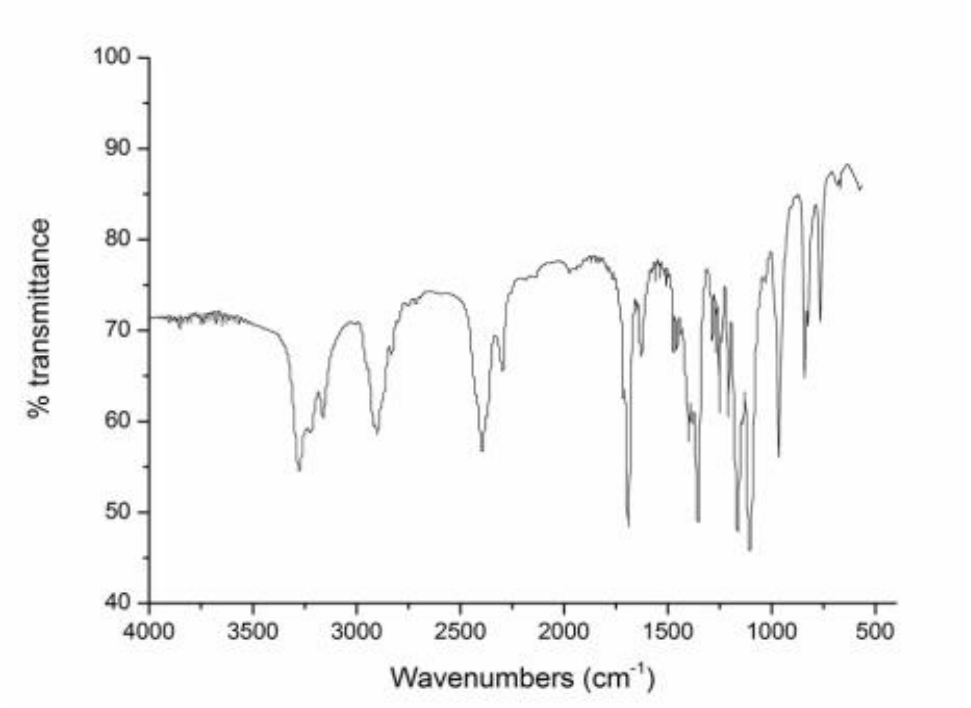

Figure S2d. FTIR spectrum of $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**).

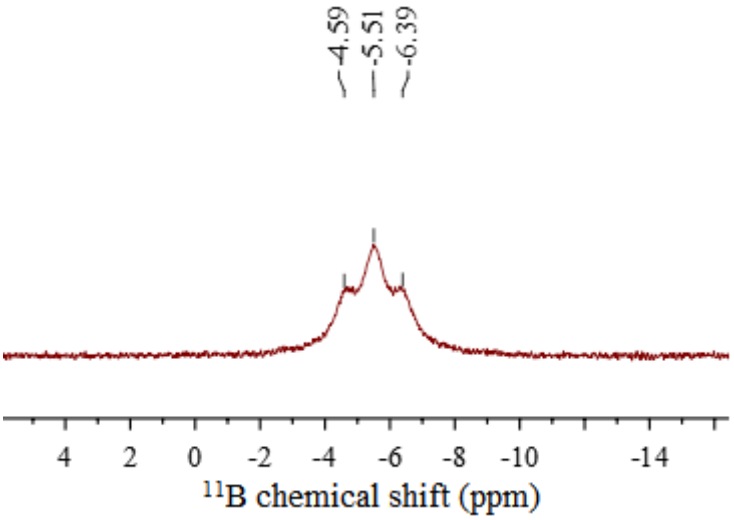

Figure S3a. ^{11}B NMR spectrum of $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**) in CD_3CN.

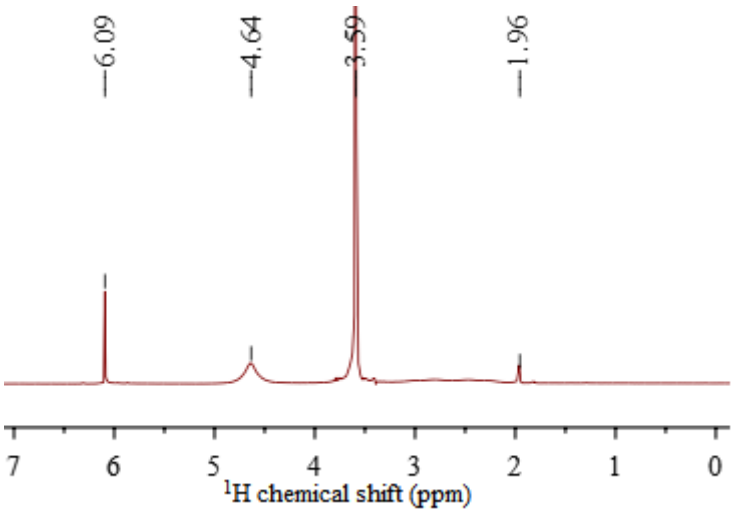

Figure S3b. ^{1}H NMR spectrum of $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**) in CD_3CN.

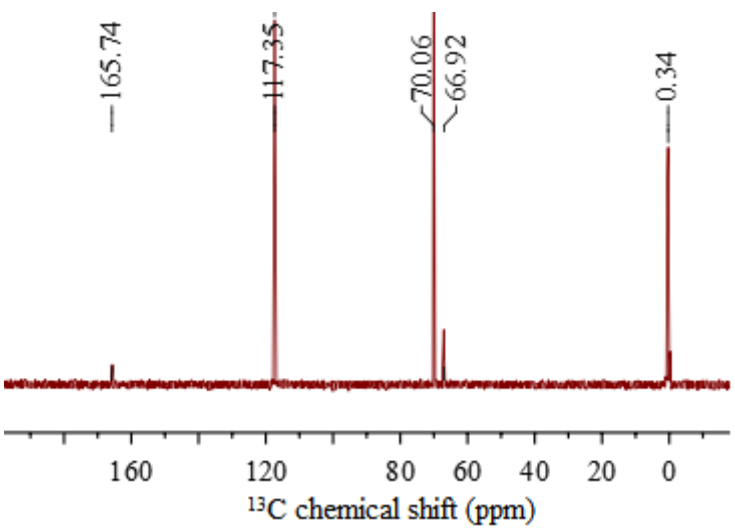

Figure S3c. ^{13}C NMR spectrum of $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**) in CD_3CN.

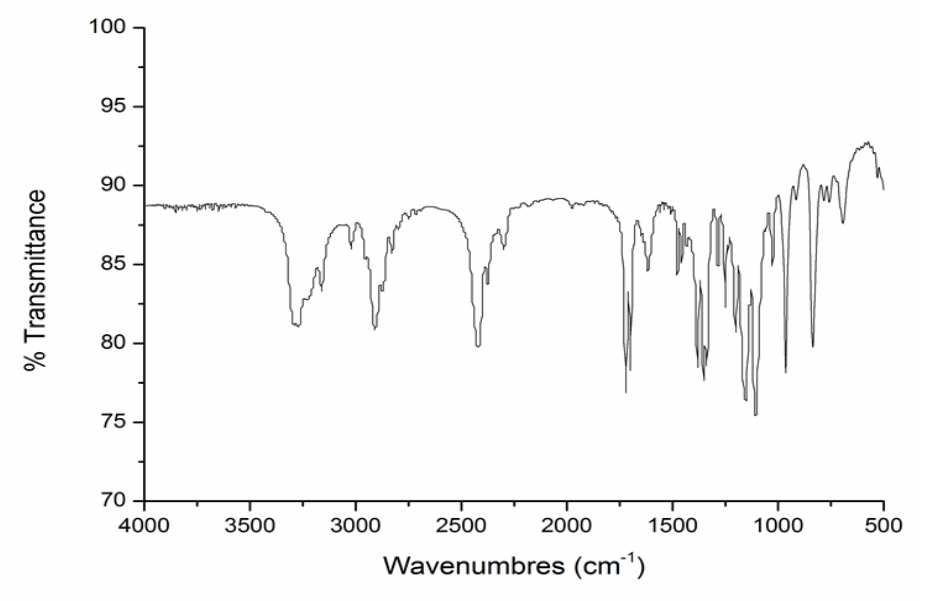

Figure S3d. FTIR spectrum of $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**).

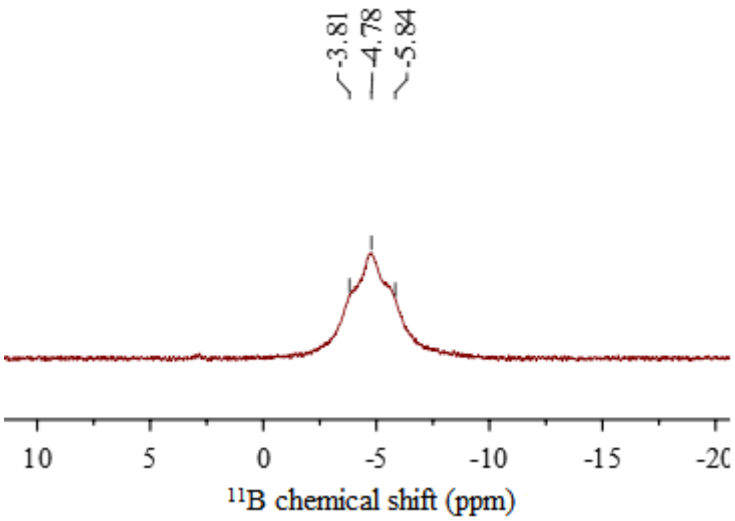

Figure S4. ^{11}B NMR spectrum of $NH_3BH_2OOCCCl_3$ in CD_3CN.

Table S1. The chemical shifts of B in the ammonia B-monoacyloxy boranes.

Ammonia B-monoacyloxy boranes	δ (BH_2), ppm
$NH_3BH_2OOCCH_3$	-6.5
$NH_3BH_2OOCCH_2Cl$	-5.7
$NH_3BH_2OOCCHCl_2$	-5.5
$NH_3BH_2OOCCCl_3$	-4.8

Table S2. Crystallographic data for $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**) and $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**).

Complexes	$2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$	$2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$
Chemical formula	$C_8H_{19}BClNO_5$	$C_8H_{18}BCl_2NO_5$
Fw (g/mol)	255.50	289.94
T (K)	103.0 (2)	153.0 (2)
Wavelength (Å)	0.71073	0.71073
cryst syst	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$
a, (Å)	10.312 (2)	8.616 (1)
b, (Å)	12.187 (2)	11.914 (2)
c, (Å)	10.604 (2)	13.693 (2)
α, (deg)	90	90
β, (deg)	100.686(6)	99.807(3)
γ, (deg)	90	90
V, (Å^3)	1309.6(4)	1385.1(3)
Z	4	4
D calc, (g/cm^3)	1.296	1.390
μ (mm^{-1})	0.296	0.476
F(000)	544.0	608.0
2θ range, (deg)	6.06-62.16	5.90-55.00
reflns collected	21063	13711
indep reflns/R_{int}	4181/0.1584	3186/0.0703
Data/restraints/parameters	4181/0/145	3186/694/313
GOF on F^2	0.983	0.907
Coverage of independent reflections	99.1%	99.9%
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
R_1,wR_2 [I>2σ(I)] [a]	0.0842, 0.1926	0.0557, 0.1271
R_1,wR_2(all data) [a]	0.1320, 0.2281	0.1074, 0.1465
Largest diff. peak/hole (eÅ^{-3})	0.69/-0.64	0.467/-0.467

[a] $R1 = \sum ||F_o|-|F_c|| / \sum |F_o|$; $wR_2 = \{\sum [w(F_o^2-F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

Table S3. Bond lengths (Å) and bond angles ( ) of $2NH_3BH_2OOCCH_2Cl$ $C_{12}H_{24}O_6$ (**1**).

Bond lengths (Å)		Bond angles ( )	
B(1)-N(1)	1.581(3)	O(1)-B(1)-N(1)	102.66(5)
B(1)-O(1)	1.505(3)	C(1)-C(2)-Cl(1)	117.5(2)
C(1)-C(2)	1.505(4)	O(2)-C(1)-O(1)	125.5(3)
C(2)-Cl(1)	1.779(3)	O(2)-C(1)-C(2)	116.9(2)
C(2)-O(1)	1.303(3)	O(1)-C(1)-C(2)	117.5(2)
C(1)-O(2)	1.217(3)	C(1)-O(1)-B(1)	118.1(2)

Table S4. Bond lengths (Å) and bond angles ( ) of $2NH_3BH_2OOCCHCl_2$ $C_{12}H_{24}O_6$ (**2**).

Bond lengths (Å)		Bond angles ( )	
B(1)-N(1)	1.590(7)	O(1)-B(1)-N(1)	109.1(5)
B(1)-O(1)	1.513(7)	C(1)-C(2)-Cl(2)	109.0(6)
C(1)-C(2)	1.536(9)	C(1)-C(2)-Cl(1)	110.1(5)
C(2)-Cl(2)	1.724(7)	Cl(2)-C(2)-Cl(1)	113.2(4)
C(2)-Cl(1)	1.750(7)	O(2)-C(1)-O(1)	126.9(7)
C(1)-O(2)	1.205(9)	O(2)-C(1)-C(2)	123.6(7)
C(1)-O(1)	1.304(8)	O(1)-C(1)-C(2)	109.5(7)
		C(1)-O(1)-B(1)	120.2(5)

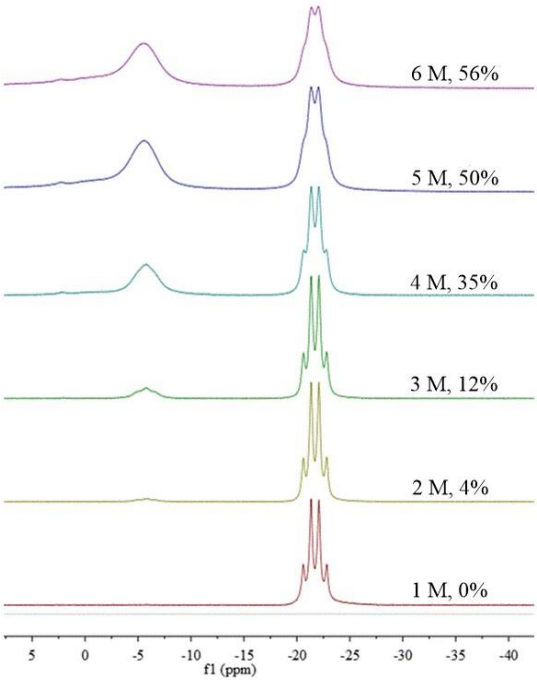

Figure S5. ^{11}B NMR spectra of the reaction mixture of AB with CH_3COOH with different concentration in 14 h (c_{AB} = 1~6 M, the conversion of AB: %).

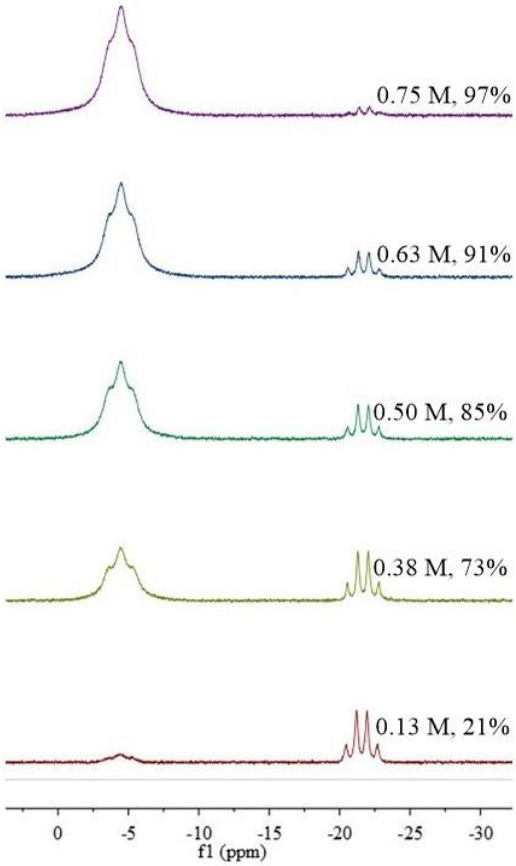

Figure S6. ^{11}B NMR spectra of the reaction mixture of AB with CCl_3COOH at a ratio of 1:1 (c_{AB} = 0.13~0.75 M, the conversion of AB: %).

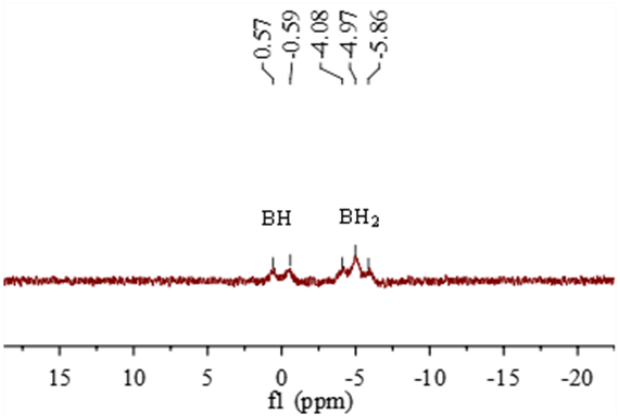

Figure S7. ^{11}B NMR spectrum of the reaction mixture of AB with excess $ClCH_2COOH$ over a period of 10 d.

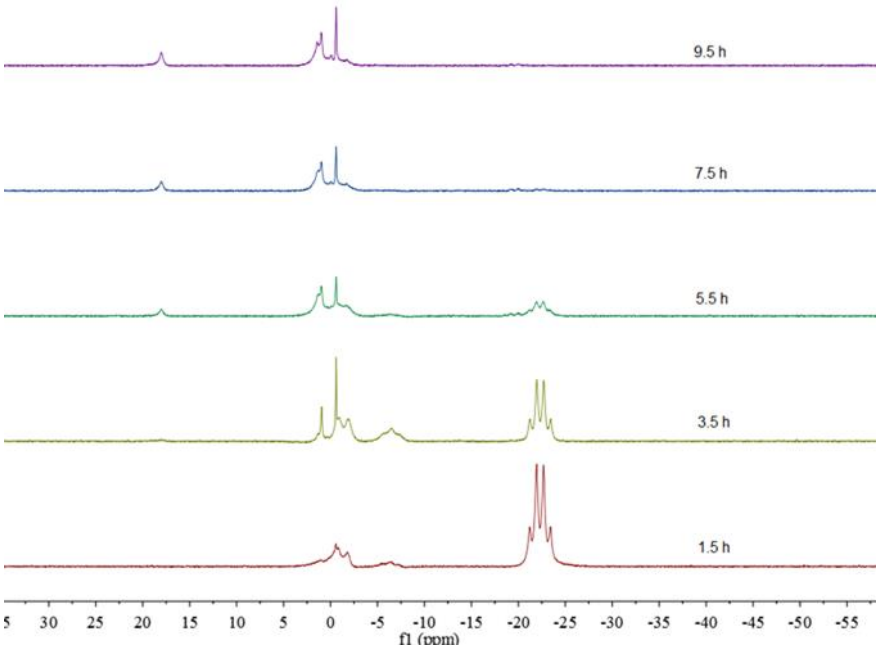

Figure S8. ^{11}B NMR spectra of the reaction of AB with CH_3COOH at 70 °C (n_{AB}: n_{acid} to 1:1, c_{AB} = 3 M).

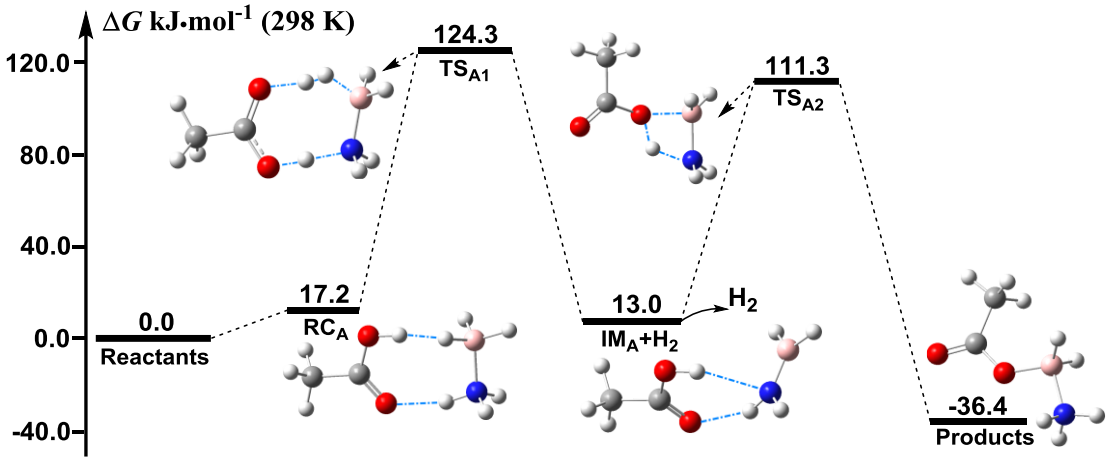

Figure S9a. Energy profile of the reaction of AB with CH_3COOH.

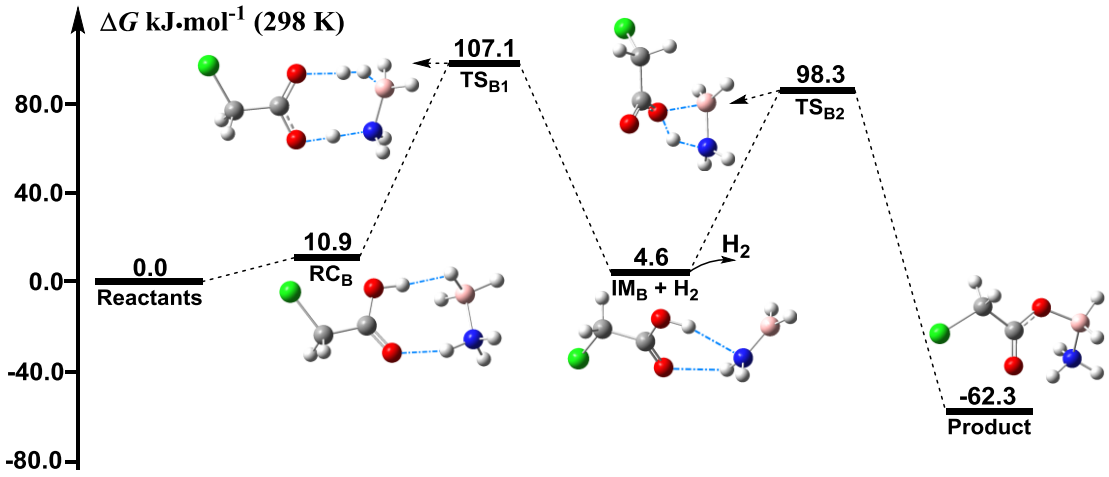

Figure S9b. Energy profile of the reaction of AB with $CH_2ClCOOH$.

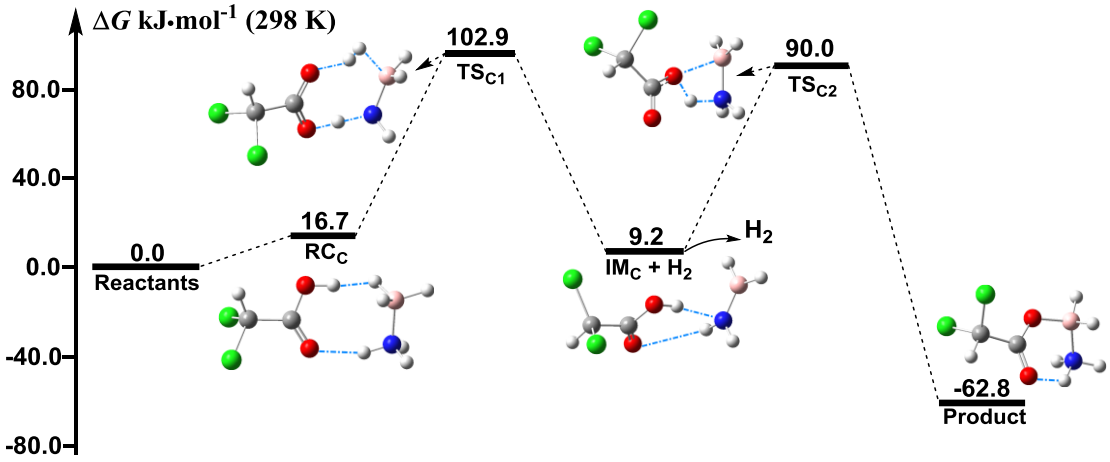

Figure S9c. Energy profile of the reaction of AB with $CHCl_2COOH$.

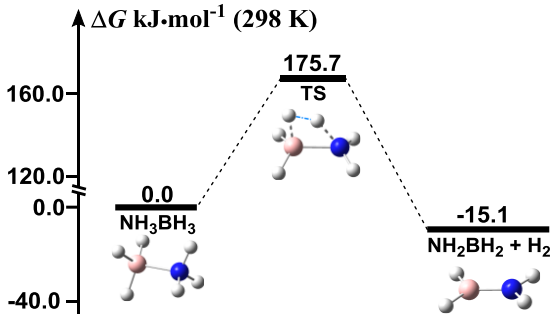

Figure S10. Energy profile of the decomposition of AB to produce hydrogen and NH_2BH_2.

Table S5. The relative energies {Δ(E+ZPE)/(kJ·mol^{-1})}, enthalpies {ΔH (298 K)/(kJ·mol^{-1})}, free energy changes {ΔG (298 K)/(kJ·mol^{-1})} and entropy {S (298 K)(J·mol^{-1})} for the reactions of AB with CH_3COOH.

Species	Δ*E*	Δ(*E* + ZPE)	Δ*H*	Δ*G*	S
AB + CH_3COOH	0.0	0.0	0.0	0.0	538.1
RC_A	-32.2	-25.9	-26.4	17.2	392.5
TS_{A1}	92.5	78.2	75.3	124.3	374.5
$IM_A + H_2$	27.2	2.1	10.0	13.0	527.6
TS_{A2}	127.2	92.5	96.2	111.3	487.0
Product	-36.8	-54.8	-50.2	-36.4	491.6

Table S6. The relative energies {Δ(E + ZPE)/(kJ·mol^{-1})}, enthalpies {ΔH (298 K)/(kJ·mol^{-1})}, free energy changes {ΔG (298 K)/(kJ·mol^{-1})} and entropy {S (298 K)(J·mol^{-1})} for the reactions of AB with $CH_2ClCOOH$.

Species	Δ*E*	Δ(*E* + ZPE)	Δ*H*	Δ*G*	S
AB + $CH_2ClCOOH$	0.0	0.0	0.0	0.0	545.2
RC_B	-32.6	-26.8	-24.7	10.9	425.9
TS_{B1}	78.7	64.4	64.0	107.1	400.4
$IM_B + H_2$	23.4	-2.5	8.0	4.6	556.1
TS_{B2}	119.2	83.7	90.8	98.3	519.7
Product	-61.9	-79.1	-72.8	-62.3	510.4

Table S7. The relative energies {Δ(E + ZPE)/(kJ·mol^{-1})}, enthalpies {ΔH (298 K)/(kJ·mol^{-1})}, free energy changes {ΔG (298 K)/(kJ·mol^{-1})} and entropy {S (298 K)(J·mol^{-1})} for the reactions of AB with $CHCl_2COOH$.

Species	Δ***E***	Δ(***E*** + ZPE)	Δ***H***	Δ***G***	S
AB + $CHCl_2COOH$	0.0	0.0	0.0	0.0	595.8
RC_C	-33.5	-27.2	-27.2	16.7	448.1
TS_{C1}	70.7	56.5	54.0	102.9	431.8
$IM_C + H_2$	23.4	-2.1	5.9	9.2	585.3
TS_{C2}	108.0	72.0	77.4	90.0	554.0
Product	-66.5	-83.3	-79.1	-62.8	541.0

Table S8. The relative energies {Δ(E + ZPE)/(kJ·mol^{-1})}, enthalpies {ΔH (298 K)/(kJ·mol-1)}, free energy changes {ΔG (298 K)/(kJ·mol^{-1})} and entropy {S (298 K) (J·mol-1)} for the reactions of AB with CCl_3COOH.

Species	Δ***E***	Δ(***E*** + ZPE)	Δ***H***	Δ***G***	S
AB + CCl_3COOH	0.0	0.0	0.0	0.0	619.2
RC_D	-34.3	-28.5	-28.5	14.6	474.0
TS_{D1}	64.0	49.4	47.3	94.6	459.8
$IM_D + H_2$	23.4	-3.4	5.4	5.4	618.0
TS_{D2}	99.6	63.6	69.0	80.3	580.7
Product	-69.5	-86.6	-82.0	-66.5	567.4

Table S9. The relative energies {Δ(E + ZPE)/(kJ·mol^{-1})}, enthalpies {ΔH (298 K)/(kJ·mol^{-1})}, free energy changes {ΔG (298 K)/(kJ·mol^{-1})} and entropy {S (298 K) (J·mol^{-1})} for the reactions of AB release hydrogen without catalyst.

Species	Δ*E*	Δ(*E* + ZPE)	Δ*H*	Δ*G*	S
AB	0.0	0.0	0.0	0.0	248.5
TS	192.5	175.3	174.9	175.7	245.2
$NH_2BH_2 + H_2$	41.4	10.5	17.6	-15.1	358.6

Table S10. The total rate constants for the reactions of AB with acids.

T/*K*	k_r	k_1	k_2	k_3	k_4
258	1.95E-20	8.70E-31	2.94E-27	1.54E-26	6.03E-25
278	1.02E-18	1.09E-29	2.55E-26	9.65E-26	3.05E-24
298	4.79E-17	1.00E-28	1.70E-25	4.83E-25	1.27E-23
318	1.84E-15	7.08E-28	9.09E-25	2.01E-24	4.47E-23
338	5.52E-14	4.02E-27	4.06E-24	7.16E-24	1.38E-22
358	1.26E-12	1.91E-26	1.56E-23	2.24E-23	3.79E-22
378	2.22E-11	7.75E-26	5.26E-23	6.29E-23	9.46E-22
398	3.05E-10	2.76E-25	1.59E-22	1.61E-22	2.18E-21

The *r* is the decomposition of AB into AoB and H_2, and the 1-4 are the reactions of AB react with CH_3COOH, $CH_2ClCOOH$, $CHCl_2COOH$ and CCl_3COOH, respectively.

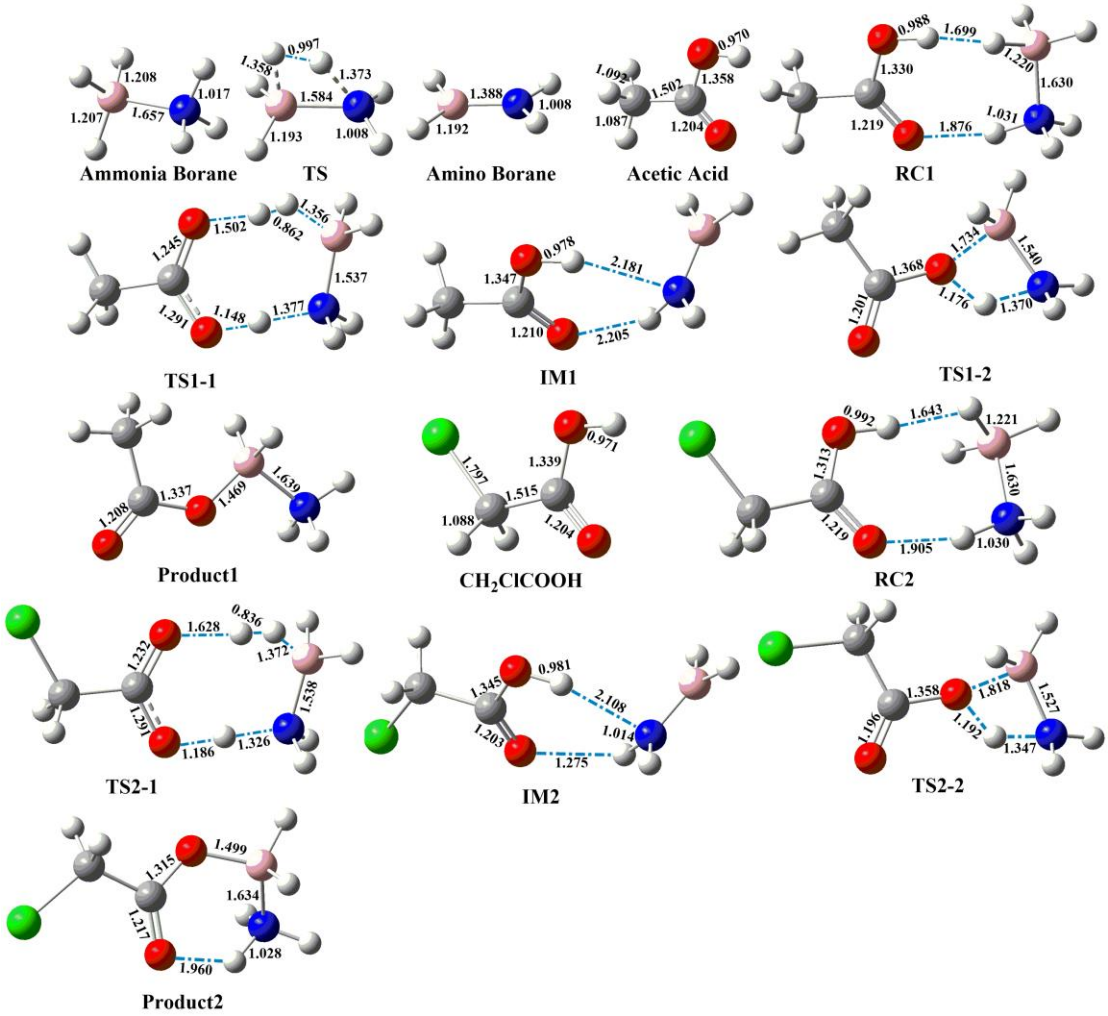

Figure S11a. The optimized geometry constructions of the reactions for AB, AB with acetic acid and AB with $CH_2ClCOOH$.

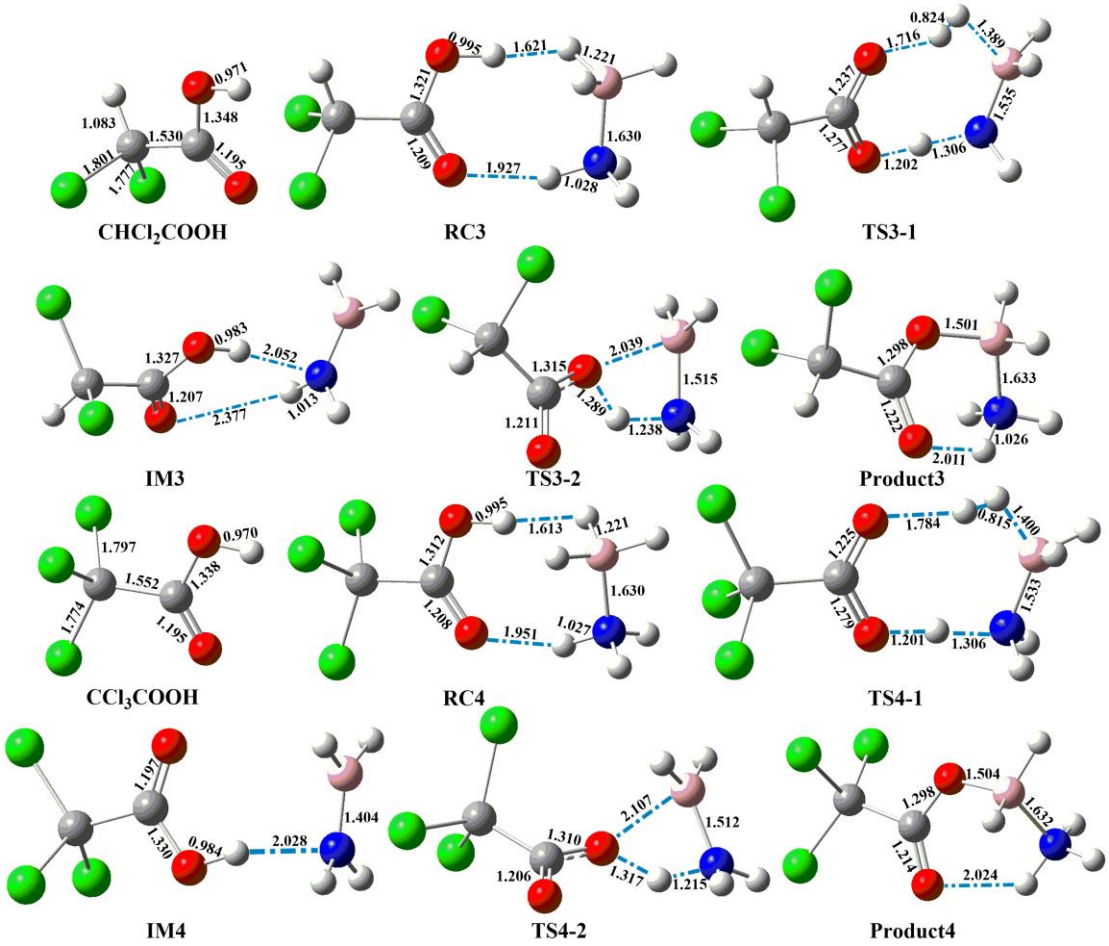

Figure S11b. The optimized geometry constructions of the reactions for AB with $CHCl_2COOH$ and AB with CCl_3COOH.

2. The optimized cartesian coordinates of all species

Ammonia Borane

N	0.72745900	0.00001600	0.00000000
H	1.09314700	-0.73111300	-0.60538100
H	1.09313000	-0.15863800	0.93587600
B	-0.92948300	0.00009900	0.00016500
H	-1.24146900	0.89752800	0.74500600
H	-1.24116700	-1.09462100	0.40439100
H	1.09300100	0.88978400	-0.33066000
H	-1.24144000	0.19645100	-1.15006000

TS

N	0.76209200	0.00000000	0.01356800
H	1.26116400	0.83823000	-0.24032500
H	1.26116400	-0.83823000	-0.24032600
B	-0.81291400	0.00000000	-0.15199500
H	-1.26869200	-1.03187000	-0.53981700
H	-1.26869200	1.03187000	-0.53981600
H	-0.13228800	0.00000000	1.05476100
H	-1.12273100	0.00000000	1.17052200

NH_2BH_2

N	0.00000000	0.00000000	0.61065500
H	0.00000000	0.84353800	1.16284600
H	0.00000000	-0.84353800	1.16284600
B	0.00000000	0.00000000	-0.77775100
H	0.00000000	-1.04237500	-1.35576100
H	0.00000000	1.04237500	-1.35576100

CH_3COOH

C	-0.08853400	0.12698900	-0.00000500
O	-0.62190700	1.20624200	-0.00000100
O	-0.79628700	-1.03164100	-0.00000700
H	-1.73486500	-0.78603300	0.00005200
C	1.39216500	-0.12774300	-0.00000200
H	1.66707300	-0.71260100	0.87978300
H	1.66702700	-0.71310300	-0.87946400
H	1.92453300	0.81945000	-0.00026600

RC1

N	2.68138300	-0.78397500	0.10922600
H	1.73157100	-1.12874800	-0.03357400
H	2.95418200	-1.00655000	1.06361000
B	2.75987200	0.83795100	-0.17438200
H	3.88809600	1.17018300	0.08602300
H	1.95409600	1.33679400	0.58637500
H	3.30298300	-1.28965000	-0.51693600
H	2.46512400	0.97681400	-1.33530500
C	-1.55343500	0.19222000	0.02000500
O	-1.94386200	1.32639200	0.09358700
O	-0.23372500	-0.12923400	0.03787200
H	0.29703900	0.69266200	0.10351500
C	-2.42272900	-1.02975300	-0.10227200
H	-2.20523800	-1.54613700	-1.03958000
H	-2.21083000	-1.72411200	0.71300800
H	-3.46838300	-0.73525100	-0.07788300

TS1-1

N	-2.01671600	-0.78732300	0.01456500
H	-0.65027100	-0.94633200	-0.05594100
H	-2.44975200	-1.26564200	-0.76978600
B	-2.41464200	0.69436900	0.11322100
H	-3.39657700	1.02419700	-0.49288100
H	-1.64260000	1.42640700	-0.72822100
H	-2.30287400	-1.28600900	0.85152100
H	-2.30817300	1.14565100	1.21370400
C	1.12027300	0.05749900	-0.02427400
O	0.49138500	-1.06805000	-0.08232000
O	0.56539900	1.17230000	-0.03963900
H	-0.91101000	1.26396400	-0.30158300
C	2.61966200	-0.04160500	0.07248600
H	3.07044800	0.94737900	0.05136700
H	2.88669900	-0.55094900	1.00073500
H	3.00045100	-0.64860400	-0.75057500

IM1

N	2.25236600	0.34993000	-0.39747200
H	0.41929300	-0.82663600	-0.29692400
H	2.45821900	0.36961800	-1.38591100
B	3.06260200	-0.32029100	0.51741200
H	3.96946100	-0.97970900	0.11369300
H	1.50746800	0.98589900	-0.13231500
H	2.80904100	-0.23679700	1.67853100
C	-1.21392600	0.08746300	0.00314800
O	-0.53125400	-1.04903800	-0.23675000
O	-0.67732200	1.16821400	0.09936300
C	-2.69028900	-0.15763100	0.13349500
H	-3.20565300	0.78551800	0.29329700
H	-3.06657100	-0.64595600	-0.76721100
H	-2.87693100	-0.83239600	0.97131900

TS1-2

N	2.31230500	-0.37445500	0.15100800
H	1.09813500	-0.74144000	-0.36750800
H	3.10640100	-0.41364500	-0.47520800
B	1.46954200	0.91503400	0.15500700
H	1.78389500	1.74571100	-0.63802300
H	2.55746200	-0.77574300	1.04712600
H	1.06996400	1.25253300	1.22821700
C	-1.03883200	-0.26316600	-0.07168100
O	0.20315900	-0.01037900	-0.58539200
O	-1.39773700	-1.38612100	0.15679300
C	-1.86493200	0.97732000	0.12226600
H	-2.85342100	0.70637100	0.48425100
H	-1.37271700	1.64026600	0.83658100
H	-1.94436100	1.51904200	-0.82225500

Product1

N	2.57372300	-0.23754100	0.00031800
H	2.59194100	-0.83992200	0.82198000
H	2.59273900	-0.84001000	-0.82125200
B	1.20619900	0.66505700	-0.00021500
H	1.24822200	1.32264900	-1.01365000
H	3.40921900	0.34274600	0.00067500
H	1.24741000	1.32244100	1.01337800
C	-1.12698300	-0.25498000	0.00004500
O	0.20148800	-0.40698800	-0.00070200

O	-1.85588800	-1.21885900	0.00019200
C	-1.64285200	1.16737100	0.00014200
H	-2.72981000	1.15637600	-0.00007900
H	-1.27650400	1.70259800	0.87911700
H	-1.27606600	1.70306200	-0.87836300

$CH_2ClCOOH$

C	-1.04471400	-0.06543500	0.00035600
O	-2.10561900	-0.63491400	-0.00869500
O	-0.90992900	1.26709400	0.00521400
H	-1.80579800	1.64144000	-0.00025800
C	0.25126600	-0.84951300	0.01034700
H	0.25762300	-1.47205300	0.90246700
H	0.25566900	-1.49782600	-0.86298300
Cl	1.77515100	0.10357000	-0.00444700

RC2

N	3.41598700	0.45999000	-0.10153800
H	2.51092500	0.94981900	-0.08230200
H	3.85944800	0.64219100	-0.99844100
B	3.16998800	-1.13300800	0.13890900
H	4.22655500	-1.69549300	0.01778700
H	2.39768300	-1.47732700	-0.74131200
H	4.01296100	0.85292200	0.62161600
H	2.69584600	-1.23651000	1.24483300
C	-0.24025900	0.38794900	0.01321000
O	0.62831500	1.24057400	-0.05488800
O	-0.04019200	-0.90954300	-0.01861500
H	0.92681300	-1.11295300	-0.10700800
C	-1.68013200	0.82976900	0.18317000
H	-1.79508100	1.20859800	1.19797100
H	-1.86953400	1.64184600	-0.51344800
Cl	-2.93588800	-0.42838400	-0.07139600

TS2-1

N	-3.04958800	-0.47787600	0.01949600
H	-1.79763000	-0.91035000	-0.04256800
H	-3.56916900	-0.85509100	-0.76797100
B	-3.13662600	1.05336500	0.12750700
H	-4.03697100	1.58103900	-0.46115900
H	-2.27513800	1.62439400	-0.77550400
H	-3.43726100	-0.90692500	0.85496600
H	-2.90888900	1.47496200	1.21834300
C	0.17788800	-0.32007100	-0.03543200
O	-0.67373000	-1.28948400	-0.07042200
O	-0.09638000	0.88115100	-0.05924000
H	-1.63775500	1.34002000	-0.31511500
C	1.60843100	-0.82873800	0.04901500
H	1.72868900	-1.38762700	0.97498900
H	1.79687900	-1.50024400	-0.78564200
Cl	2.85943800	0.45750900	0.01655600

IM2

N	-3.14198700	-0.52084700	-0.39319700
H	-1.56163800	0.86444800	-0.22906000
H	-3.38589600	-0.45539800	-1.37126500
B	-3.99599800	-0.07458300	0.61704700
H	-4.98334400	0.52033900	0.31738600
H	-2.33420800	-1.11006300	-0.22429200
H	-3.69485900	-0.27415400	1.75169100

C	0.22439900	0.24276900	-0.08214300
O	-0.66150600	1.25046100	-0.17211500
O	-0.07087700	-0.92301100	-0.09338300
C	1.62255200	0.81801700	0.03679300
H	1.81911100	1.46597900	-0.81528300
H	1.68517100	1.41590500	0.94453400
Cl	2.89452500	-0.43485500	0.09938300

TS2-2

N	3.19229900	0.16482900	-0.33921800
H	2.12281100	0.60975500	0.34734300
H	3.33799700	0.61057300	-1.23632200
B	2.26361300	-1.04632800	-0.28711700
H	1.66180100	-1.28271300	-1.28718600
H	4.06174700	0.11688600	0.17671400
H	2.57196700	-1.92016700	0.45567700
C	-0.05622700	0.45458800	0.26779200
O	1.15371000	0.00880200	0.69302800
O	-0.25663200	1.58806700	-0.05853600
C	-1.07350700	-0.66966200	0.30983000
H	-0.73104000	-1.48903600	-0.31978000
H	-1.15887700	-1.03346600	1.33245000
Cl	-2.70169300	-0.17755900	-0.24708500

Product2

N	2.81244400	0.77713600	0.33213300
H	2.05994400	1.40531100	0.02177400
H	3.70771400	1.09986500	-0.02545800
B	2.43971300	-0.69368700	-0.27381700
H	2.54971600	-0.58162700	-1.46705800
H	2.84938200	0.79133300	1.34925700
H	3.16706100	-1.49954700	0.23668100
C	0.04960300	-0.13530000	-0.11141200
O	1.02550400	-0.98321500	0.13009200
O	0.18612800	1.03470300	-0.41816000
C	-1.29467600	-0.82791500	0.04393600
H	-1.43851900	-1.50226000	-0.79925600
H	-1.30208300	-1.41317300	0.95983100
Cl	-2.68832400	0.29976300	0.08692800

$CHCl_2COOH$

C	1.14646000	-0.32213100	0.07149500
O	1.35268800	-0.93432400	1.07672800
O	2.10371800	0.15305400	-0.75034600
H	2.96259600	-0.06400200	-0.35300400
C	-0.22738300	0.06251700	-0.48000300
H	-0.19082600	0.20967300	-1.55263300
Cl	-1.43230100	-1.19810900	-0.13863800
Cl	-0.68166800	1.64882500	0.24132200

RC3

N	-3.57885700	0.42165000	-0.88448500
H	-4.04929600	1.31995600	-0.96000900
H	-3.91900900	-0.16755800	-1.64056500
B	-3.83740200	-0.25661100	0.57424500
H	-5.01064200	-0.50300900	0.66900600
H	-3.44820100	0.54281600	1.39135100
H	-2.57048000	0.56909500	-1.01993200
H	-3.18424900	-1.28835800	0.57133100
C	-0.14315400	-0.08234700	0.26151200

O	-0.67699300	0.44740400	-0.68466000
O	-0.74679600	-0.74426900	1.23183000
H	-1.72791800	-0.78257100	1.07313700
C	1.37101400	-0.08872700	0.48297700
H	1.61385300	-0.34811800	1.50583400
Cl	2.07679200	-1.37207600	-0.56145900
Cl	2.07368400	1.51270000	0.14297200

TS3-1

N	-3.15730900	0.18827600	-0.95404300
H	-3.34255700	1.12459500	-1.30268300
H	-3.48976500	-0.45907800	-1.66306800
B	-3.82559800	-0.01034700	0.41329900
H	-4.81943100	-0.67729900	0.43455700
H	-3.83074900	0.95813500	1.10557500
H	-1.85511000	0.10243300	-0.89732300
H	-3.20275100	-1.05952000	1.07713000
C	-0.21661700	-0.07938300	0.34695800
O	-0.65597900	0.04809700	-0.84505500
O	-0.88941900	-0.23557600	1.37257500
H	-2.56504900	-0.54693100	1.17066000
C	1.30477900	-0.03822900	0.52219900
H	1.55560900	-0.12707200	1.57099500
Cl	2.06548200	-1.43209100	-0.32075000
Cl	1.97058700	1.52762300	-0.05096400

IM3

N	-3.58330800	-0.46470700	0.02247800
H	-3.71575300	-1.41704300	-0.28804800
H	-3.09141000	-0.40187700	0.90610800
B	-4.28048900	0.60580000	-0.54565700
H	-4.17021600	1.68474100	-0.05559500
H	-4.93539000	0.41241700	-1.52078300
H	-1.67882600	-0.11589000	-0.65704700
C	-0.17392500	-0.12715500	0.47743900
O	-0.70234900	-0.03194900	-0.73583600
O	-0.79268500	-0.29286900	1.50085100
C	1.34636200	-0.01299000	0.49473700
H	1.68732200	-0.08846400	1.51917800
Cl	2.08648300	-1.37136500	-0.41595200
Cl	1.87325300	1.58251100	-0.13028600

TS3-2

N	3.33904700	-0.20081500	-0.37967500
H	2.23868100	-0.76751900	-0.35069200
H	3.83466400	-0.30149200	0.49851500
B	2.43626300	1.00436200	-0.54970700
H	2.20130800	1.63314100	0.42384200
H	3.91884400	-0.47831100	-1.16266200
H	2.28831900	1.41206500	-1.64910200
C	0.25716400	-0.62909100	0.58595800
O	0.99945000	-0.44032900	-0.48317800
O	0.60906500	-1.19991800	1.59447800
C	-1.17543400	-0.08973700	0.50155400
H	-1.68695000	-0.27890700	1.43629900
Cl	-1.18666000	1.68951700	0.24406100
Cl	-2.09028200	-0.94834800	-0.78555600

Product3

N	3.24741300	-0.38978300	-0.07204700

H	2.89209300	-0.43697300	0.88956400
H	4.22652500	-0.11543100	-0.06586900
B	2.34448700	0.72716100	-0.84944700
H	2.58714300	1.77123700	-0.30544000
H	3.17753400	-1.31549300	-0.49023500
H	2.61821800	0.67242800	-2.01456300
C	0.41053800	0.07679800	0.50662500
O	0.91011500	0.32650000	-0.66459900
O	1.02897300	-0.06748400	1.55110100
C	-1.11024400	-0.08314600	0.53101300
H	-1.43758900	-0.22068500	1.55323400
Cl	-1.93492800	1.37377500	-0.10556200
Cl	-1.58464300	-1.56768300	-0.37284700

CCl_3COOH

C	1.26219000	0.47181700	-0.00017600
O	1.58313100	1.62242800	-0.00026800
O	2.10725500	-0.56590600	-0.00018000
H	3.00800000	-0.20500300	-0.00022100
C	-0.21114600	-0.01715000	-0.00001400
Cl	-1.31319400	1.37311700	-0.00025400
Cl	-0.48582300	-1.00972500	-1.47204600
Cl	-0.48553400	-1.00899100	1.47259000

RC4

N	-4.02664200	-0.78887300	0.04309500
H	-3.05592500	-1.12334000	0.03584100
H	-4.52796000	-1.23870600	-0.71879700
B	-4.04466200	0.83315500	-0.11902600
H	-3.55409500	1.06853000	-1.19657300
H	-1.88296900	1.24586300	0.20232900
H	-4.45998900	-1.08635700	0.91394000
H	-5.18392700	1.20423000	-0.02064500
C	-0.44543900	0.00415600	0.06900900
O	-0.88990800	1.23570300	0.14500500
O	-1.10831600	-1.00522300	0.06242000
H	-3.37671300	1.25782000	0.81086500
C	1.10810000	-0.03303900	-0.00927700
Cl	1.63525600	0.89909800	-1.44895600
Cl	1.76627900	0.71366100	1.48651400
Cl	1.68441800	-1.70936200	-0.14057500

TS4-1

N	-3.59272200	-0.75869000	-0.03754500
H	-2.29395000	-0.86359100	0.05622100
H	-3.82622200	-1.23167300	-0.90638500
B	-4.07911200	0.69474700	-0.08060000
H	-4.00064500	1.21414100	-1.14836300
H	-2.75646900	1.37470500	0.33726300
H	-4.01011100	-1.30217700	0.71282900
H	-5.05242400	0.95979700	0.56304400
C	-0.49805600	0.15082300	0.04263500
O	-1.00661100	1.26502900	0.00628700
O	-1.09980200	-0.97486200	0.11874700
H	-3.37110100	1.44168000	0.86891500
C	1.05887400	0.01596700	-0.00461000
Cl	1.85283900	1.60553400	-0.10965400
Cl	1.60379300	-0.82067800	1.49291500
Cl	1.50465800	-0.96590700	-1.44479900

IM4

N	-4.15616100	-0.59927600	-0.00104500
H	-2.12781000	-0.57621500	0.00006700
H	-4.21889500	-1.15324100	-0.84397100
B	-4.39769000	0.78407500	0.00152100
H	-4.48739300	1.34815400	-1.04077600
H	-4.21823600	-1.15630100	0.83991400
H	-4.48617600	1.34445200	1.04593600
C	-0.45999700	0.31572900	-0.00026100
O	-0.90382200	1.42706500	-0.00115400
O	-1.17107000	-0.80800200	0.00059900
C	1.06475800	0.00722300	0.00008000
Cl	1.99761100	1.51655800	0.00019700
Cl	1.45965700	-0.94722300	1.47221700
Cl	1.45982900	-0.94712900	-1.47217500

TS4-2

N	3.70847800	0.34717100	0.18031400
H	2.61002900	0.44479200	0.69088200
H	3.95080900	1.20019200	-0.31148500
B	3.01191400	-0.74438700	-0.60004000
H	2.59569700	-0.45815800	-1.66796700
H	4.43228400	0.07962900	0.83718000
H	3.15266500	-1.85125800	-0.21247300
C	0.50741000	0.67266400	0.13881000
O	0.65943900	1.82699500	-0.17519600
O	1.42263300	-0.12142400	0.63545900
C	-0.88752000	-0.02326900	-0.00239500
Cl	-2.07852600	1.06369900	-0.75346400
Cl	-0.71294800	-1.50226800	-1.01469700
Cl	-1.45184000	-0.48286500	1.64470700

Product4

N	3.52275200	0.49402300	0.29719500
H	3.51316100	0.45935300	1.31491200
H	2.98809500	1.31462800	-0.00755000
B	2.82317700	-0.81102400	-0.38913900
H	2.97742800	-0.67494600	-1.57269400
H	4.48855200	0.58122800	-0.00921700
H	3.31890900	-1.78877400	0.09292800
C	0.64301000	0.28794400	-0.21936300
O	1.03211900	1.39716600	-0.52230000
O	1.36776600	-0.76827900	-0.01278500
C	-0.87468700	0.00391600	0.00781300
Cl	-1.85000500	1.45100700	-0.33485700
Cl	-1.39215500	-1.33533900	-1.06768500
Cl	-1.10315200	-0.47312600	1.73177400