Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary information for

Metal-Free, Polyether-Mediated H_2-Releases from Ammonia Borane: Roles of Hydrogen Bonding Interactions on Dehydrogenation

Yongmin Kim,[a] Hyunjae Baek,[a] Jin Hee Lee,[a] Shinyoung Yeo,[a] Kibum Kim,[a] Son-Jong Hwang,[b] Bit Eun,[a] Suk Woo Nam,[a,c] Tae-Hoon Lim,[a,c] and Chang Won Yoon*[a,d]

[a] Fuel Cell Research Center, Korea Institute of Science and Technology, 39-1 Hawolgok-dong, Sungbuk-gu, Seoul 136-791, Republic of Korea

[b] Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, United States.

[c] Green School, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 136-791, Republic of Korea.

[d] Department of Clean Energy and Chemical Engineering, University of Science and Technology, Daejeon, Republic of Korea

Contents

Table S1 Detailed amounts of reagents for Figure 1. In all cases, 0.12 g of AB (4.0 mmol) was employed with various amounts of promoters.

AB:promoter (mmol)		4.0:0.5	4.0:1.0	4.0:2.3
promoter (g)	EGDE	0.045	0.090	0.21
	DEGDE	0.067	0.13	0.31
	T3EGDE	0.089	0.18	0.41
	T4EGDE	0.11	0.22	0.51

Table S2 Detailed amounts of reagents for Figure 4 and Figure S3. In all cases, 0.12 g of AB (4.0 mmol) was employed with various amounts of promoters.

AB:promoter (mmol)		4.0:1.0	4.0:2.0	4.0:3.0	4.0:4.0	4.0:5.0	4.0:6.0	4.0:7.0	4.0:8.0
Promoter/AB (molar ratio)		0.25	0.5	0.75	1	1.25	1.5	1.75	2
Solvent (g)	EGDE	0.090	0.18	0.27	0.36	0.45	0.54	0.63	0.72
	DEGDE	0.13	0.27	0.40	0.54	0.67	0.80	0.94	1.1
	T3EGDE	0.18	0.36	0.53	0.71	0.89	1.0	1.2	1.4
	T4EGDE	0.22	0.44	0.67	0.89	1.1	1.3	1.6	1.8

Table S3 Calculated stabilization energies for AB·L (L = promoter).

Reactions					Stablization Energy (ΔE, kcal/mol)
AB	+	T4EGDE	→	AB·T4EGDE (**1**)	-23.5
AB	+	T3EGDE	→	AB·T3EGDE (**2**)	-19.0
AB	+	DEGDE	→	AB·DEGDE (**3**)	-15.9

Table S4 Computed energies of the DFT-optimized geometries in Figure 9.

	Energy (in Hartree)	Relative Energy (in kcal/mol)
NH_3	-56.35931382	-
2AB	-165.7240037	0.0
TS1	-165.7010630	14.4
4 + NH_3	-165.7079138	10.1
TS2	-165.6742325	31.2
DADB	-165.7258196	-1.1
T4EGDE	-767.8133821	-
2AB + T4EGDE	-933.5373858	0.0
1 + AB	-933.5748512	-23.5
TS3	-933.5527244	-9.6
5 + NH_3	-933.5661071	-18.0
TS4	-933.5305927	4.3
DADB-T4EGDE	-933.5676417	-19.0

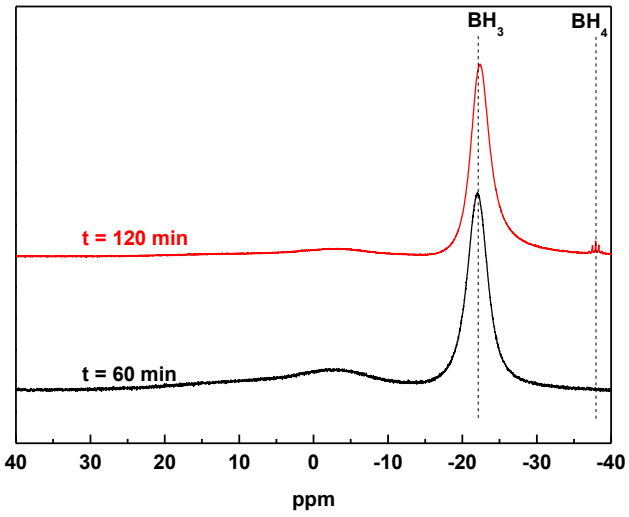
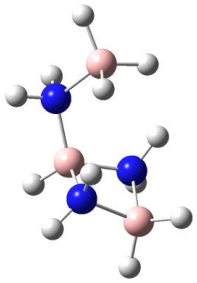
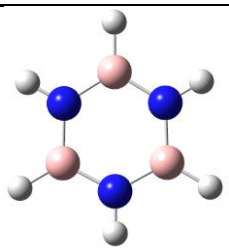


Fig. S1 ^{11}B NMR spectra of the reaction residues following the dehydrogenations of neat AB (0.12 g, 4.0 mmol) at 85 ^{o}C with time. The NMR spectra were obtained by dissolving the residues in T4EGDE (0.5 g).



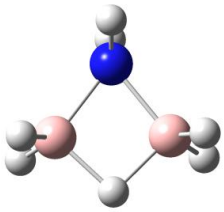
***DFT-optimized* geometry of BCDB**

	Observed wave number (cm^{-1})	Calculated wave number (cm^{-1})
N-H(cm^{-1})	~3300	3355, 3477
B-H(cm^{-1})	~2300	2326, 2343, 2401, 2446, 2461, 2508



DFT-optimized geometry of Borazine

	Observed wave number (cm^{-1})	Calculated wave number (cm^{-1})
N-H(cm^{-1})	~3500	3515
B-H(cm^{-1})	~2500	2541
N-B (cm^{-1})	~1500	1431



***DFT-optimized* geometry of μ-aminodiborane**

	Observed wave number (cm^{-1})	Calculated wave number (cm^{-1})
N-H(cm^{-1})	~3500	3444 (weak) 3528 (weak)
B-H (cm^{-1})	~1600 ~2550 ~2580	1681 2485 2575

Fig. S2 Comparison of the observed IR frequencies with the calculated ones of borazine, BCDB, and μ-aminodiborane (atom colors: pink, boron; blue, nitrogen; gray, hydrogen). The calculated IR frequencies were scaled.

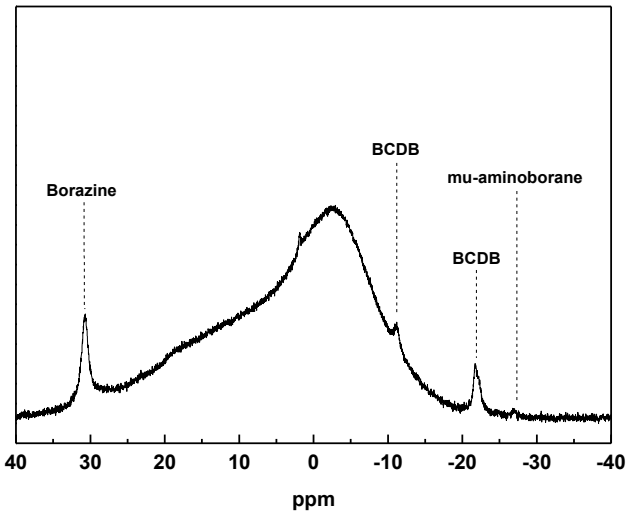


Fig. S3 $^{11}B\{^{1}H\}$ NMR spectrum of the gaseous by-products following the dehydrogenation of AB (0.123 g) with T4EGDE (0.05 g) at 85 ^{o}C for 3 hours. The gaseous by-products were trapped in the T4EGDE solvent (0.5 g) before conducting ^{11}B NMR spectroscopy.

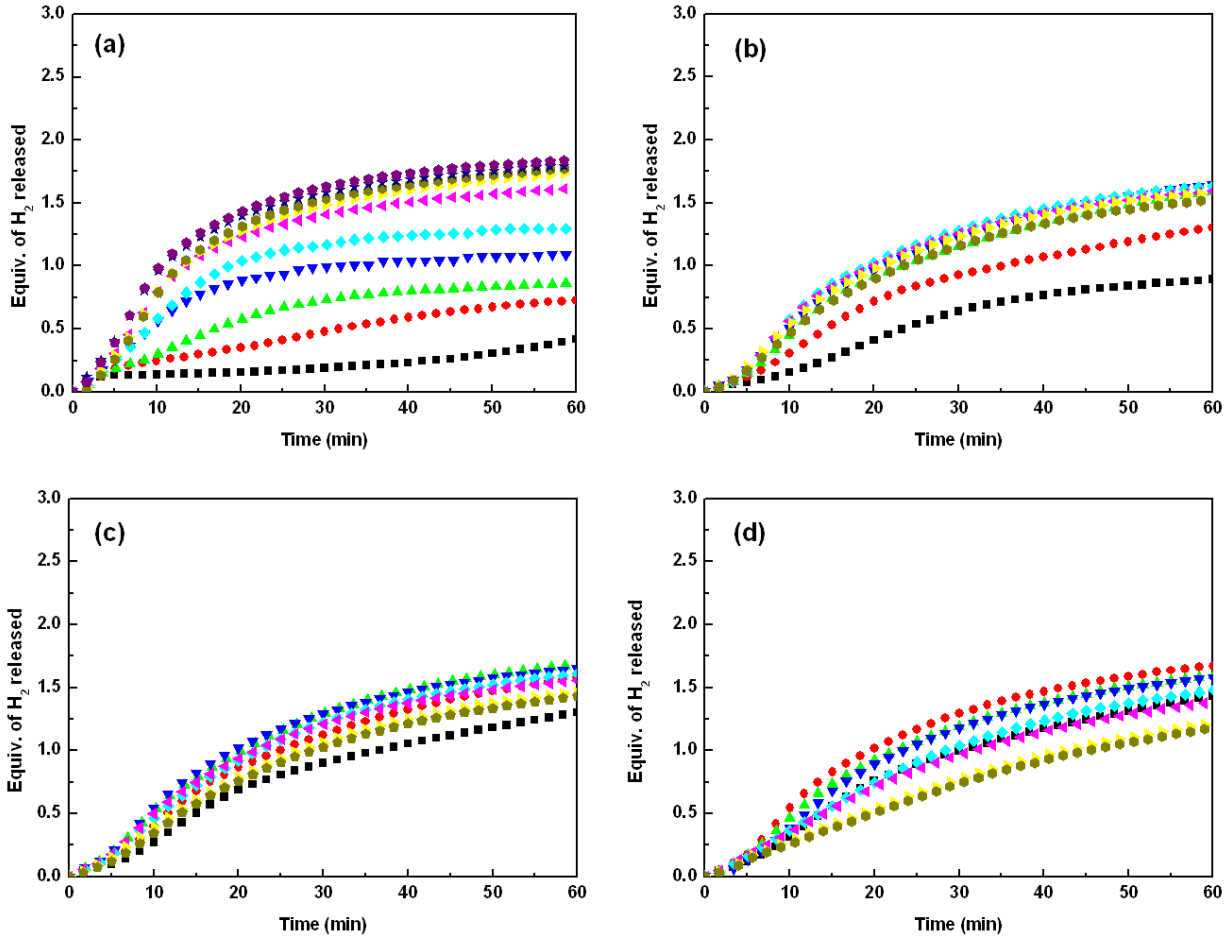


Fig. S4 H_2-releases from AB at 85 °C in the presence of different amounts of various solvents with respect to 4.0 mmol of AB, (a) EGDE, (b) DEGDE, (c) T3EGDE and (d) T4EGDE; (■) 1 mmol, (●) 2 mmol, (▲) 3 mmol, (▼) 4 mmol, (◆) 5 mmol, (◀) 6 mmol, (▶) 7 mmol, and (⬢) 8 mmol.

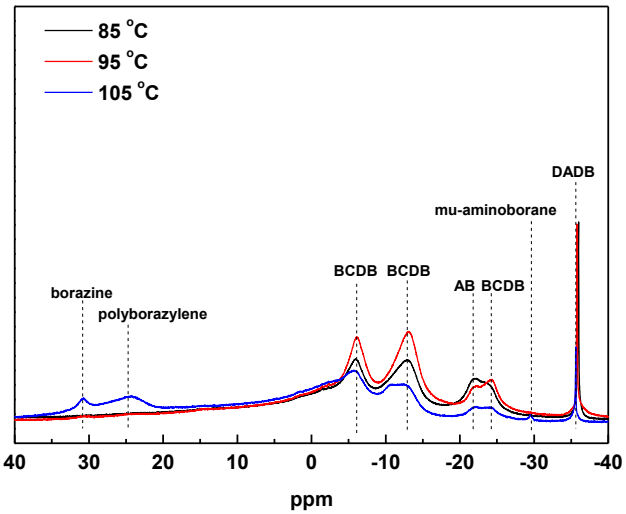
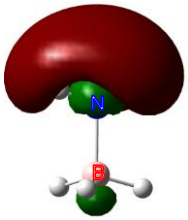


Fig. S5 The product distribution after the dehydrogenation of AB (0.12 g, 4.0 mmol) in the presence of T4EGDE (0.050 g, 0.23 mmol) upon increasing the temperatures from 85 °C to 105 °C, as characterized by $^{11}B\{^{1}H\}$ NMR spectroscopy. The NMR spectra were obtained by dissolving the residues in T4EGDE (0.5 g).

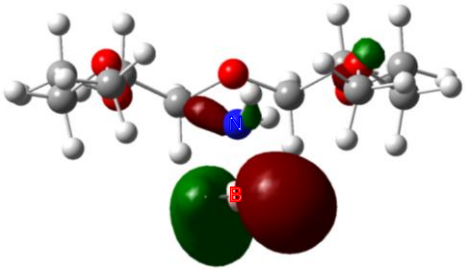
The calculated HOMOs and LUMOs of AB and **1**.

(a) AB

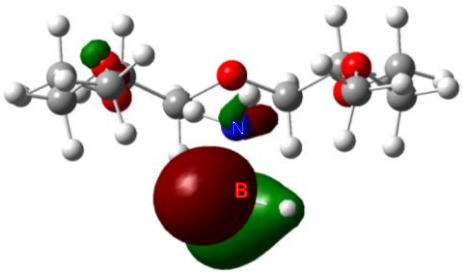


LUMO

(b) AB•T4EGDE (**1**)



HOMO



HOMO-1

Fig. S6 The calculated HOMOs and LUMOs of AB and **1**.

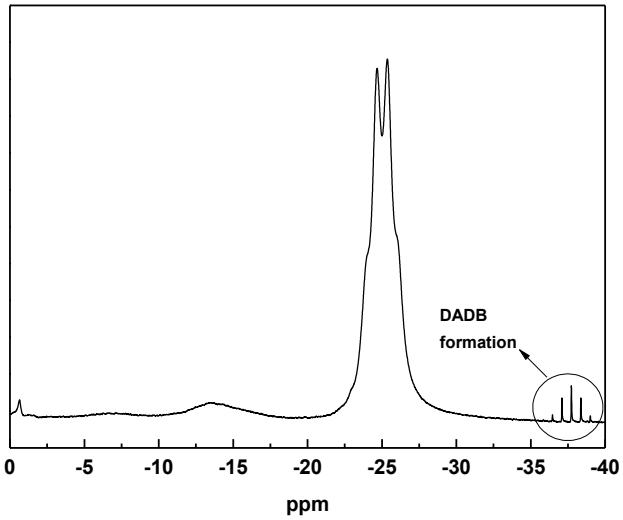


Fig. S7 ^{11}B NMR Spectrum of spent-fuels following the dehydrogenations of AB (1.2 g) at 25 ^{o}C in the presence of T4EGDE (AB:T4EGDE=4:2, mmol) after 11 days. The formation of DADB (-36 ppm) was confirmed in the NMR spectra.

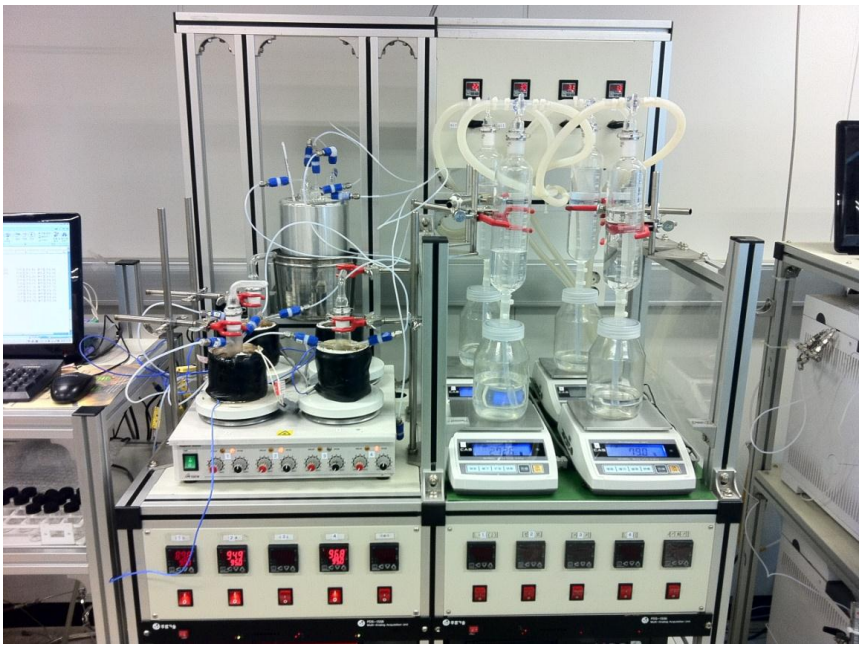


Fig. S8 An experimental setup for H_2 measurement.

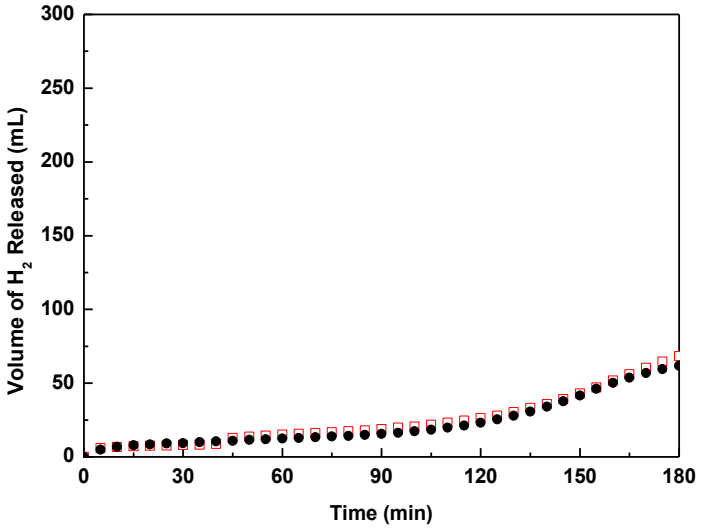


Fig. S9 H_2-releases from AB (0.12 g) at 85 ^oC with and without the added H_2O: □ H_2O (0.005 g), ● pristine AB.

Cartertian coordinates for the DFT-optimized geometries:

AB

B	-0.93800300	0.00040200	0.00009300
H	-1.24574600	-0.35545100	1.11682500
H	-1.24529000	-0.78988100	-0.86562600
H	-1.24598300	1.14490800	-0.25075300
N	0.73307600	0.00016400	0.00018400
H	1.09607300	-0.93033300	0.20048200
H	1.10190900	0.63831200	0.70331000
H	1.09751700	0.28928600	-0.90599500

NH3

N	0.00000000	0.00000000	0.10817100
H	0.00000000	0.94937700	-0.25239900
H	-0.82218500	-0.47468900	-0.25239900
H	0.82218500	-0.47468900	-0.25239900

AB·T4EGDE (**1**)

C	2.37834700	-2.23357300	0.07996600
H	3.27659500	-2.84840800	-0.09924500
H	2.18431200	-2.20301500	1.16188900
C	1.19502500	-2.86927400	-0.62115900
H	1.19034200	-3.94977700	-0.40289200
H	1.28264500	-2.73546400	-1.71047500
O	-0.00069800	-2.27516500	-0.13814400
O	2.57713300	-0.92062200	-0.42543400
C	-1.19191700	-2.86728000	-0.63400300
H	-1.18839500	-3.94911700	-0.42233900
H	-1.27117700	-2.72694300	-1.72315200
C	-2.38119000	-2.23716600	0.06205800
H	-3.27823700	-2.84943100	-0.13141600
H	-2.19731300	-2.21755200	1.14605600
C	3.55441600	-0.19041900	0.30316000
H	4.52326200	-0.71737800	0.27533000
H	3.24605300	-0.08326200	1.35357600
C	3.73694100	1.17499400	-0.32538500
H	4.62234800	1.65508500	0.12230400
H	3.90987000	1.06941500	-1.40782900
O	-2.57426600	-0.91915800	-0.43207200
O	2.58581700	1.97475600	-0.08995300
C	-3.55966100	-0.19650700	0.29286600
H	-4.52742500	-0.72451500	0.25105900
H	-3.26205900	-0.09785200	1.34727100
C	-3.73813200	1.17418400	-0.32535700
H	-4.62868200	1.64881300	0.11793900
H	-3.90043300	1.07790600	-1.41030700
C	2.69471500	3.28067700	-0.62968700
H	2.80869500	3.25325800	-1.72369500
H	1.77497500	3.81212100	-0.37655300
H	3.54966500	3.82026700	-0.19562500
O	-2.59074600	1.97345800	-0.07141700
C	-2.69776200	3.28547400	-0.59670400
H	-1.78138200	3.81565900	-0.32922000

H	-2.80227800	3.27073900	-1.69189900
H	-3.55757000	3.81808800	-0.16364700
N	0.00098800	0.60478800	0.93227600
H	0.82738300	1.11253200	0.60759300
H	-0.83092600	1.11092400	0.61952100
H	-0.00164600	-0.29686400	0.44825600
B	0.01183200	0.40629800	2.54766100
H	-0.99556300	-0.22127200	2.83201200
H	1.02370000	-0.22000700	2.81910600
H	0.01457700	1.51822500	3.04377100

AB·T3EGDE (**2**)

C	-0.58037600	2.55768700	-0.15290600
H	-0.51036200	2.64589500	-1.24776000
H	-1.05983000	3.46971100	0.23878500
C	0.80775400	2.44140900	0.44285700
H	1.32896200	3.40573500	0.32138700
H	0.73265100	2.22512000	1.51963000
C	2.81744600	1.18823300	0.30856100
H	3.42880200	2.10124400	0.21361800
H	2.75649600	0.92301500	1.37500500
C	3.49493000	0.06949200	-0.45589900
H	4.55693900	0.03591200	-0.16349100
H	3.44012400	0.26696500	-1.53782300
C	-2.67367300	1.43519100	-0.30719900
H	-3.22736200	2.27443200	0.14373600
H	-2.66028700	1.57329400	-1.39876400
C	-3.38049500	0.13790400	0.03016800
H	-4.46342400	0.28326500	-0.11974400
H	-3.20956500	-0.12196800	1.08552600
C	-3.57693600	-2.13707200	-0.58082000
H	-3.17960600	-2.85656700	-1.30039400
H	-3.38572000	-2.49747300	0.43821600
H	-4.66158900	-2.03770400	-0.73903800
C	3.49567300	-2.28495900	-0.76387600
H	2.95088900	-3.17430000	-0.44144600
H	3.45625300	-2.20853500	-1.86044900
H	4.54556300	-2.37303500	-0.44881600
O	-2.91263800	-0.90027400	-0.82002200
O	2.87124000	-1.16841000	-0.14685700
O	1.51933900	1.40921200	-0.22314300
O	-1.34376600	1.41431700	0.20193300
H	-0.39283300	-0.34947000	0.59248600
H	-0.62740900	-1.71047500	-0.24248400
H	0.89069800	-1.33098200	0.30253600
H	-1.60834300	-2.05755000	2.12255300
H	-0.06770700	-3.30206000	1.72014900

H	0.24400200	-1.61497000	2.79558000
B	-0.40956900	-2.15004900	1.92026200
N	-0.10412100	-1.32932900	0.54415400

AB·DEGDE (**3**)

C	-2.38429200	-1.14888500	-0.01787800
H	-2.31687400	-1.81464000	-0.89216000
C	-1.18771300	-1.35889200	0.88581900
H	-1.19199400	-0.61441500	1.69486400
H	-1.25762300	-2.36381500	1.33510600
O	-0.00022500	-1.24507800	0.11326900
C	1.18737800	-1.35927300	0.88561400
H	1.25710400	-2.36426400	1.33477500
H	1.19199200	-0.61485600	1.69470600
C	2.38383500	-1.14942900	-0.01827800
H	2.31614700	-1.81508300	-0.89261900
O	-2.43135900	0.20835500	-0.44221500
H	-3.30116500	-1.39768300	0.53998200
O	2.43106000	0.20784700	-0.44245400
H	3.30075500	-1.39845700	0.53940300
B	0.00177200	2.47762900	1.68479000
H	1.01498200	3.13224000	1.83442500
H	0.00159500	1.46393500	2.36058300
H	-1.01025000	3.13370100	1.83613800
N	0.00002500	1.98442300	0.11935900
H	0.82461800	1.41742100	-0.10268200
H	-0.00017800	2.79123200	-0.50122500
H	-0.82563800	1.41833400	-0.10099500
C	3.54576600	0.49628600	-1.27104900
H	3.49773000	1.55839900	-1.52019900
H	4.49172300	0.29512500	-0.74745500
H	3.51749600	-0.09530700	-2.19791700
C	-3.54615600	0.49686500	-1.27067000
H	-4.49206500	0.29578000	-0.74696100
H	-3.49807300	1.55896800	-1.51985500
H	-3.51803600	-0.09474700	-2.19752800

TS1 (Figure 10)

B	-0.63406000	0.52296200	0.00040100
B	2.09896600	0.80125300	-0.00035100
H	-1.08282000	1.62967200	0.00629900
H	0.92909900	1.19554200	0.00265000
H	-0.49080600	-0.06021700	-1.04064500
H	-0.48948300	-0.07029900	1.03563800
H	2.64955800	1.12384600	-1.02478800
H	2.65453300	1.12413800	1.02133300
N	2.01432600	-0.83135400	0.00003800
H	2.93937900	-1.25707600	-0.00298400
H	1.50234500	-1.15539200	0.82049800
H	1.49697700	-1.15527400	-0.81713200
H	-3.31306800	-1.18620100	-0.06002600
N	-3.04611800	-0.20751600	-0.00053900
H	-3.45692400	0.28310300	-0.78955100
H	-3.44077800	0.17916800	0.85196300

NH3BH2(μ-H)BH3 (**4**) (Figure 10)

B	-1.65107400	-0.24188000	0.00217100
B	0.39149400	0.94323300	-0.00065800
H	-1.38562700	-0.71948400	1.07961900
H	-0.86622700	0.85759000	-0.16696800
H	-2.68337200	0.36869200	-0.05123500
H	-1.39781300	-0.93012500	-0.96034100
H	0.75579800	1.53349600	-0.98157400
H	0.58674300	1.46538900	1.05992400
N	1.08600900	-0.50967600	0.00076200
H	2.09856600	-0.42889800	0.08928100
H	0.72172000	-1.06780500	0.77491600
H	0.86604700	-1.01789000	-0.85652600

TS2 (Figure 10)

B	2.66686100	-0.37963700	0.04676400
B	-0.22473600	-0.54805100	-0.07973300
H	3.67334700	-0.99018400	-0.23088900
H	1.65540500	-1.07530600	-0.20171300
H	2.57771000	0.61983700	-0.70694500
H	2.61631500	-0.01485100	1.21310600
H	-0.32732200	-1.00295700	-1.17097800
H	-0.25311800	-1.15776000	0.93501700
N	0.21244700	0.94867000	-0.01190600
H	-0.28155600	1.55322900	-0.66503000
H	0.15727100	1.34657500	0.92376500
H	1.25763900	0.91691300	-0.27636800
N	-2.36573300	-0.20758000	0.03607900
H	-2.64788400	-1.18492000	0.00090200
H	-2.83733500	0.26546800	-0.73324900
H	-2.72809800	0.17476300	0.90801800

DADB (Figure 10)

B	1.40984900	-0.00052300	-0.25690200
H	1.56314800	-0.00052600	-1.44943300
H	2.43216000	-0.00053800	0.38056200
N	0.53512700	1.28609200	0.12678000
H	0.93021500	2.10766700	-0.32939700
H	0.50394700	1.47953500	1.12787100
H	-0.47151100	1.18669200	-0.18054700
N	0.53433900	-1.28610100	0.12686200
H	0.92812500	-2.10803600	-0.32980500
H	-0.47224700	-1.18512100	-0.18038500
H	0.50307200	-1.47987900	1.12788300
B	-2.27809700	0.00027900	-0.06353300
H	-1.89386000	-0.99578700	-0.69975500
H	-1.89617400	1.00194700	-0.69239700
H	-3.48639600	-0.00132600	-0.01453000
H	-1.78549900	-0.00334800	1.06661100

TS3 (Figure 10)

B	3.56462400	-0.06934300	1.60258000
B	0.62668100	-0.18649900	2.13893700
H	3.64302100	1.05139600	2.01503900
H	1.85975800	-0.18427700	2.20226500
H	3.84507700	-0.99775300	2.30349200
H	3.25533600	-0.26317400	0.45798100
H	0.19664200	-1.26074500	2.51398600
H	0.17257800	0.75673600	2.75299500
N	0.24460500	-0.00913300	0.58371300
H	-0.76933200	0.00297700	0.44273300
H	0.60645600	0.87175900	0.20695300
H	0.61618300	-0.78063300	0.02238600
H	6.24529100	0.73991300	0.39241100
N	5.91146400	0.02491800	1.03248600
H	6.23696700	-0.87979000	0.70488100
H	6.31986700	0.19842300	1.94606000
C	-3.55251900	-1.22702000	0.22965800
H	-3.81661500	-1.34772000	-0.83213100
C	-2.67748100	-2.38093200	0.67311900
H	-2.25190400	-2.16370600	1.66376300
H	-3.29813000	-3.28974600	0.75133200
O	-1.64459600	-2.57356800	-0.28169600
C	-0.70545300	-3.56729700	0.10602000
H	-1.20618900	-4.54518100	0.20835800
H	-0.24892800	-3.30437700	1.07111300
C	0.36909100	-3.68325300	-0.95457000
H	-0.09085700	-3.82120900	-1.94598200
O	-2.85906300	-0.00225000	0.43193700
H	-4.48202600	-1.22999400	0.82209400
O	1.17680400	-2.51639800	-0.94429600
H	0.98739000	-4.56851300	-0.73308800
C	-3.58743400	1.13816600	0.00306700
H	-4.57382200	1.16067200	0.49508700
H	-3.74516200	1.10556600	-1.08605700
C	-2.83290300	2.39583000	0.38100500

H	-3.49619600	3.26402900	0.22701200
H	-2.55848700	2.35505800	1.44589700
O	-1.67135100	2.51768600	-0.42541000
C	-0.89971900	3.66788100	-0.11123000
H	-0.62073800	3.66385900	0.95311600
H	-1.48237100	4.58233900	-0.31467600
C	0.35460400	3.68722900	-0.95976600
H	0.09580800	3.53666800	-2.01987500
H	0.83318200	4.67509400	-0.85790500
O	1.24133900	2.67393500	-0.51501700
C	2.28293800	-2.58636300	-1.82768100
H	2.85798200	-1.66890400	-1.69036000
H	2.92438200	-3.44791300	-1.58919500
H	1.95436400	-2.66505100	-2.87518500
C	2.49970900	2.68613300	-1.17275700
H	3.09849700	1.89544700	-0.71788500
H	2.38696800	2.49721900	-2.25120400
H	3.00594900	3.65277000	-1.03172400

T4EGDE---NH3BH2(μ-H)BH3 (**5**) (Figure 10)

B	0.13916300	-3.02031000	2.33720500
B	-0.24347700	-0.68863100	2.32913000
H	1.32052500	-2.81428500	2.24759600
H	-0.51885800	-1.89578100	2.66791400
H	-0.20192300	-3.64106100	3.31371000
H	-0.40982900	-3.34706900	1.30649200
H	-1.30199800	-0.17979900	2.61711300
H	0.70342900	-0.27420700	2.93716100
N	-0.01852400	-0.58403600	0.76567300
H	0.02244200	0.39950900	0.47702200
H	0.85922600	-1.02299000	0.46391000
H	-0.79589200	-1.01320500	0.25035100
C	-1.22661700	3.12564600	-0.14755600
H	-1.29633100	3.23898700	-1.24001700
C	-2.40256200	2.31647000	0.35645800
H	-2.25866000	2.06651600	1.41813400
H	-3.31607800	2.92770000	0.26426400
O	-2.52096600	1.13489800	-0.42140600
C	-3.60287900	0.30627500	-0.01886200
H	-4.55978100	0.83776000	-0.15421200
H	-3.50274700	0.03354000	1.04190700
C	-3.61540100	-0.94712900	-0.86820200
H	-3.58707700	-0.68009800	-1.93631200
O	-0.01063300	2.47569900	0.20262800
H	-1.25828700	4.12821300	0.30889300
O	-2.50054800	-1.75844100	-0.53091800
H	-4.55050800	-1.49645800	-0.67311400
C	1.14128300	3.15300300	-0.28126900
H	1.16739600	4.18054100	0.11665900
H	1.11655800	3.20722100	-1.38027300
C	2.38971300	2.42486500	0.16905300
H	3.26565900	3.05325000	-0.06449000
H	2.35960100	2.26827800	1.25817600
O	2.47884900	1.18196100	-0.50894300
C	3.64525900	0.44463600	-0.17064200

H	3.69916900	0.28968900	0.91740300
H	4.54672000	0.99486400	-0.48843900
C	3.61500800	-0.89849000	-0.86932400
H	3.43064700	-0.76130600	-1.94661200
H	4.59856200	-1.38006100	-0.74578200
O	2.60503900	-1.70710900	-0.28945200
C	-2.49367100	-3.01688400	-1.19014600
H	-1.63508400	-3.57001400	-0.80633700
H	-3.41077900	-3.58087400	-0.96688600
H	-2.40403800	-2.89468600	-2.27982000
C	2.60804300	-3.05071800	-0.75364800
H	1.83061900	-3.57543700	-0.19684000
H	2.39725200	-3.09868800	-1.83247000
H	3.57832100	-3.52919700	-0.55693000

TS4 (Figure 10)

B	0.00071100	4.52727700	0.59986100
B	0.00028500	1.81919700	1.83889300
H	-1.01673500	5.18741500	0.71325100
H	0.00110700	3.64276000	1.49213400
H	1.01812800	5.18757300	0.71253400
H	0.00036200	3.94673300	-0.50374400
H	1.05326500	1.96347900	2.36400500
H	-1.05248300	1.96450500	2.36414200
N	0.00003800	1.49195200	0.31591400
H	-0.84727300	1.00202100	0.01566100
H	0.00024100	2.42879400	-0.14621600
H	0.84701600	1.00157500	0.01547500
H	-0.82062100	-0.50370000	2.97880700
N	-0.00094400	-0.37948800	2.39083400
H	0.81739800	-0.50422600	2.98055400
H	-0.00045100	-1.11396200	1.68047200
C	1.17912600	-3.29635400	-0.38471700
H	1.17961400	-3.23362900	-1.48302800
C	2.41482700	-2.60904700	0.15487700
H	2.35443300	-2.52494800	1.25217200
H	3.28846600	-3.23881300	-0.08373700
O	2.55681500	-1.33223400	-0.44095600
C	3.77492800	-0.69082700	-0.08366500
H	4.62984000	-1.33539500	-0.34757700
H	3.80535600	-0.50448100	1.00107700
C	3.90587600	0.62069000	-0.82760600
H	3.78464600	0.45402100	-1.91018600
O	-0.00011000	-2.69577100	0.13772300
H	1.21237600	-4.36080400	-0.09922000
O	2.94182400	1.53990600	-0.35208100
H	4.92180100	1.01295000	-0.65504600
C	-1.17897800	-3.29610100	-0.38583200
H	-1.21241000	-4.36070400	-0.10092100
H	-1.17870600	-3.23280400	-1.48411100
C	-2.41507200	-2.60916300	0.15332300

H	-3.28852300	-3.23879100	-0.08633900
H	-2.35545000	-2.52580700	1.25071800
O	-2.55669800	-1.33194100	-0.44173500
C	-3.77508300	-0.69085100	-0.08481600
H	-3.80627700	-0.50532900	1.00004700
H	-4.62978400	-1.33525700	-0.34979800
C	-3.90558800	0.62122600	-0.82784800
H	-3.78366100	0.45539100	-1.91047500
H	-4.92163000	1.01333300	-0.65563400
O	-2.94186000	1.54010900	-0.35101600
C	3.14587100	2.86709200	-0.84133700
H	2.37935000	3.50385900	-0.39783700
H	4.14009100	3.23357900	-0.54837700
H	3.06087800	2.89738500	-1.93730400
C	-3.14574000	2.86769700	-0.83927700
H	-2.37931500	3.50410100	-0.39509900
H	-3.06043200	2.89886500	-1.93519400
H	-4.14004100	3.23396500	-0.54630500

T4EGDE---DADB (Figure 10)

B	1.39044800	4.81453900	0.20484900
B	0.25637100	0.93198200	2.22467800
H	0.47538500	5.62989100	0.21136400
H	1.45215300	4.28338800	1.33394600
H	2.47146500	5.34364500	-0.01916800
H	1.17064600	3.94836800	-0.65203200
H	1.25486600	0.76878500	2.87979100
H	-0.69821900	1.30855400	2.85830800
N	0.53054100	1.87733700	1.00344000
H	-0.30508300	2.00572700	0.42251500
H	0.84509600	2.85270500	1.23669900
H	1.28215700	1.51709200	0.40497500
H	-0.32523300	-1.18040500	2.26111000
N	-0.12686500	-0.48159300	1.54747500
H	0.61771900	-0.87540000	0.95581500
H	-0.95932500	-0.44279800	0.94263400
C	0.19097900	-3.58239900	-0.59766600
H	0.21800200	-3.28270200	-1.65546900
C	1.52886100	-3.26980800	0.04361900
H	1.49056700	-3.46401700	1.12710500
H	2.28639800	-3.93817800	-0.39225700
O	1.87439300	-1.91106500	-0.21564900
C	3.23639200	-1.58384600	0.09090100
H	3.88146800	-2.43310000	-0.17828300
H	3.34708000	-1.39228500	1.16794900
C	3.69551200	-0.38039700	-0.70944700
H	3.48267800	-0.54267500	-1.77834500
O	-0.84300300	-2.88297200	0.08301100
H	0.01562500	-4.66927800	-0.54773900
O	3.08145800	0.81143400	-0.25734400
H	4.78881300	-0.30426300	-0.58918400
C	-2.10005400	-2.92569400	-0.58018100
H	-2.52611500	-3.94077900	-0.53081900
H	-1.97894300	-2.64968700	-1.63785500
C	-3.05768600	-1.95465800	0.08250500

H	-4.06017700	-2.10598900	-0.34544400
H	-3.11732000	-2.15385100	1.16409500
O	-2.61895500	-0.62187200	-0.16553100
C	-3.55016500	0.39549400	0.22853300
H	-3.40728300	0.64462800	1.28968100
H	-4.57688900	0.02502900	0.09534300
C	-3.38311700	1.63263300	-0.63278700
H	-3.45195200	1.35382400	-1.69674000
H	-4.22066700	2.31300600	-0.40541500
O	-2.15295100	2.27967000	-0.37101100
C	3.67887700	1.98509600	-0.83259600
H	3.12736900	2.85510500	-0.47179000
H	4.73275300	2.05589500	-0.53080300
H	3.61388600	1.95121300	-1.92860000
C	-2.02933300	3.52889800	-1.06895600
H	-1.06415800	3.96524800	-0.80353500
H	-2.07559500	3.36595200	-2.15479400
H	-2.83610800	4.21107600	-0.76844800