Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Catalyst-free CO_2 Hydrogenation with BH_3NH_3 in Water: DFT Mechanistic Insights

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DOI:

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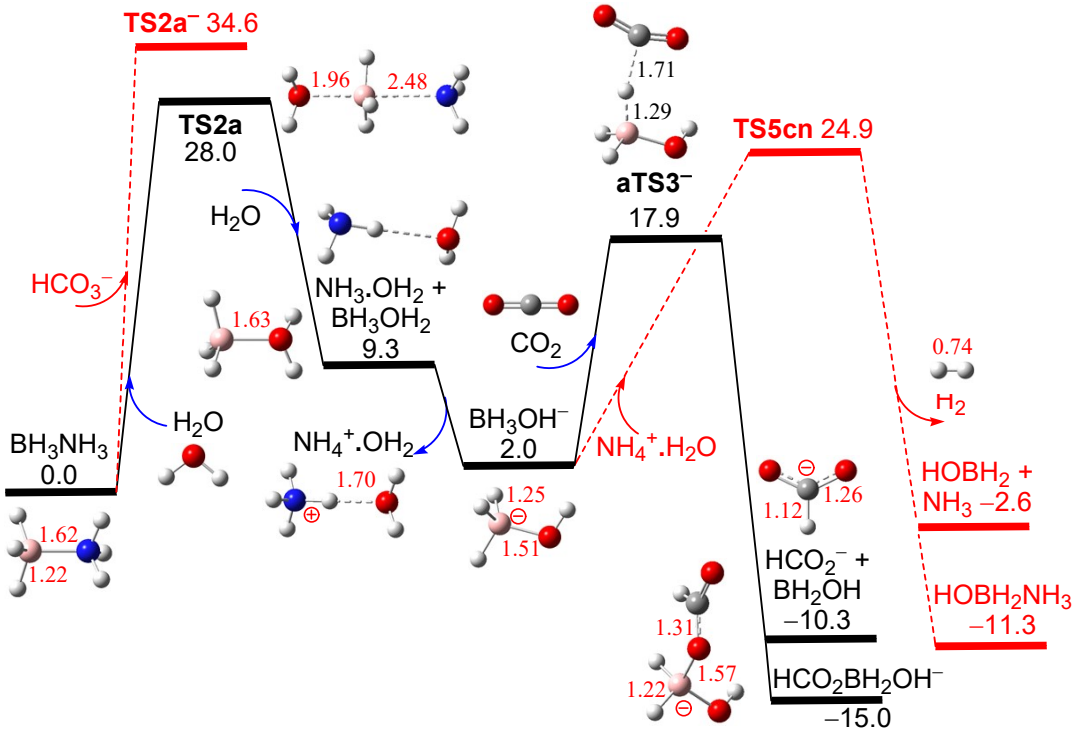

Figure S1. DFT computed free energy path (in kcal/mol, at 298 K and 1 M) for the first hydride transfer from BH_3NH_3 to CO_2 in water, initiated by S_N2 replacement with H_2O or HCO_3^-.

Though S_N2 replacement of NH_3 group of BH_3NH_3 with H_2O is possible over a moderate free energy barrier (via **TS2a**) of 28.0 kcal/mol, direct transfer hydrogenation of CO_2 with BH_3NH_3 is kinetically 2.1 kcal/mol more favourable over a barrier of 25.9 kcal/mol (via **TS2**). Even though, when reductive borate anion such as BH_3OH^- is reached via hydrolysis, hydride transfer to CO_2 becomes very facile. Moreover, OH-substituted ammonia borane $HOBH_2NH_3$ may also be formed from water hydrolysis, and it turns out to be more reactive than BH_3NH_3 for transfer hydrogenation of CO_2. These results suggest more efficient hydrogenation of CO_2 with borate salts and alkoxyl-substituted borane ammonia complexes (see Table S1 below).

In contrast, S_N2 replacement of NH_3 group of BH_3NH_3 with bicarbonate anion HCO_3^- is prevented by a high barrier (via **TS2a**$^-$) of 34.6 kcal/mol, while transfer hydrogenation of HCO_3^- with BH_3NH_3 is forbidden over a very high barrier (via **TS2c**$^-$) of 47.4 kcal/mol, clearly excluding HCO_3^- as the key intermediate for CO_2 reduction. Similarly, S_N2 replacement of NH_3 group of BH_3NH_3 with formate anion HCO_2^- is prevented by a high barrier (via **TS2b**$^-$) of 32.3 kcal/mol, which is kinetically also unfavourable (see Table S1 below).

Table S1. DFT-computed energies for the base-assisted hydrogenation of CO_2 with BH_3NH_3 in water. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in water solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95 (E_P)); total PW6B95-D3 Gibbs free energies ($G_P = E_P + Gc + Gsol$), relative electronic energies (ΔE_T and ΔE_P) and final Gibbs free-energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels. Each structure is labeled either by its molecular formula or a specific name in bold, with singly charged cation and anion species indicated by the + and − superscripts, respectively. Transition structures (with only one imaginary frequency) are indicated by the "**TS**" prefix. See also main-text figures for structural labelings.

Reactions in 1M water solution	ImF cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95 E_h	G_P E_h	ΔE_T kcal /mol	ΔE_P kcal /mol	*ΔG_P kcal /mol*	ΔG_T kcal /mol
Water as pure solvent: 2.4 kcal/mol higher free energy due to high concentration													
H_2O (1 M)	0	12.99	15.36	1.90	-10.53	-6.21	-76.47338	-76.54981	-76.55367	0.00	0.00	*0.00*	0.00
H_2O (solvent)	0	12.99	15.36	1.90	-11.06	-1.93	-76.47338	-76.54981	-76.54986	0.00	0.00	*2.39*	2.39
Solvation of molecules in water													
No water molecule is tighty bound to ammonia borane BH_3NH_3													
$BH_3NH_3 + H_2O$	0	56.77	62.01	31.71	-29.32	-17.28	-159.75130	-159.90846	-159.88246	0.00	0.00	*0.00*	0.00
$BH_3NH_3.OH_2$	0	58.74	63.45	40.93	-26.02	-19.26	-159.76318	-159.91948	-159.88194	-7.46	-6.92	*0.33*	-0.21
H-bonded complexes may coexist with "freely" solvated NH_3													
$NH_3 + H_2O$	0	34.11	38.87	11.70	-25.05	-8.46	-133.06794	-133.20185	-133.19367	0.00	0.00	*0.00*	0.00
$NH_3.H_2O$ (N..H)	0	36.71	40.48	20.86	-19.34	-12.25	-133.07856	-133.21034	-133.19360	-6.67	-5.33	*0.05*	-1.30
$NH_3.OH_2$ (H..O)	0	36.09	40.41	19.52	-25.83	-14.61	-133.07138	-133.20485	-133.19401	-2.16	-1.88	*-0.21*	-0.49
In average, only one H_2O is bound to ammonium cation NH_4^+													
$NH_4^+ + H_2O$	0	43.98	48.74	22.04	-85.77	-77.81	-133.40897	-133.54109	-133.62695	0.00	0.00	*0.00*	0.00
$NH_4^+.OH_2$	0	46.30	50.07	30.43	-70.43	-68.28	-133.44176	-133.57204	-133.62935	-20.57	-19.42	*-1.50*	-2.66
$NH_4^+.OH_2 + H_2O$	0	59.28	65.43	32.33	-81.48	-70.21	-209.91514	-210.12185	-210.17921	0.00	0.00	*0.00*	0.00
$NH_4^+.(OH_2)_2$	0	61.40	66.93	42.50	-69.94	-64.22	-209.94197	-210.14743	-210.17902	-16.84	-16.05	*0.12*	-0.67
Strong base Dbu is not tightly bound to water													
$Dbu + H_2O$	0	165.38	174.31	133.01	-34.67	-11.01	-538.87415	-539.43913	-539.24169	0.00	0.00	*0.00*	0.00
$Dbu.H_2O$ (N..H)	0	167.59	175.93	144.28	-26.73	-13.51	-538.89030	-539.45246	-539.24106	-10.14	-8.37	*0.40*	-1.37
..and protonated $DbuH^+$ is also not tightly bound to water													
$DbuH^+ + H_2O$	0	174.39	183.50	141.88	-59.61	-43.43	-539.29261	-539.85756	-539.69766	0.00	0.00	*0.00*	0.00
$DbuH^+.OH_2$	0	176.44	185.19	152.81	-52.83	-42.57	-539.31089	-539.87468	-539.69599	-11.47	-10.75	*1.05*	0.32

..while bicarbonate HCO_3^- and formate HCO_2^- anions are also "freely" solvated													
HCO_2^- + H_2O	0	25.56	30.40	-0.06	-128.85	-88.30	-265.79437	-266.05902	-266.19681	0.00	0.00	*0.00*	0.00
HCO_2^-.H_2O	0	27.60	31.84	9.61	-105.22	-78.89	-265.82292	-266.08560	-266.19299	-17.92	-16.68	*2.40*	1.16
HCO_3^- + H_2O	0	28.97	34.14	1.72	-129.37	-88.85	-341.09234	-341.43498	-341.57082	0.00	0.00	*0.00*	0.00
HCO_3^-.H_2O	0	31.26	35.57	12.92	-107.96	-81.00	-341.12010	-341.46015	-341.56563	-17.42	-15.80	*3.26*	1.63
..No stable $NH_4^+HCO_3^-$ and $NH_4^+HCO_2^-$ contact ion pairs exist in water													
NH_4^+.OH_2 + HCO_2^-	0	58.87	65.11	28.47	-188.21	-154.64	-322.76275	-323.08125	-323.27630	0.00	0.00	*0.00*	0.00
$NH_4^+HCO_2^-$ + H_2O	0	57.68	64.05	28.98	-53.36	-31.53	-322.94711	-323.26446	-323.26550	-115.69	-114.97	*6.78*	6.05
Proton H^+ is tightly bound to two H_2O in water													
$H_5O_2^+$ + H_2O	0	48.76	54.48	22.76	-124.68	-86.33	-229.75449	-229.97904	-230.07734	0.00	0.00	*0.00*	0.00
$H(H_2O)_3^+$	0	51.78	56.61	33.69	-99.93	-74.73	-229.79270	-230.01492	-230.07731	-23.97	-22.51	*0.01*	-1.45
*Formic acid HCO_2H-aided H_2-release from BH_3NH_3 is slightly endergonic over a barrier (**TS0**) of 28.5 kcal/mol*													
BH_3NH_3 + HCO_2H	0	64.46	69.92	35.36	-31.83	-22.16	-273.16105	-273.43056	-273.40350	0.00	0.00	*0.00*	0.00
TS0	180i	62.94	68.18	43.16	-38.43	-25.01	-273.12681	-273.38999	-273.35806	21.49	25.46	*28.51*	24.55
BH_2NH_2 + H_2 + HCO_2H	0	56.74	64.01	20.78	-18.69	-7.42	-273.16128	-273.43050	-273.40017	-0.14	0.04	*2.09*	1.91
*..while weak base NH_3-bridged H_2-release from BH_3NH_3 is slower over a higher barrier (**TS0a**)*													
BH_3NH_3 + NH_3.OH_2	0	79.87	87.07	49.33	-44.09	-29.96	-216.34930	-216.56350	-216.52661	0.00	0.00	*0.00*	0.00
$BH_3NH_2^-$ + NH_4^+.OH_2	0	79.80	86.42	49.45	-175.59	-150.75	-216.13386	-216.34616	-216.50157	135.19	136.38	*15.72*	14.52
TS0a + H_2O	685i	74.54	81.70	45.41	-35.70	-18.98	-216.31118	-216.51854	-216.47342	23.92	28.21	*33.38*	29.09
BH_2NH_2 + H_2 + NH_3.OH_2	0	72.15	81.15	34.75	-30.95	-15.22	-216.34952	-216.56344	-216.52328	-0.14	0.04	*2.09*	1.91
.. single H_2O-bridged H_2-release from BH_3NH_3 is even more difficult													
BH_3NH_3 + H_2O	0	56.77	62.01	31.71	-29.32	-17.28	-159.75130	-159.90846	-159.88246	0.00	0.00	*0.00*	0.00
TS0b	1091i	53.61	57.39	36.87	-14.39	-7.66	-159.72217	-159.86872	-159.81915	18.28	24.94	*39.73*	33.06
BH_2NH_2 + H_2 + H_2O	0	49.05	56.10	17.13	-16.18	-2.54	-159.75152	-159.90840	-159.87913	-0.14	0.04	*2.09*	1.91
*Hydration of CO_2 is 2.7 kcal/mol endergonic over a barrier (**TS1**) of 19.0 kcal/mol mediated by three H_2O.*													
CO_2 + $2H_2O$	0	33.11	40.09	-2.05	-23.46	-2.30	-341.65219	-341.99353	-341.99743	0.00	0.00	*0.00*	0.00
TS1a	645i	36.40	40.51	18.36	-45.71	-26.83	-341.62110	-341.95459	-341.96507	19.51	24.43	*20.31*	15.39
TS1 - H_2O	500i	38.33	41.73	29.24	-27.72	-22.01	-341.65086	-341.98174	-341.96721	0.83	7.40	*18.96*	12.40
H_2CO_3 + H_2O	0	36.96	42.29	10.02	-34.79	-14.09	-341.64618	-341.98971	-341.99320	3.77	2.39	*2.66*	4.04
..while overall reaction with NH_3 is -5.5 kcal/mol exergonic to form NH_4^+ and dicarbonate HCO_3^-													
CO_2 + H_2O + NH_3.H_2O	0	56.21	65.15	15.57	-38.23	-14.97	-398.25019	-398.64856	-398.64158	0.00	0.00	*0.00*	0.00

$H_2CO_3 + NH_3.H_2O$	0	60.06	67.34	27.64	-49.56	-26.77	-398.24418	-398.64475	-398.63734	3.77	2.39	*2.66*	4.04
$NH_4^+HCO_3^- + H_2O$	0	60.97	67.85	31.36	-65.99	-40.84	-398.23259	-398.62782	-398.63991	11.05	13.01	*1.05*	-0.92
$NH_4^+.OH_2 + HCO_3^-$	0	62.28	68.85	30.25	-188.74	-155.20	-398.06072	-398.45721	-398.65030	118.89	120.07	*-5.47*	-6.66
..for comparison, reaction of formic acid HCO_2H with NH_3 is slightly more exergonic in water													
$HCO_2H + NH_3.H_2O$	0	56.76	63.68	25.07	-39.40	-21.42	-322.95451	-323.27676	-323.26491	0.00	0.00	*0.00*	0.00
$NH_4^+HCO_2^- + H_2O$	0	57.68	64.05	28.98	-53.36	-31.53	-322.94711	-323.26446	-323.26550	4.64	7.71	*-0.37*	-3.45
$NH_4^+.OH_2 + HCO_2^-$	0	58.87	65.11	28.47	-188.21	-154.64	-322.76275	-323.08125	-323.27630	120.33	122.68	*-7.15*	-9.50
CO_2 itself cannot replace the NH_3 group from ammonia borane BH_3NH_3													
$BH_3NH_3 + CO_2$	0	50.92	56.03	23.96	-19.61	-13.78	-271.98334	-272.25255	-272.23031	0.00	0.00	*0.00*	0.00
TS20	156i	46.85	52.99	25.87	-7.95	-2.86	-271.93962	-272.20868	-272.16900	27.44	27.53	*38.48*	38.38
$BH_3OCO + NH_3$	0	47.46	53.67	18.95	-17.32	-6.46	-271.93424	-272.20294	-272.17700	30.82	31.13	*33.45*	33.13
*..Transfer hydrogenation of CO_2 with BH_3NH_3 is possible over a sizable barrier (**TS2**) of 25.9 kcal/mol, followed by facile addition overB=N bond*													
$BH_3NH_3 + CO_2$	0	50.92	56.03	23.96	-19.61	-13.78	-271.98334	-272.25255	-272.23031	0.00	0.00	*0.00*	0.00
TS2	757i	49.26	53.50	31.05	-23.35	-15.98	-271.95397	-272.21606	-272.18903	18.43	22.90	*25.90*	21.44
$BH_2NH_3^+ + HCO_2^-$	0	50.64	55.90	21.72	-187.41	-155.04	-271.71813	-271.98905	-272.19548	166.43	165.35	*21.86*	22.93
$BH_2NH_2 + HCO_2H$	0	50.40	55.60	21.66	-18.01	-8.72	-271.98068	-272.25456	-272.22792	1.67	-1.26	*1.50*	4.43
TS3a	172i	51.48	55.74	33.30	-9.45	-4.96	-271.98650	-272.25619	-272.20801	-1.98	-2.28	*13.99*	14.30
$HCO_2BH_2NH_3$	0	54.42	58.60	36.48	-19.87	-14.47	-272.01375	-272.28560	-272.24751	-19.08	-20.74	*-10.79*	-9.13
..Hydrolysis of BH_3NH_3 via S_N2 replacement in water is 2.0 kcal/mol endergonic over a higher barrier of 28.0 kcal/mol													
$BH_3NH_3 + 2H_2O$	0	69.75	77.37	33.61	-40.38	-19.22	-236.22468	-236.45827	-236.43232	0.00	0.00	*0.00*	0.00
TS2a + H_2O	306i	68.99	76.58	39.63	-32.95	-15.95	-236.19793	-236.42840	-236.38766	16.79	18.74	*28.03*	26.07
$BH_3OH_2 + NH_3.OH_2$	0	70.89	78.17	39.69	-54.10	-33.05	-236.20113	-236.43417	-236.41756	14.78	15.12	*9.26*	8.91
$BH_3OH^- + NH_4^+.OH_2$	0	72.13	78.70	41.85	-175.66	-151.53	-236.02988	-236.26033	-236.42909	122.24	124.21	*2.03*	0.05
..S_N2 replacement of BH_3NH_3 with dicaronate HCO_3^- is kinetically much less favorable													
$BH_3NH_3 + HCO_3^-$	0	59.76	65.43	29.63	-136.58	-102.27	-347.89688	-348.24382	-348.35356	0.00	0.00	*0.00*	0.00
TS2a$^-$	395i	57.93	64.19	37.09	-115.40	-87.15	-347.87880	-348.22174	-348.29850	11.35	13.86	*34.55*	32.04
$BH_3OCO_2H^- + NH_3$	0	57.48	63.76	28.55	-104.61	-80.26	-347.91494	-348.26351	-348.33990	-11.33	-12.36	*8.57*	9.60
$NH_4^+BH_3OCO_2^-$	0	59.82	65.23	40.12	-145.96	-110.38	-347.88540	-348.22817	-348.33714	7.21	9.82	*10.31*	7.69
..formate anion HCO_2^- is also less bound to BH_3 than NH_3													
$BH_3NH_3 + HCO_2^-$	0	56.36	61.70	27.85	-136.05	-101.72	-272.59890	-272.86786	-272.97955	0.00	0.00	*0.00*	0.00
TS2b$^-$	0	54.80	60.58	34.81	-112.70	-85.14	-272.58651	-272.85098	-272.92817	7.78	10.59	*32.25*	29.43

$HCO_2BH_3^-$ + NH_3	0	54.01	59.97	25.96	-94.79	-73.33	-272.62924	-272.89929	-272.96875	-19.03	-19.72	*6.78*	7.47
*..Transfer hydrogenation of bicaronate HCO_3^- is not feasible over a very high barrier (**TS2c⁻**) of 47.4 kcal/mol*													
BH_3NH_3 + HCO_3^-	0	59.76	65.43	29.63	-136.58	-102.27	-347.89688	-348.24382	-348.35356	0.00	0.00	*0.00*	0.00
$BH_3NH_2^-$ + H_2CO_3	0	57.48	63.28	27.14	-128.90	-94.64	-347.86490	-348.21402	-348.31555	20.07	18.70	*23.85*	25.22
TS2c⁻	519i	57.50	62.67	38.25	-106.81	-79.19	-347.87573	-348.21576	-348.27799	13.27	17.61	*47.42*	43.09
$HCO(OH)_2^-$ + BH_2NH_2	0	58.31	64.45	27.90	-130.91	-90.99	-347.87112	-348.21938	-348.31390	16.17	15.34	*24.89*	25.72
..transient BH_2NH_2 does not exist in water due to very rapid water addition													
BH_2NH_2 + $2H_2O$	0	55.70	63.05	19.90	-26.56	-5.78	-235.04431	-235.28227	-235.25675	0.00	0.00	*0.00*	0.00
TS3	895i	58.66	62.82	41.08	-21.25	-12.22	-235.06122	-235.28884	-235.23982	-10.61	-4.12	*10.62*	4.13
TS3b - H_2O	885i	60.66	63.78	52.35	-19.96	-15.88	-235.07711	-235.30064	-235.23952	-20.58	-11.52	*10.81*	1.75
$HOBH_2NH_3$ + H_2O	0	60.31	66.12	33.13	-39.81	-21.82	-235.06381	-235.29879	-235.27776	-12.23	-10.37	*-13.19*	-15.05
*Further hydrolysis aided by base NH_3 is still facile over a low barrier (**TS4**) of 18.1 kcal/mol to form another borate anion*													
$HOBH_2NH_3$ + H_2O	0	60.31	66.12	33.13	-39.81	-21.82	-235.06381	-235.29879	-235.27776	0.00	0.00	*0.00*	0.00
TS4	164i	59.07	65.47	38.72	-27.73	-16.14	-235.05251	-235.28797	-235.24898	7.09	6.79	*18.06*	18.36
$HOBH_2OH_2$ + NH_3	0	59.61	65.55	32.10	-46.80	-26.85	-235.04664	-235.28155	-235.26715	10.77	10.82	*6.66*	6.61
$BH_2(OH)_2^-$ + NH_4^+	0	60.94	66.66	34.03	-193.46	-164.10	-234.84309	-235.07697	-235.27821	138.50	139.20	*-0.28*	-0.98
*..while transfer hydrogenation with $HOBH_2NH_3$ (via **TS4a**) is kinetically much more favorable than with BH_3NH_3!*													
$HOBH_2NH_3$ + CO_2	0	54.46	60.14	25.38	-30.10	-18.32	-347.29586	-347.64289	-347.62561	0.00	0.00	*0.00*	0.00
TS4a	340i	53.85	59.24	33.99	-23.59	-16.94	-347.28498	-347.62555	-347.59538	6.82	10.88	*18.97*	14.92
HCO_2H + $HOBHNH_2$	0	54.29	59.94	23.65	-27.83	-14.74	-347.30920	-347.66259	-347.64236	-8.37	-12.37	*-10.51*	-6.52
..and even 1.6 kcal/mol more favorable with alkoxyl-substituted $MeOBH_2NH_3$													
CO_2 + $MeOBH_2NH_3$	0	72.33	78.68	41.95	-23.84	-14.07	-386.62217	-387.00759	-386.95714	0.00	0.00	*0.00*	0.00
TS4b	382i	71.06	77.53	49.64	-19.28	-13.45	-386.61241	-386.99019	-386.92950	6.13	10.92	*17.34*	12.55
$MeOBHNH_2.HCO_2H$	0	73.16	79.61	51.70	-19.53	-10.89	-386.64131	-387.02896	-386.96091	-12.01	-13.41	*-2.36*	-0.97
$MeOBHNH_2$ + HCO_2H	0	71.84	78.39	39.67	-22.25	-10.00	-386.63659	-387.02748	-386.97416	-9.05	-12.48	*-10.68*	-7.25
In contrast, transfer hydrogenation with BH_3NHMe_2 is less favorable than with BH_3NH_3													
CO_2 + BH_2NHMe_2	0	86.48	92.71	56.41	-16.70	-8.07	-350.65373	-351.00214	-350.91907	0.00	0.00	*0.00*	0.00
TS4c	694i	83.76	89.89	63.21	-20.92	-11.10	-350.62051	-350.96110	-350.87504	20.85	25.75	*27.63*	22.73
BH_2NMe_2 + HCO_2H	0	85.68	92.23	53.43	-18.27	-6.61	-350.64273	-350.99517	-350.91453	6.90	4.37	*2.85*	5.38
..In contrast, formate anion HCO_2^- cannot replace NH_3 from $HOBH_2NH_3$													
$HOBH_2NH_3$ + HCO_2^-	0	59.90	65.80	29.27	-146.54	-106.26	-347.91141	-348.25819	-348.37485	0.00	0.00	*0.00*	0.00

TS4$^-$	216i	57.73	64.77	35.67	-124.51	-90.63	-347.90506	-348.25050	-348.33506	3.98	4.83	*24.97*	24.13
$HCO_2BH_2OH^-$ + NH_3	0	57.79	64.40	28.39	-108.08	-78.96	-347.94540	-348.29377	-348.36833	-21.33	-22.32	*4.09*	5.09
Competive channels for H_2-release via hydrolysis are also possible but kinetically less favorable													
$HCO_2BH_2OH^-$ + H_2O	0	49.65	56.24	20.49	-105.14	-74.36	-367.82422	-368.19154	-368.27438	0.00	0.00	*0.00*	0.00
TS5a$^-$	141i	50.08	56.90	28.25	-133.66	-97.31	-367.77879	-368.14431	-368.25135	28.51	29.64	*14.45*	13.32
HCO_2^- + $HOBH_2OH_2$	0	51.07	57.08	20.34	-150.60	-106.68	-367.77306	-368.13872	-368.27029	32.10	33.14	*2.57*	1.53
HCO_2H + $BH_2(OH)_2^-$	0	50.62	56.55	19.45	-132.33	-95.03	-367.79063	-368.15760	-368.27202	21.08	21.30	*1.48*	1.26
TS5b$^-$	669i	47.99	53.89	27.15	-94.99	-71.15	-367.81942	-368.17866	-368.24576	3.01	8.08	*17.96*	12.89
$BH(OH)_2$ + HCO_2^- + H_2	0	44.89	52.30	7.76	-135.45	-93.46	-367.81840	-368.18456	-368.31210	3.66	4.38	*-23.67*	-24.39
BH_3NH_3 + $2H_2O$	0	69.75	77.37	33.61	-40.38	-19.22	-236.22468	-236.45827	-236.43232	0.00	0.00	*0.00*	0.00
BH_3OH^- + $NH_4^+.OH_2$	0	72.13	78.70	41.85	-175.66	-151.53	-236.02988	-236.26033	-236.42909	122.24	124.21	*2.03*	0.05
TS5cn	347i	69.23	75.51	49.16	-18.21	-9.86	-236.23338	-236.45824	-236.39261	-5.46	0.02	*24.92*	19.44
BH_2OH + $NH_3.OH_2$ + H_2	0	64.25	73.16	26.56	-36.53	-17.56	-236.22855	-236.45985	-236.43646	-2.43	-0.99	*-2.60*	-4.04
..and HCO_2H aided H_2 release from $HOBH_2NH_3$ is kinetically less favorable than H_2O hydrolysis													
$HOBH_2NH_3$ + HCO_2H	0	68.00	74.03	36.79	-42.33	-26.70	-348.47356	-348.82089	-348.79880	0.00	0.00	*0.00*	0.00
TS5d	400i	65.19	71.16	44.63	-42.22	-28.20	-348.44650	-348.78647	-348.75728	16.98	21.60	*26.05*	21.43
$HCO_2BH(OH)NH_3$ + H_2	0	63.86	70.92	37.58	-29.19	-16.77	-348.51574	-348.86234	-348.82317	-26.47	-26.01	*-15.29*	-15.75
..with H_2 release via BH_2NH_2 hydrolysis being kinetically much less favorable													
BH_2NH_2 + $2H_2O$	0	55.70	63.05	19.90	-26.56	-5.78	-235.04431	-235.28227	-235.25675	0.00	0.00	*0.00*	0.00
TS5c - H_2O	885i	59.96	62.98	51.66	-28.96	-20.10	-235.04653	-235.26989	-235.21659	-1.39	7.77	*25.20*	16.04
TS5ca	1097i	57.31	61.76	39.45	-29.76	-15.82	-235.02752	-235.25435	-235.21368	10.54	17.52	*27.02*	20.04
$HOBHNH_2$ + H_2 + H_2O	0	52.94	60.44	19.12	-25.99	-8.56	-235.08004	-235.31643	-235.29357	-22.42	-21.44	*-23.11*	-24.09
..Further hydrolysis of $BH(OH)_2$ with water is still facile													
$BH(OH)_2$ + $3H_2O$	0	64.94	74.92	16.29	-50.15	-14.19	-406.73696	-407.14885	-407.14249	0.00	0.00	*0.00*	0.00
$BH(OH)_3^-$ + $H_5O_2^+$	0	69.32	76.64	37.19	-240.39	-174.79	-406.51721	-406.92331	-407.13657	137.89	141.53	*3.71*	0.08
TS6	606i	68.45	75.10	47.61	-60.33	-34.45	-406.73367	-407.13224	-407.10826	2.06	10.42	*21.48*	13.12
$B(OH)_3$ + $2H_2O$ + H_2	0	62.26	72.39	16.97	-45.73	-14.27	-406.77581	-407.18773	-407.17740	-24.38	-24.40	*-21.91*	-21.89
..less likely with only one H_2O as proton bridge													
$BH(OH)_2$ + H_2O	0	38.97	44.21	12.49	-28.03	-10.33	-253.79020	-254.04922	-254.04277	0.00	0.00	*0.00*	0.00
$BH(OH)_2.H_2O$	0	40.75	45.73	22.13	-27.32	-15.36	-253.79685	-254.05528	-254.04149	-4.17	-3.80	*0.80*	0.43
TS6a	945i	40.50	43.24	32.71	-31.65	-20.76	-253.77191	-254.02142	-253.99936	11.48	17.45	*27.23*	21.26

$B(OH)_3 + H_2$	0	36.29	41.67	13.16	-23.62	-10.40	-253.82905	-254.08810	-254.07768	-24.38	-24.40	*-21.91*	-21.89
..which is energetically more favorable than trimer $(BH_2NH_2)_3$ formation													
BH_2NH_2	0	29.73	32.33	16.10	-4.44	-1.91	-82.09755	-82.18265	-82.15702	0.00	0.00	*0.00*	0.00
$1/3(BH_2NH_2)_3$	0	32.88	34.47	26.93	-6.18	-4.96	-82.12138	-82.20524	-82.16923	-14.95	-14.17	*-7.66*	-8.44
$(BH_2NH_2)_3$	0	98.64	103.40	80.78	-18.53	-14.89	-246.36413	-246.61571	-246.50770				
.. hydride transfer from $HCO_2BH_2OH^-$ to CO_2 is also possible but kinetically less favorable													
$HCO_2BH_2OH^- + CO_2$	0	43.80	50.26	12.74	-95.43	-70.86	-480.05627	-480.53563	-480.62223	0.00	0.00	*0.00*	0.00
TS7⁻	435i	43.32	49.53	21.87	-71.76	-57.41	-480.06233	-480.53657	-480.59019	-3.80	-0.59	*20.11*	16.89
$HCO_2BHOH + HCO_2^-$	0	45.18	51.24	13.32	-124.11	-88.58	-480.03955	-480.52229	-480.63619	10.50	8.37	*-8.76*	-6.64
$(HCO_2)_2BHOH^-$	0	46.56	52.56	25.54	-88.97	-66.38	-480.10561	-480.58900	-480.65108	-30.96	-33.49	*-18.10*	-15.57
*Hydride transfer from $BH_2(OH)_2^-$ to CO_2 is facile over a low barrier (**TS8⁻**)*													
$CO_2 + BH_2(OH)_2^-$	0	37.08	42.66	8.04	-120.10	-86.65	-366.61293	-366.97959	-367.09884	0.00	0.00	*0.00*	0.00
TS8⁻	300i	36.45	41.93	16.26	-95.84	-72.03	-366.62675	-366.98905	-367.07491	-8.67	-5.94	*15.01*	12.28
$HCO_2BH(OH)_2^-$	0	40.28	45.12	21.29	-106.40	-77.62	-366.67350	-367.04411	-367.13086	-38.01	-40.49	*-20.10*	-17.62
$HCO_2^- + BH(OH)_2$	0	38.56	43.89	8.63	-134.77	-94.76	-366.63780	-367.00862	-367.13986	-15.61	-18.22	*-25.74*	-23.13
..followed by base NH_3 assisted hydrolysis of $BH(OH)_2$													
$BH(OH)_2 + H_2O$	0	38.97	44.21	12.49	-28.03	-10.33	-253.79020	-254.04922	-254.04277	0.00	0.00	*0.00*	0.00
$BH(OH)_2.OH_2$	0	40.75	45.73	22.13	-27.32	-15.36	-253.79685	-254.05528	-254.04149	-4.17	-3.80	*0.80*	0.43
$BH(OH)_2 + NH_3.OH_2$	0	62.07	69.26	30.11	-42.81	-23.01	-310.38820	-310.70426	-310.68691	0.00	0.00	*0.00*	0.00
$BH(OH)_2.NH_3 + H_2O$	0	63.68	70.16	35.30	-47.16	-24.69	-310.38686	-310.70156	-310.68163	0.84	1.69	*3.31*	2.46
$BH(OH)_3^- + NH_4^+.OH_2 - H_2O$	0	66.86	72.23	44.86	-186.14	-156.74	-310.20447	-310.51631	-310.68858	115.29	117.94	*-1.05*	-3.70
..and further facile hydride transfer from borate $BH(OH)_3^-$ to CO_2 to form neutral $B(OH)_3$													
$CO_2 + BH(OH)_3^-$	0	40.69	46.89	10.48	-128.12	-88.83	-441.94152	-442.38798	-442.50681	0.00	0.00	*0.00*	0.00
TS9⁻	303i	40.01	46.29	18.51	-103.48	-74.78	-441.95374	-442.39498	-442.48164	-7.67	-4.39	*15.79*	12.52
$HCO_2B(OH)_3^-$	0	43.03	48.88	22.81	-114.57	-81.13	-441.99882	-442.45032	-442.54023	-35.95	-39.12	*-20.98*	-17.81
$HCO_2^- + B(OH)_3$	0	42.53	48.30	12.08	-140.72	-98.07	-441.96944	-442.42137	-442.55238	-17.52	-20.95	*-28.60*	-25.17
With BH_4^- anion as reductant in water													
*In neutral water (pH = 7), H_2 release is prevented by a sizeable barrier (**aTS1**) of 29.4 kcal/mol, partially due to low H^+ concentration (+9.5 kcal/mol)*													
$BH_4^- + H_5O_2^+$	0	57.25	63.03	31.31	-210.42	-164.82	-180.56561	-180.73637	-180.94311	0.00	0.00	*0.00*	0.00
aTS1	-724	57.41	62.93	38.44	-29.89	-19.04	-180.77893	-180.94538	-180.91145	-133.86	-131.15	*19.87*	17.16
$BH_3OH_2 + H_2O + H_2$	0	54.12	61.52	21.20	-40.01	-19.07	-180.78372	-180.95508	-180.94566	-136.87	-137.24	*-1.60*	-1.23

*Hydride transfer from borate anion BH_4^- to CO_2 is facile over a moderate barrier (**aTS1⁻**) of 19.8 kcal/mol*													
$CO_2 + BH_4^-$	0	28.61	33.28	4.60	-98.14	-78.85	-215.98992	-216.20104	-216.31334	0.00	0.00	*0.00*	0.00
aTS1⁻	0	28.62	33.27	10.09	-67.32	-59.65	-216.00098	-216.20581	-216.28177	-6.94	-2.99	*19.81*	15.87
$HCO_2BH_3^-$	0	32.89	36.46	16.16	-80.79	-66.80	-216.03468	-216.24725	-216.32494	-28.08	-29.00	*-7.28*	-6.37
..followed by facile S_N2 replacement with H_2O to release formate anion HCO_2^-													
$HCO_2BH_3^- + H_2O$	0	45.87	51.82	18.06	-91.85	-68.73	-292.50806	-292.79706	-292.87480	0.00	0.00	*0.00*	0.00
aTS2⁻	305i	46.75	52.53	26.60	-126.22	-93.71	-292.45363	-292.73769	-292.84162	34.15	37.26	*20.82*	17.71
$HCO_2^- + BH_3OH_2$	0	47.38	52.80	18.21	-146.06	-104.80	-292.45074	-292.73853	-292.87050	35.97	36.73	*2.70*	1.94
$HCO_2H + BH_3OH^-$	0	46.51	51.90	16.98	-118.81	-90.06	-292.47125	-292.76020	-292.87064	23.10	23.13	*2.61*	2.57
..and facile hydride transfer from BH_3OH^- to CO_2													
$CO_2 + BH_3OH^-$	0	32.97	38.01	5.57	-106.58	-81.69	-291.29355	-291.58219	-291.69746	0.00	0.00	*0.00*	0.00
aTS3⁻	396i	32.98	37.68	14.02	-79.51	-65.07	-291.31018	-291.59383	-291.67218	-10.44	-7.31	*15.86*	12.73
$HCO_2^- + BH_2OH$	0	34.41	39.38	5.95	-127.81	-90.61	-291.29757	-291.58827	-291.71716	-2.52	-3.81	*-12.36*	-11.07
$HCO_2BH_2OH^-$	0	36.66	40.88	18.59	-94.09	-72.43	-291.35084	-291.64173	-291.72452	-35.95	-37.36	*-16.98*	-15.58
Water-aided hydrolysis of BH_3 is facile for the first B-H bond to relase H_2.													
$BH_3.OH_2 + 2H_2O$	0	60.77	68.47	23.97	-50.38	-22.30	-256.07651	-256.32895	-256.32328	0.00	0.00	*0.00*	0.00
$BH_3OH^- + H_5O_2^+$	0	61.61	67.75	32.28	-218.86	-167.65	-255.86924	-256.11752	-256.32722	130.07	132.67	*-2.48*	-5.08
$BH_3.OH_2$	0	34.80	37.76	20.17	-28.27	-18.44	-103.12975	-103.22932	-103.22355	0.00	0.00	*0.00*	0.00
aTS4 – $2H_2O$	844i	36.22	36.62	39.56	-5.86	-12.45	-103.15535	-103.24283	-103.19662	-16.06	-8.48	*16.90*	9.31
aTS4a – H_2O	1005i	33.90	35.21	28.38	-15.90	-13.14	-103.12913	-103.22007	-103.19278	0.39	5.80	*19.31*	13.89
aTS4b	1503i	31.49	34.19	17.04	-9.48	-5.38	-103.09854	-103.19408	-103.17250	19.59	22.12	*32.04*	29.51
$BH_2OH + H_2$	0	28.16	32.74	7.04	-10.70	-2.95	-103.15717	-103.25500	-103.24245	-17.21	-16.11	*-11.86*	-12.96
..also facile for the second BH bond													
$BH_2OH + H_2O$	0	34.81	39.69	9.81	-21.08	-6.18	-178.44996	-178.62887	-178.62007	0.00	0.00	*0.00*	0.00
$BH_2OH.OH_2$	0	38.49	42.04	22.30	-32.81	-20.32	-178.45208	-178.62951	-178.62334	-1.33	-0.40	*-2.05*	-2.98
$BH_2OH.OH_2 + 2H_2O$	0	64.46	72.76	26.10	-54.92	-24.18	-331.39884	-331.72914	-331.72306	0.00	0.00	*0.00*	0.00
$BH_2(OH)_2^- + H_5O_2^+$	0	65.72	72.40	34.75	-232.38	-172.61	-331.18862	-331.51492	-331.72860	131.92	134.42	*-3.48*	-5.98
*..via H_2-release from $BH_2OH.OH_2$ complex mediated by two additional H_2O (via **TS5a**)*													
$BH_2OH.OH_2$	0	38.49	42.04	22.30	-32.81	-20.32	-178.45208	-178.62951	-178.62334	0.00	0.00	*0.00*	0.00
TS5a - $2H_2O$	749i	39.27	40.38	41.52	-21.05	-19.76	-178.47060	-178.63643	-178.59875	-11.62	-4.34	*15.43*	8.15
TS5b - H_2O	1016i	37.22	39.15	30.51	-27.81	-19.65	-178.44573	-178.61453	-178.59422	3.99	9.40	*18.27*	12.86

$BH(OH)_2 + H_2$	0	32.31	37.26	9.72	-17.66	-7.10	-178.49741	-178.67535	-178.66515	-28.45	-28.77	*-26.24*	-25.92
..and can be easily replaced by water from BH_3.Thf, leading to facile hydrolysis of BH bonds for H_2 release													
BH_3.THF + H_2O	0	106.06	113.14	76.40	-25.30	-10.17	-335.74653	-336.08403	-335.97547	0.00	0.00	*0.00*	0.00
$BH_3.OH_2$ + THF	0	107.09	113.65	75.55	-39.45	-22.01	-335.73356	-336.07140	-335.98007	8.14	7.92	*-2.88*	-2.67
THF is not bound to borane BH_2OH in water													
BH_2OH + THF	0	94.12	100.23	63.29	-21.20	-7.82	-334.58040	-334.92113	-334.82672	0.00	0.00	*0.00*	0.00
BH_2OH.THF	0	96.66	102.10	76.89	-22.15	-11.46	-334.59265	-334.93190	-334.82462	-7.69	-6.76	*1.32*	0.39
..while H_2O is bound by 2.1 kcal/mol													
$BH_2OH + H_2O$	0	34.81	39.69	9.81	-21.08	-6.18	-178.44996	-178.62887	-178.62007	0.00	0.00	*0.00*	0.00
$BH_2OH.OH_2$	0	38.49	42.04	22.30	-32.81	-20.32	-178.45208	-178.62951	-178.62334	-1.33	-0.40	*-2.05*	-2.98
..and NH_3 is bound even stronger, thus may stabilize borane in water													
$BH_2OH + NH_3.OH_2$	0	57.92	64.75	27.43	-35.85	-18.86	-235.04796	-235.28391	-235.26422	0.00	0.00	*0.00*	0.00
$HOBH_2NH_3 + H_2O$	0	60.31	66.12	33.13	-39.81	-21.82	-235.06381	-235.29879	-235.27776	-9.94	-9.34	*-8.50*	-9.10
Effect of strong but bulky base Dbu in water													
*The S_N2 replacement with Dbu is kinetically slower due to a high barrier (**TS2b**) of 30.8 kcal/mol*													
Dbu + BH_3NH_3	0	196.18	205.61	160.92	-41.88	-24.43	-545.67869	-546.24797	-546.02444	0.00	0.00	*0.00*	0.00
TS2b	0	193.90	204.19	168.30	-22.54	-11.00	-545.66436	-546.22910	-545.97542	8.99	11.84	*30.76*	27.91
Dbu.BH_3 + NH_3	0	194.73	204.71	161.16	-38.49	-20.29	-545.69302	-546.26305	-546.03255	-9.00	-9.47	*-5.09*	-4.62
..with Dbu being 13.0 kcal/mol more basic than NH_3 in water													
$DbuH^+ + NH_3.OH_2$	0	197.49	208.56	159.50	-74.38	-56.11	-595.89061	-596.51259	-596.34181	0.00	0.00	*0.00*	0.00
Dbu + $NH_4^+.OH_2$	0	198.69	209.02	161.54	-94.04	-77.36	-595.84253	-596.46136	-596.32118	30.17	32.15	*12.95*	10.96
..and Dbu is still bound to borane BH_2OH													
Dbu + BH_2OH	0	174.22	183.29	139.03	-33.63	-13.33	-564.37735	-564.96838	-564.76204	0.00	0.00	*0.00*	0.00
Dbu.BH_2OH	0	177.45	185.77	154.30	-37.36	-20.44	-564.40693	-564.99728	-564.78095	-18.56	-18.14	*-11.86*	-12.28
..but not bound to borane $BH(OH)_2$ in water													
Dbu + $BH(OH)_2$	0	178.38	187.80	141.71	-40.59	-17.48	-639.71759	-640.38873	-640.18474	0.00	0.00	*0.00*	0.00
Dbu.$BH(OH)_2$	0	180.36	189.61	156.22	-41.01	-20.92	-639.73097	-640.40147	-640.18285	-8.40	-8.00	*1.18*	0.78

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in water solution. Each structure is labeled by the specific name (See also **Table S1** and main-text figures), followed by the number of atoms, the total energy, and the detailed atomic coordinates (in double-column text list).

$(BH_2NH_2)_3$: BH_2NH_2 trimer
18
Energy = -246.3690482353
B -1.4087080 0.6640462 0.2762259
H -2.4032518 1.1329076 -0.2440978
H -1.4524526 0.6849797 1.4865752
N -1.2124548 -0.8414228 -0.1972049
H -1.3119824 -0.9109651 -1.2137237
H -1.9980970 -1.3866400 0.1631911
B 0.1291485 -1.5520163 0.2764348
H 0.2202396 -2.6478008 -0.2438167
H 0.1334118 -1.6001058 1.4867640
N 1.3347818 -0.6293511 -0.1974161
H 2.1997927 -1.0370401 0.1629915
H 1.4449112 -0.6809801 -1.2139396
B 1.2794849 0.8878182 0.2763128
H 1.3190186 0.9153788 1.4866445
H 2.1828800 1.5146992 -0.2438580
N -0.1224204 1.4706948 -0.1974452
H -0.2018682 2.4236897 0.1629799
H -0.1324398 1.5921450 -1.2139356

BH_2NH_2 : transient aminoborane
6
Energy = -82.09624344404
B 0.0000504 0.0000065 -0.7828147
H 0.0000054 1.0457937 -1.3675041
H -0.0000584 -1.0457951 -1.3675051
N 0.0000648 -0.0000018 0.6061148
H 0.0000082 -0.8436869 1.1675195
H -0.0000705 0.8436834 1.1675087

$BH_2NH_3^+$: cation from hydride transfer
7
Energy = -82.51079979808
B -0.7885745 -0.0229234 -0.3100080
H -1.3059147 1.0217209 -0.5011621
H -1.3056756 -1.0843659 -0.3472536
N 0.7074073 -0.0019007 -0.0252353
H 1.2137051 -0.0696495 -0.9234902
H 1.0374407 0.8657433 0.4108693
H 1.0369291 -0.7946970 0.5358802

BH_2NMe_2 : transient aminoborane
12
Energy = -160.7505876654
B 0.0011708 0.0043940 -0.7788880
H 0.0014102 1.0493078 -1.3662432
H 0.0016963 -1.0462504 -1.3574976
N 0.0002374 0.0073747 0.6095717
C -0.0005018 -1.2365606 1.4079386
H 0.0018448 -0.9894806 2.4720849
H -0.8919095 -1.8323477 1.1923408
H 0.8880599 -1.8353543 1.1890925
C -0.0005410 1.2344449 1.4123752
H -0.8895460 1.2721846 2.0538186
H 0.8875168 1.2723760 2.0551197
H -0.0001732 2.0999349 0.7477837

$BH_2(OH)_2^-$: borate anion
7
Energy = -178.0035467822
B 0.0004169 0.6685633 -0.1283136
H 0.0142857 1.3354139 0.9278756
H 0.2870663 1.3813479 -1.0983088
O 1.0441748 -0.4050630 -0.0703041
H 0.9990839 -0.8588708 0.7848819
O -1.3791822 0.1420112 -0.3832330
H -1.7418428 -0.2334267 0.4333719

BH_2OH.THF : unstable THF adduct of borane
18
Energy = -334.5862759891
O -0.4356952 -0.1893230 1.1717805
C -0.2578680 1.0959170 0.4419894
C 0.2689787 0.7023118 -0.9342656
C -0.2346587 -0.7398829 -1.1067065
C -0.0520540 -1.3124268 0.2863067
H 0.4311698 1.7069662 1.0263396
H -1.2452705 1.5594782 0.4115255
H 1.3628979 0.7236255 -0.9438171
H -0.0995614 1.3774907 -1.7097508
H -1.2918838 -0.7529099 -1.3900672
H 0.3362575 -1.3014433 -1.8498794
H -0.7066839 -2.1437328 0.5420264
H 0.9904123 -1.5649739 0.5052881
B 0.2091199 -0.2171527 2.7060037
H 1.4060248 -0.1227652 2.5043124
H -0.3177781 0.7649720 3.1924719
O -0.1286543 -1.4862937 3.2797182
H -1.0319658 -1.4898032 3.6302346

BH_2OH : borane
5
Energy = -101.9752070405
B 0.7136038 0.0062622 0.0767498
H 1.2207871 1.0852808 0.1974580
H 1.3430759 -1.0116425 0.0964637
O -0.6280385 -0.1218878 -0.0916837
H -1.1044552 0.7258091 -0.1026020

$MeOBH_2NH_3$: alkoxyl-substituted
12
Energy = -197.9258970825
O 1.3157514 -0.2275530 -0.0093465
B 0.1890350 0.7069513 -0.0714239
H 0.1260746 1.4642170 0.8939852
H 0.1236387 1.3272037 -1.1300626
N -1.1152927 -0.2410865 -0.0059020
H -1.9817296 0.2987903 -0.0456880
H -1.1462065 -0.7901461 0.8560864
H -1.1433698 -0.9061664 -0.7820382
C 2.5849804 0.4060399 -0.0484565
H 2.7157325 1.0964139 0.8010178
H 3.3619837 -0.3643932 0.0015066
H 2.7176974 0.9828104 -0.9785147

$BH_3NH_2^-$: anion from *N*-deprotonation
7
Energy = -82.78981351946
B -0.8362612 0.0132696 -0.0091548
H -1.2686346 0.0925217 1.1490709
H -1.3368352 0.9618312 -0.6553901
H -1.2690374 -1.0354487 -0.5066916
N 0.7245490 -0.0232780 0.0156802
H 1.1079678 -0.0673716 -0.9305855
H 1.1082362 0.8398694 0.4056270

$BH_3NH_3.OH_2$: loose H-bonded
11
Energy = -159.7759548914
B -2.4205671 0.9226756 -1.4211752
H -3.4281621 0.4229124 -0.9541916
H -2.1216064 1.9522703 -0.8429375
H -1.4944594 0.1319450 -1.4364291
N -2.7462265 1.3058827 -2.9578979
H -3.0090704 0.4752139 -3.5158393
H -3.5156393 1.9746502 -3.0320154
H -1.9463392 1.7394758 -3.4234813
O -3.4527656 -1.1715876 -4.4018312
H -2.7237389 -1.7971902 -4.2547469
H -4.2097218 -1.5698570 -3.9403736

BH_3NH_3 : ammonia borane
8
Energy = -83.29471634154
B -0.9052404 0.0000137 0.0000280
H -1.2622537 0.0861285 1.1607809
H -1.2622369 0.9621928 -0.6549765
H -1.2621776 -1.0483009 -0.5057737
N 0.7154744 0.0000129 0.0000668
H 1.1032084 -0.0697793 -0.9424343
H 1.1032105 0.8511258 0.4108650
H 1.1030791 -0.7813375 0.5318249

BH_3NHMe_2 : *N*-methylated ammonia borane
14
Energy = -161.9522049343
B -0.8925241 0.0023213 0.0075149
H -1.2542236 0.0927513 1.1671375
H -1.2354527 0.9647756 -0.6544841
H -1.2388539 -1.0494010 -0.4984028
N 0.7264501 0.0014740 0.0320399
H 1.0483659 -0.0724194 -0.9356034
C 1.2811784 1.2729668 0.5835338
H 2.3733758 1.2486297 0.5550101
H 0.9052085 2.1042697 -0.0131726
H 0.9355344 1.3734562 1.6138927
C 1.2772122 -1.1741345 0.7690723
H 0.8989716 -2.0846514 0.3039402
H 2.3694641 -1.1575176 0.7379763
H 0.9309686 -1.1174479 1.8025387

$BH_3OCO_2H^-$: borane bicarbonate anion adduct
9
Energy = -291.4009584996
B -1.9973102 0.0011029 -0.0003273
H -2.1220314 0.6850600 1.0067295
H -2.1245719 0.6828841 -1.0086475
H -2.7860460 -0.9332462 0.0015559
O -0.6003942 -0.6712217 -0.0016374
C 0.4716794 0.0619732 0.0002351
O 0.5638996 1.2882911 0.0033956
O 1.5856658 -0.7418660 -0.0015947
H 2.3577717 -0.1471493 0.0008388

BH_3OCO : borane CO_2 adduct
7
Energy = -215.3321365463
B 1.9510064 0.4495244 0.0003583
H 1.6941568 1.0328684 -1.0119278
H 1.8196142 1.0177998 1.0445196
H 2.6561854 -0.5135217 -0.0494967
O 0.2405598 -0.5925171 0.1024175
C -0.8564032 -0.1783038 0.0042578
O -1.9454824 0.2084791 -0.0902257

$BH_3.OH_2$: borane water adduct
7
Energy = -103.1439334585
B -0.9280118 0.0142522 -0.0100603
H -1.2138676 0.0962567 1.1631896
H -1.2781911 0.9733738 -0.6654805
H -1.2153204 -1.0489947 -0.5121456
O 0.7020887 0.0027774 -0.0034792
H 1.0813188 -0.0631677 -0.8990825
H 1.0819680 0.8068958 0.3956144

BH_3OH^- : borate anion
6

Energy = -102.6869469525
B -0.8139242 0.0033328 -0.0207625
H -1.2139491 0.0925208 1.1447759
H -1.2827531 0.9574901 -0.6705030
H -1.2690279 -1.0471837 -0.5124438
O 0.6914984 0.0169248 0.0171518
H 1.0361722 -0.0485873 -0.8852768

BH_3.THF : BH_3 and THF adduct
17
Energy = -259.2699515878
O -0.4422079 -0.1488731 1.1271746
C -0.1937529 1.1290674 0.3975917
C 0.2943250 0.7049088 -0.9840956
C -0.2273734 -0.7360703 -1.1313803
C -0.0484064 -1.2879041 0.2679243
H 0.5383740 1.6905884 0.9784497
H -1.1536206 1.6467157 0.3856103
H 1.3873610 0.7137306 -1.0198496
H -0.0845255 1.3713207 -1.7617238
H -1.2849536 -0.7440096 -1.4119707
H 0.3377561 -1.3124666 -1.8669699
H -0.7074693 -2.1111552 0.5406735
H 0.9929800 -1.5336163 0.4983322
B 0.0087631 -0.2066126 2.6499046
H 1.2222783 -0.0930515 2.6593195
H -0.5592769 0.7255813 3.1788303
H -0.3709389 -1.2894051 3.0433615

BH_4^- : borate anion
5
Energy = -27.38674964591
B -1.3639611 -0.0000113 0.0002553
H -1.7720089 1.1574900 -0.0999143
H -1.7936394 -0.4980793 1.0411156
H -1.7572688 -0.6586405 -0.9629895
H -0.1327688 -0.0006448 0.0226229

$BH(OH)_2.NH_3$: unstable adduct
10
Energy = -233.9253996628
B -0.1870304 -0.4282313 0.0520072
H -0.4572791 -1.5525487 0.4548633
O -0.2307210 -0.4294530 -1.4060988
H 0.1624137 0.3887392 -1.7524345
O 1.0010465 0.1866657 0.6445779
H 1.7740882 -0.3807146 0.5095168
N -1.3859690 0.5494959 0.6079601
H -2.2957286 0.2801075 0.2303124
H -1.4630273 0.5241053 1.6269207
H -1.2293852 1.5264367 0.3455506

$BH(OH)_2.OH_2$: loose water adduct
9
Energy = -253.7955272862
B 0.7762479 -0.4683169 0.4167867
H 0.2794950 -1.2212371 1.1979685
O -0.0656231 0.2921809 -0.3586244
H 0.3945635 0.8900101 -0.9739978
O -2.8664024 0.6023744 -0.0183574
H -1.8976090 0.5043608 -0.1439479
H -3.2580220 0.1196258 -0.7633370
O 2.1270751 -0.3302702 0.2591382
H 2.6422587 -0.9072490 0.8453341

$BH(OH)_2$: borane
6
Energy = -177.3147792428
B 0.7744730 -0.4633520 0.4116487
H 0.2840354 -1.2202678 1.1955408
O -0.0706219 0.2926208 -0.3557930
H 0.3970248 0.8849533 -0.9712587
O 2.1304674 -0.3294590 0.2584079
H 2.6386383 -0.9093775 0.8480595

$BH(OH)_3^-$: borate anion
8
Energy = -253.3271145916
B -0.0215494 -0.0030741 -0.3909130
H -0.1205250 -0.0005069 -1.6394557
O 1.0927033 0.8572423 0.0812165
H 0.9016503 1.7727694 -0.1699959
O -1.3532265 0.4730492 0.0848556
H -1.3361747 0.4966658 1.0568462
O 0.3259101 -1.3469885 0.1363299
H -0.3912022 -1.9588282 -0.0854835

$HOBHNH_2$: aminoborane
7
Energy = -157.4256939944
O 0.8837868 -1.1540612 -0.4881783
H 0.6364883 -1.4676165 0.3977560
B 1.6989115 -0.0336551 -0.4777148
H 2.0271361 0.3871174 -1.5498304
N 2.1405164 0.6061868 0.6919349
H 1.9072787 0.3116630 1.6332739
H 2.7359457 1.4235528 0.6677525

$MeOBHNH_2.HCO_2H$: loose HCO_2H adduct
15
Energy = -386.6356839022
B -1.7677592 0.4585481 -0.3149657
H -1.6625836 0.8622232 -1.4366989
N -1.4515892 -0.9081200 -0.0129961
H -1.5028347 -1.5912032 -0.7624781
H 0.2660682 -0.9393319 0.3098889
H -1.7695551 -1.3075162 0.8671987
H 1.3464263 -0.4254483 -1.4614293
C 1.9615346 -0.6602723 -0.5765548
O 1.2639910 -0.9745849 0.5146942

O 3.1782852 -0.6349554 -0.5906427
O -2.1143743 1.2818574 0.7145334
C -2.3384876 2.6884721 0.4897578
H -3.3324386 2.9399921 0.8678143
H -1.5828700 3.2522072 1.0432161
H -2.2736696 2.9266397 -0.5764455

$MeOBHNH_2$: aminoborane
10
Energy = -196.7463925354
B -0.5781397 0.4140136 -0.0043429
H -0.3998897 1.6005556 -0.0163112
N -1.8835095 -0.1043928 0.0018683
H -2.7042098 0.4853603 -0.0041814
H -2.0949295 -1.0952576 0.0122057
O 0.4892789 -0.4623946 0.0022044
C 1.8281667 0.0708714 0.0027587
H 2.0078600 0.6599221 0.9083391
H 2.5143646 -0.7784233 -0.0198737
H 1.9948678 0.6974252 -0.8798180

BOf_3 : or $B(OCHO)_3$
13
Energy = -592.8200902380
B 0.1459150 0.0670239 0.5306402
O 0.2803935 1.3859602 0.9193202
O 1.2492458 -0.6405474 0.0957803
O -1.0918902 -0.5437343 0.5795419
C -0.7706975 2.1632745 1.3535251
C 2.5158381 -0.1038746 0.0185604
C -1.3132527 -1.8485876 0.1966338
O -0.5844093 3.3031296 1.6815033
H -1.7366980 1.6442309 1.3606029
O 3.4330022 -0.7734657 -0.3709130
H 2.5777679 0.9437094 0.3370457
O -2.4137972 -2.3221157 0.2728761
H -0.4165462 -2.3666395 -0.1642739

$B(OH)_2Of$: or $B(OH)_2OCHO$
9
Energy = -366.0403007489
B 0.1224877 0.1082686 0.5364658
O 0.3632688 1.3980721 0.9046353
O 1.1981373 -0.6968513 0.0958545
O -1.1226618 -0.4445507 0.5753514
C 2.4695023 -0.2288694 0.0234306
O 3.3739679 -0.9352838 -0.3556703
H 2.5860885 0.8181177 0.3332732
H -0.4339139 1.8720248 1.1931334
H -1.1491092 -1.3715615 0.2857533

$B(OH)_3.NH_3$: loose NH_3 adduct
11
Energy = -309.2544097870
B -0.7678104 -0.0187450 0.0267088
O -2.1228109 0.2852528 -0.0039217
O 0.1749705 0.9382404 -0.1950306
O -0.4042357 -1.3311971 0.2910017
H -2.2785107 1.2239446 -0.1949965
H 1.1448309 0.6001955 -0.1435036
H -1.1774939 -1.9017614 0.4274558
N 2.7305020 0.1080760 -0.0699142
H 2.7724385 -0.9004784 0.0789333
H 3.2557474 0.2989934 -0.9235923
H 3.2505729 0.5376140 0.6956752

$B(OH)_3$: boric acid
7
Energy = -252.6447631493
B -0.0000353 -0.0000399 0.0004253
O 1.3554852 -0.2467016 0.0004547
H 1.5650945 -1.1945953 -0.0005894
O -0.8914225 -1.0505950 0.0004256
H -1.8170629 -0.7580184 -0.0005633
O -0.4641026 1.2972742 0.0004156
H 0.2520436 1.9526760 -0.0005685

$BOHOf_2$: or $HOB(OCHO)_2$
11
Energy = -479.4318166242
B 0.1556085 0.1054071 0.5288712
O 0.3489036 1.3898120 0.8990754
O 1.2165186 -0.6911099 0.0955587
O -1.1197528 -0.4611107 0.5705749
C 2.5006454 -0.2263384 0.0235727
C -1.3836358 -1.7535546 0.2118508
O 3.3917784 -0.9415229 -0.3560469
H 2.6191032 0.8189661 0.3356633
O -2.5054363 -2.1889229 0.2684503
H -0.5033840 -2.3203558 -0.1164059
H -0.4575487 1.8513570 1.1844554

Cl^- : chloride anion
1
Energy = -460.4091180604
Cl 0.0000000 0.0000000 0.0000000

CO_2 : carbon dioxide
3
Energy = -188.6986489612
C 0.0000179 0.0000101 0.0000008
O 1.1685142 0.0000318 0.0000684
O -1.1683972 -0.0000353 -0.0000663

$Dbu.BH_2OH$: Dbu borane adduct
32
Energy = -564.3963759449
C 2.1688097 1.4026370 -0.0970006
C 0.9672414 1.4840110 0.8747000
C 2.9876711 0.1174197 0.0590871

H	1.8066043	1.5029946	-1.1272941
H	2.8199171	2.2616663	0.0989664
H	1.2585311	1.0822956	1.8519922
H	0.6723000	2.5217114	1.0300868
C	-0.2427742	0.7419389	0.3747661
C	2.1897833	-1.1752668	-0.1451069
H	3.4204596	0.1011254	1.0692560
H	3.8282420	0.1379020	-0.6445556
N	-0.2060091	-0.6051868	0.4269514
N	-1.2614488	1.4311557	-0.1138097
C	1.0124290	-1.3386251	0.8261475
H	2.8608818	-2.0294691	0.0036665
H	1.8122640	-1.2402363	-1.1736270
C	-1.3375763	-1.4290907	-0.0299068
C	-2.4379161	0.7073194	-0.6335412
H	1.3056974	-1.0432348	1.8403467
H	0.7150526	-2.3874664	0.8714965
H	-1.3743322	-2.3152706	0.6092098
H	-1.1560153	-1.7621985	-1.0598686
C	-2.6242026	-0.6289395	0.0670738
H	-3.3038153	1.3536381	-0.4829092
H	-2.3177907	0.5643627	-1.7157316
H	-3.4442995	-1.1868447	-0.3931667
H	-2.8748724	-0.4617897	1.1206242
B	-1.2763418	3.0389092	-0.2840330
H	-1.0623693	3.5391663	0.8163613
H	-2.4079202	3.2867407	-0.6683754
O	-0.3250223	3.4916089	-1.3208053
H	0.5645639	3.6073997	-0.9580330

$Dbu.BH_3$: Dbu borane adduct
31
Energy = -489.0867973547

C	2.2146521	1.3538532	-0.0439385
C	1.0083580	1.4372681	0.9187765
C	3.0108935	0.0512386	0.0908085
H	1.8608230	1.4851108	-1.0738239
H	2.8788909	2.1975565	0.1727496
H	1.2850888	1.0200788	1.8941643
H	0.7247607	2.4773875	1.0720329
C	-0.2029280	0.7132115	0.3988029
C	2.1957997	-1.2280082	-0.1339878
H	3.4425171	0.0112895	1.1009692
H	3.8530398	0.0692425	-0.6112855
N	-0.1921726	-0.6361913	0.4400186
N	-1.2061993	1.4225458	-0.0862687
C	1.0141387	-1.3891356	0.8335741
H	2.8562676	-2.0927291	0.0016872
H	1.8185320	-1.2722951	-1.1637593
C	-1.3251958	-1.4217260	-0.0716153
C	-2.4303998	0.7451802	-0.5551166
H	1.3097314	-1.1062789	1.8507563
H	0.7040057	-2.4348418	0.8685664
H	-1.3645901	-2.3513940	0.5014653
H	-1.1534013	-1.6799046	-1.1250097
C	-2.6058209	-0.6200597	0.0903132
H	-3.2692964	1.4018364	-0.3141766
H	-2.3871520	0.6592719	-1.6484984
H	-3.4409390	-1.1504058	-0.3753831
H	-2.8293222	-0.5023596	1.1566094
B	-1.1868733	3.0030556	-0.2582729
H	-1.3550802	3.5461240	0.8293404
H	-0.1308890	3.3631104	-0.7532935
H	-2.1147479	3.2692010	-1.0049561

$Dbu.H_2O$: H-bonded
30
Energy = -538.8706145503

C	2.2253777	1.3189162	-0.1422329
C	0.9942517	1.4995048	0.7739681
C	3.0133230	0.0294311	0.1168935
H	1.8984853	1.3616047	-1.1895196
H	2.8940296	2.1731822	0.0152539
H	1.2536332	1.2065258	1.7995203
H	0.7044891	2.5521804	0.7929495
C	-0.2189727	0.7357521	0.2958147
C	2.2058375	-1.2631622	-0.0468263
H	3.4062612	0.0628833	1.1433520
H	3.8826877	-0.0011219	-0.5514519
N	-0.1946593	-0.6226941	0.4184016
N	-1.1914830	1.4306222	-0.2273475
C	0.9918913	-1.3515724	0.8902776
H	2.8605263	-2.1163341	0.1702902
H	1.8631358	-1.3767760	-1.0834953
C	-1.3279103	-1.4298675	-0.0561928
C	-2.3658083	0.7193151	-0.7422202
H	1.2677709	-1.0035678	1.8940699
H	0.6786202	-2.3934032	0.9889720
H	-1.4084950	-2.3045366	0.5965474
H	-1.1313660	-1.7910609	-1.0756869
C	-2.6066184	-0.6030942	-0.0176670
H	-3.2321606	1.3819771	-0.6379767
H	-2.2343361	0.5356836	-1.8190727
H	-3.4239536	-1.1639632	-0.4821951
H	-2.8812713	-0.4047475	1.0251733
O	-1.3920031	4.1264475	-0.0042025
H	-1.2924397	3.1166559	-0.0905093
H	-1.5544652	4.2730236	0.9406036

$DbuH^+.OH_2$: H-bonded
31
Energy = -539.3484080719

C	2.2199974	1.2918050	-0.1398929
C	0.9774584	1.4747730	0.7625355
C	3.0141158	0.0146341	0.1545522
H	1.9090044	1.3180035	-1.1917016
H	2.8701052	2.1577841	0.0210639
H	1.2224672	1.2039898	1.7960175
H	0.6698958	2.5229349	0.7641718
C	-0.1981593	0.6621031	0.3031224

C	2.2248514	-1.2893982	-0.0084165
H	3.3885374	0.0675781	1.1862690
H	3.8931424	-0.0149821	-0.4993128
N	-0.1844821	-0.6638345	0.4004574
N	-1.2221827	1.3128712	-0.2322567
C	1.0003762	-1.3915354	0.9083000
H	2.8833625	-2.1314313	0.2333118
H	1.9037519	-1.4232297	-1.0491532
C	-1.3283129	-1.4742746	-0.0716253
C	-2.4329819	0.6579243	-0.7403144
H	1.2357269	-1.0309254	1.9158318
H	0.6833387	-2.4310163	0.9990785
H	-1.3886782	-2.3497527	0.5778315
H	-1.1207129	-1.8187689	-1.0913910
C	-2.6183878	-0.6664424	-0.0118518
H	-3.2725640	1.3337240	-0.5658447
H	-2.3333625	0.5049551	-1.8208510
H	-3.4259459	-1.2390546	-0.4735700
H	-2.8854533	-0.4780268	1.0329638
H	-1.1740170	2.3425572	-0.2605083
O	-1.2259327	4.1435022	-0.3457787
H	-0.5607102	4.6000720	-0.8866306
H	-1.2323252	4.6258420	0.4974545

$DbuH^+$: N-protonated Dbu
28
Energy = -462.8648172736

C	2.2268202	1.3381491	-0.1198438
C	0.9907561	1.5038390	0.7950507
C	3.0180242	0.0524557	0.1422054
H	1.9092885	1.3895643	-1.1686264
H	2.8790573	2.1991030	0.0577844
H	1.2409382	1.2071622	1.8202291
H	0.6878283	2.5533128	0.8254994
C	-0.1890488	0.7057504	0.3255846
C	2.2250177	-1.2443103	-0.0559400
H	3.3926619	0.0772090	1.1748723
H	3.8966303	0.0381811	-0.5127179
N	-0.1811825	-0.6199072	0.3789142
N	-1.2215179	1.3716114	-0.1822736
C	1.0025803	-1.3694677	0.8600775
H	2.8812377	-2.0946520	0.1614243
H	1.9019565	-1.3485632	-1.0994347
C	-1.3321028	-1.4106918	-0.1113827
C	-2.4456692	0.7437993	-0.6952226
H	1.2406013	-1.0404334	1.8776836
H	0.6794861	-2.4092357	0.9194782
H	-1.3867037	-2.3090228	0.5062540
H	-1.1337902	-1.7169583	-1.1448762
C	-2.6201237	-0.6041468	-0.0085758
H	-3.2771850	1.4169288	-0.4803019
H	-2.3622697	0.6302660	-1.7815477
H	-3.4334047	-1.1598594	-0.4805364
H	-2.8748224	-0.4514378	1.0450029
H	-1.1629490	2.3822190	-0.1760516

Dbu : 1,8-Diazabicyclo[5.4.0]undec-7-ene
27
Energy = -462.3809967830

C	2.1975313	1.3549237	-0.0716959
C	0.9770565	1.4899708	0.8663186
C	2.9939847	0.0580483	0.1158942
H	1.8558262	1.4435771	-1.1115416
H	2.8673694	2.2028081	0.1143546
H	1.2528599	1.1597335	1.8765977
H	0.6783334	2.5387505	0.9293165
C	-0.2419024	0.7438978	0.3709636
C	2.1886529	-1.2298007	-0.0912700
H	3.4036396	0.0463067	1.1364619
H	3.8526215	0.0620167	-0.5671062
N	-0.2064126	-0.6252029	0.4484141
N	-1.2155663	1.4596668	-0.1124717
C	0.9932588	-1.3620971	0.8656221
H	2.8517528	-2.0884763	0.0731521
H	1.8253475	-1.2978485	-1.1250736
C	-1.3239852	-1.4190628	-0.0767905
C	-2.3840238	0.7513310	-0.6496048
H	1.2901993	-1.0506319	1.8757593
H	0.6900237	-2.4098886	0.9328616
H	-1.3954997	-2.3324420	0.5226571
H	-1.1237386	-1.7184767	-1.1162733
C	-2.6119371	-0.6102014	0.0056492
H	-3.2622855	1.3934073	-0.5121393
H	-2.2581760	0.6220794	-1.7358332
H	-3.4257568	-1.1542606	-0.4854354
H	-2.8859628	-0.4701062	1.0584249

H_2CO_3 : carbonic acid
6
Energy = -265.1719501371

C	0.0070130	-0.0454969	0.3442346
O	0.0728088	-1.1114489	-0.2395634
O	0.4680532	0.2061262	1.5797583
H	0.8650526	-0.6161650	1.9236023
O	-0.5393831	1.0831220	-0.1353036
H	-0.8735444	0.8954019	-1.0325883

$H_2O.H_2O$: H-bonded water dimer
6
Energy = -152.9589854991

O	0.3694783	0.4592079	-0.3092859
O	0.7734567	2.2949521	1.7574631
H	0.6790955	1.6379315	1.0256950
H	0.7013984	-0.4225586	-0.0714089
H	0.8739115	0.7012793	-1.1037853
H	1.7264206	2.3283341	1.9358883

H_2O : water
3
Energy = -76.47649206796

O 0.0000000 0.0000001 0.1370316
H 0.0000000 0.7646592 -0.4614238
H 0.0000000 -0.7646591 -0.4614238

H_2 : dihydrogen
2
Energy = -1.180150698198
H 0.0278424 0.0000000 0.0000000
H 0.7721576 0.0000000 0.0000000

$H_5O_2^+$: proton bound to two H_2O
7
Energy = -153.3879169353
O 0.4152649 0.6206513 -0.1677944
O 0.7951201 2.0790810 1.7270849
H 0.6493159 1.3656969 0.7581753
H 0.5934300 -0.3091232 0.0679224
H 0.9640246 0.8240463 -0.9479607
H 1.7066054 2.4187940 1.7971388
H 0.2063846 2.8561028 1.6901456

$HBOf_2OH^-$: or $HB(OCHO)_2OH^-$ anion
12
Energy = -480.1638432997
B 1.9775936 0.1505221 0.5565605
H 1.9318856 -0.4491879 1.6150038
O 2.7168096 1.4813905 0.7672252
O 2.8214710 -0.5878749 -0.4586577
O 0.7131305 0.3982830 -0.0937514
C 3.2116798 1.7929657 1.9430983
C 3.4554810 -1.6911554 -0.1245039
O 3.8150092 2.8385247 2.1692093
H 3.0397276 1.0374184 2.7303949
O 4.1604992 -2.3239005 -0.9030036
H 3.3023516 -2.0110329 0.9212612
H 0.0408622 0.6646044 0.5502401

$HBOf_3^-$: or $HB(OCHO)_3^-$ anion
14
Energy = -593.5762295318
B 0.1163449 0.1179371 0.3644324
H 0.3143635 -0.2421998 1.5009850
O -0.4375950 1.5042004 0.2873906
O 1.3604045 0.1228438 -0.4640932
O -0.8570961 -0.7572960 -0.3568040
C -0.6595700 2.1991312 1.3909111
C 2.5187932 -0.2352161 0.0649777
C -1.4026487 -1.7967615 0.2530400
O -1.1108834 3.3347631 1.3817721
H -0.4034585 1.6688672 2.3238685
O 3.5639243 -0.2457109 -0.5682433
H 2.4652407 -0.5250236 1.1281220
O -2.2030788 -2.5422827 -0.2917990
H -1.0755062 -1.9370885 1.2972680

$HBOf(OH)_2^-$: or $HB(OH)_2OCHO^-$
10
Energy = -366.7481607644
B 1.9583547 0.0448285 0.5360999
H 1.9011577 -0.4683022 1.6555139
O 2.7537363 1.4077522 0.7438704
O 2.6797887 -0.7388740 -0.4512711
O 0.6718897 0.3818049 -0.0515565
C 3.1825725 1.7616246 1.9227032
O 3.8040444 2.8036123 2.1502968
H 2.9483461 1.0477366 2.7334752
H 3.4495411 -1.1640697 -0.0476993
H 0.1221756 0.8593560 0.5861876

$HCO_2BH_2NH_3$:
11
Energy = -272.0206287943
B 0.4358297 1.0102357 0.1241347
H 1.6127425 1.0339352 0.4043293
O 0.1151093 -0.1479188 -0.8014046
N -0.3764961 0.7888432 1.4938734
H 0.0254991 2.0173577 -0.4015502
C 0.3969071 -1.3834711 -0.4392465
H -0.0851132 -0.0870212 1.9378176
H -1.3890667 0.7445024 1.3593074
H -0.2008980 1.5454226 2.1583013
O 0.8101001 -1.7358141 0.6625790
H 0.2072445 -2.0998198 -1.2532791

$HCO_2BH_2OH^-$: borate anion
9
Energy = -291.4265571247
B -1.2818009 0.5319057 0.4786271
H -1.8103049 1.5740673 0.0945232
H -1.5052704 0.2940870 1.6579754
H -0.0101356 2.4418981 -0.7061644
O -1.6407423 -0.6457936 -0.3156497
H -1.6599791 -0.4282648 -1.2597455
C 0.7539463 1.7809945 -0.2558299
O 0.2673763 0.7603635 0.3990925
O 1.9581763 2.0146442 -0.3729247

HCO_2BH_2 : borane
7
Energy = -215.3672065106
B -1.4096597 -0.2600227 -0.0122770
H -1.5726552 -1.4417687 0.0025640
H -2.2835018 0.5453971 -0.0243240
H 0.6537049 -1.6784714 0.0078871
C 0.9499790 -0.6186933 -0.0030762
O -0.1233550 0.2477631 -0.0160617
O 2.0776060 -0.2056033 -0.0044100

$HCO_2BH_3^-$: borate anion
8

Energy = -216.1116335337

B	-1.5227240	-0.2356396	0.3514929
H	-1.9277379	-0.0307431	1.4884738
H	-1.5665875	-1.4286824	0.0772358
H	-2.1582882	0.4255591	-0.4595021
H	0.5838326	-1.6082927	-0.2176387
C	0.9123737	-0.5716829	-0.0146621
O	-0.0547505	0.2502851	0.2914518
O	2.0982622	-0.2429458	-0.0780755

$HCO_2BH(OH)_2^-$: borate anion

10

Energy = -366.7476434738

B	0.9765919	0.0104339	0.4210625
H	0.7288112	0.0277547	1.6172940
H	-1.4496545	0.0110031	1.3553741
O	1.6655084	-1.2358365	0.0874177
H	1.8547323	-1.2878147	-0.8634748
C	-1.5260013	0.0066947	0.2528260
O	-0.3816386	0.0071834	-0.3722543
O	-2.6217378	0.0021221	-0.3133894
O	1.6785032	1.2399135	0.0543572
H	1.8787675	1.2591796	-0.8954398

$HCO_2BH(OH)NH_3$: ammonia borane

12

Energy = -347.3394558472

B	0.3785431	1.0295819	0.0526899
H	1.5681500	1.0811427	0.2721189
O	-0.2165877	2.1821954	-0.5610072
H	0.4390716	2.7008108	-1.0471604
H	-0.0773600	-0.0891507	1.8668052
C	0.3986951	-1.4117950	-0.4060179
O	0.8473843	-1.7144634	0.6986244
O	0.0579243	-0.2033137	-0.7989370
H	0.2281542	-2.1629816	-1.1927916
N	-0.3848003	0.7964213	1.4511389
H	-1.4015513	0.7555806	1.3414546
H	-0.1852804	1.5442961	2.1180955

$HCO_2^-.H_2O$: H-bonded anion

7

Energy = -265.9062957125

O	2.3531971	0.1264598	0.1288482
H	2.4525980	-0.0948725	-0.8100600
H	1.3869076	-0.0705528	0.3355293
C	-1.0176538	0.2897222	0.0384073
H	-0.5582367	1.0129311	-0.6788606
O	-0.1992898	-0.4045766	0.7225820
O	-2.2702616	0.2458409	0.0855696

HCO_2H : formic acid

5

Energy = -189.8826207797

C	0.0152341	-0.0600257	0.3532880
O	0.0858686	-1.1278553	-0.2206949
O	0.4793037	0.1831472	1.5903599
H	0.8798906	-0.6382260	1.9454193
H	-0.4377838	0.8487180	-0.0634205

HCO_2^- : formate anion

4

Energy = -189.4190669102

C	0.0000028	-0.0000501	0.3355594
H	-0.0000010	0.0000216	1.4577606
O	-0.0000009	1.1343085	-0.2182883
O	-0.0000009	-1.1342800	-0.2182955

$HCO_3^-.H_2O$: H-bonded anion

8

Energy = -341.2010781715

C	0.8881879	0.1591687	0.9986311
O	1.6416580	1.1453033	0.8864499
O	0.8545539	-0.8891944	0.2757065
O	-0.0282748	0.2257252	2.0545760
H	-0.5642223	-0.6046505	2.0334585
O	-1.0562782	-2.3255060	1.3703150
H	-0.3236544	-1.9161544	0.8074151
H	-1.8658486	-2.2360241	0.8423321

HCO_3^- : bicarbonate anion

5

Energy = -264.7131829931

C	0.0000065	-0.0044980	0.3411523
O	0.0000850	1.1287024	-0.1889216
O	-0.0000489	-1.1465206	-0.1848796
O	-0.0002124	0.0247403	1.7599279
H	0.0001699	-0.9073601	2.0428825

$HOBH_2NH_3$: ammonia borane

9

Energy = -158.6054607474

O	1.3716285	-0.2728957	-0.0187749
H	1.5885433	-0.5306691	0.8891459
B	0.2362983	0.6488367	-0.0490562
H	0.1612623	1.4035774	0.9105856
H	0.1977623	1.2336382	-1.1194812
N	-1.1571308	-0.2298620	-0.0021965
H	-1.9864806	0.3626619	-0.0851404
H	-1.2569953	-0.7564158	0.8684637
H	-1.1993060	-0.9097587	-0.7646321

$HOBH_2.OH_2$: borane water adduct

8

Energy = -178.4622343539

B	0.5152800	-0.5791338	0.0346001
H	0.5647739	-0.9176025	1.1976710
H	0.8589546	-1.3949289	-0.7905481
O	0.9845028	0.7336817	-0.2800473
H	0.9302306	1.3302923	0.4815678

O -1.1835820 -0.6294245 -0.2028169
H -1.6637572 -0.0583270 0.4250806
H -1.4278449 -0.3138811 -1.0931082

$HOBHOf_2^-$: or $HOBH(OCHO)_2^-$ anion
12
Energy = -480.1645021533
B 0.0773738 0.7896951 0.0083434
H 0.1628153 0.7357300 1.2180106
O -0.0306148 2.1514273 -0.4438421
O -1.1046430 -0.0357272 -0.4931175
H 2.1298430 -0.2423512 1.1607106
H -0.1016458 2.2000096 -1.4108695
C -1.9250139 -0.6154003 0.3540518
O -2.9048422 -1.2677588 0.0073693
H -1.6648419 -0.4694918 1.4169458
C 2.2596540 -0.3685199 0.0716198
O 1.2701449 0.1006344 -0.6540640
O 3.2544136 -0.9049381 -0.4069624

HOBHOf : or borane HOBH(OCHO)
8
Energy = -290.7086286819
B -1.2425086 0.4651382 -0.0110578
H -2.1639494 1.2147215 -0.0172966
O -1.4266950 -0.8717648 -0.0465678
O 0.0402046 1.0721914 0.0356740
H -0.5611543 -1.3402633 -0.0352298
C 1.1941430 0.3687622 0.0485660
O 1.2753105 -0.8450502 0.0216383
H 2.0607703 1.0394778 0.0868738

$NH_3.OH_2$: H-bonded
7
Energy = -133.0747374482
O 1.5143822 -0.1619973 0.2613739
H 1.6461149 -0.7266562 -0.5178519
H 1.8703344 0.7001773 -0.0096174
N -1.6468592 0.2444338 0.2695028
H -1.8827787 0.5244197 -0.6837601
H -2.0657913 -0.6783641 0.3949243
H -0.6314422 0.0990008 0.2786483

NH_3 : ammonia
4
Energy = -56.59634858633
N -1.3266738 0.0001256 0.0010138
H -1.7250518 0.9368036 -0.0813918
H -1.7425776 -0.4029151 0.8420993
H -1.7128708 -0.5330141 -0.7796732

$NH_4^+HCO_2^-$: H-bonded contact ion pair
9
Energy = -246.4998027258
N 2.4575882 -0.0864573 0.0005833
H 2.9690934 -0.4115748 0.8225065
H 2.9510369 -0.4009852 -0.8363490
H 1.4151904 -0.4510924 0.0089351
H 2.4366508 0.9351314 0.0070818
C -0.7637975 0.1847549 -0.0010345
O -0.0527589 -0.8811479 0.0228535
O -0.3447548 1.3628975 -0.0332891
H -1.8633924 0.0150917 0.0087040

$NH_4^+HCO_3^-.H_2O$: H-bonded contact ion pair
13
Energy = -398.2781447751
N 2.4715123 -0.2043692 -0.0147057
H 2.9233725 -0.2588060 0.8993515
H 2.9815897 -0.8023839 -0.6666114
H 1.4462123 -0.5126199 0.0516980
H 2.4819718 0.7819658 -0.3570413
C -1.0561743 -0.1152217 0.0455215
O -0.1071222 -0.9457302 0.0758469
O -0.6305941 1.2385974 0.0042618
H -1.4396659 1.7816544 -0.0167144
O -2.2837878 -0.3114149 0.0515150
O 1.7686270 2.3895154 -0.8280377
H 0.8470501 2.0893062 -0.6394824
H 1.7981068 2.5258751 -1.7896050

$NH_4^+HCO_3^-$: H-bonded contact ion pair
10
Energy = -321.7925286721
N 2.3854238 -0.0564403 -0.0004050
H 2.8978718 -0.3773021 0.8231627
H 2.8806473 -0.3744356 -0.8355336
H 1.3548818 -0.4369069 0.0094140
H 2.3729911 0.9651479 0.0016720
C -0.9708825 -0.0699835 0.0073985
O -0.0755999 -0.9723388 0.0247377
O -0.4433560 1.2264895 -0.0247585
H -1.2043496 1.8350839 -0.0343962
O -2.2078138 -0.2033130 0.0154412

$NH_4^+.OH_2$: H-bonded ammonium
8
Energy = -133.5462065183
O 1.4169754 0.0834343 -0.2514409
H 1.8510520 -0.7744588 -0.1077970
H 1.8480880 0.6861852 0.3777442
N -1.3242641 0.0009188 -0.0007670
H -1.7047242 0.9305126 -0.1906203
H -1.6211467 -0.2914402 0.9324943
H -1.7046651 -0.6545436 -0.6868017
H -0.2698285 0.0195196 -0.0605495

$OCH(OH)_2^-$: hydrogenated bicarbonate anion
7
Energy = -265.8640606858

O 1.1895512 -0.6955347 -0.0411443
O -0.0003712 1.2994181 -0.1555016
C 0.0000394 0.1061158 0.3537517
O -1.1887774 -0.6960648 -0.0409297
H 1.4558595 -0.2791624 -0.8818498
H 0.0003920 0.0015787 1.4594467
H -1.4563577 -0.2791847 -0.8809090

THF : tetrahydrofuran
13
Energy = -232.5937965276
O -0.0001678 -0.0000229 1.2607277
C -0.0973574 1.1813074 0.4190380
C 0.2601563 0.7227481 -0.9937539
C -0.2601908 -0.7227564 -0.9937716
C 0.0973454 -1.1812878 0.4190159
H 0.5833139 1.9394326 0.8189156
H -1.1261437 1.5643024 0.4665298
H 1.3463401 0.7357989 -1.1370812
H -0.2006797 1.3479246 -1.7632811
H -1.3463770 -0.7358339 -1.1370474
H 0.2006852 -1.3479324 -1.7632702
H -0.5831407 -1.9396027 0.8188665
H 1.1262163 -1.5640786 0.4665620

TS0a : NH_3-bridged H_2-release from BH_3NH_3
12
Energy = -139.8493314817
B -1.4588141 0.7496141 0.0065087
H -1.7782414 1.3175235 1.0282517
H -1.8413846 1.2512326 -1.0281847
N -1.5108805 -0.7144566 0.0554129
H -0.1034605 1.3339165 -0.0553348
H -1.2432142 -1.2446871 -0.7672573
H -1.1925849 -1.1906993 0.8929240
H 1.6176058 -1.0108226 -0.0154307
N 1.8439898 -0.0182105 -0.0503415
H 0.6431033 0.7991959 -0.0524162
H 2.4235756 0.2055341 0.7580754
H 2.3916379 0.1546953 -0.8927653

TS0b : H_2O-bridged H_2-release from BH_3NH_3
11
Energy = -159.7195261174
B -1.1980168 0.7405998 0.0330614
H -1.5430598 1.1987241 1.0931894
H -1.8226220 1.0952004 -0.9359494
N -0.8005805 -0.7362078 0.0656160
H -0.0712006 1.5299220 -0.1826794
H -1.1531774 -1.2882150 -0.7128348
H -1.0516204 -1.2172535 0.9259581
H 0.6572231 -0.5990984 -0.0308557
O 1.5986470 -0.0259573 -0.1986964
H 0.6689964 0.9818400 -0.1695034
H 2.0739919 0.0118335 0.6493047

TS0 : H_2-release from HCO_2H and BH_3NH_3
13
Energy = -273.1440154306
B -0.6033008 -1.7181724 0.0863508
H -1.3648541 -0.5646394 -0.0152985
H -0.0984466 -2.0286467 -0.9464262
H -0.6492488 -0.2856817 -0.2860540
C 0.4031298 1.9036885 0.1021719
O 1.0152987 0.8070308 -0.1399222
O -0.8097587 2.0344967 0.3800510
H 1.0305689 2.8224801 0.0483895
H -1.6001307 -2.2873502 0.4173412
H 0.9609987 -0.6115353 0.9717598
H 0.0210675 -1.3478721 2.1566519
H 1.0979917 -2.2489703 1.3038891
N 0.4331918 -1.4760325 1.2308330

TS1a : CO_2 hydration with two H_2O
9
Energy = -341.6308863358
C 0.8605420 -0.1976107 -0.0104642
O 2.0382273 -0.0508378 0.2772315
O 0.1222633 -1.1569186 -0.2970513
O 0.0703703 1.1120804 -0.0655631
H 0.4870931 1.7796743 0.5092003
H -1.1475547 0.8236301 0.0908890
O -2.1026356 0.1292642 0.0649476
H -1.5504976 -0.7045591 -0.0780934
H -2.5218817 0.0653678 0.9429185

TS1 : CO_2 hydration with three H_2O
12
Energy = -418.1251015483
C 1.3862145 -0.0670404 0.0899236
O 2.5239577 0.2512710 0.3861896
O 0.7182643 -1.0962393 0.0022157
O 0.5317316 1.1892651 -0.3381820
H 1.0188322 1.9900742 -0.0703501
H -0.6046802 1.2134150 -0.0167770
O -1.8365294 1.1579639 0.2049987
H -2.0686711 0.1628583 0.0950616
H -2.0543280 1.4173454 1.1167626
O -1.9775940 -1.3838212 -0.1432477
H -0.9857938 -1.4269693 -0.1874288
H -2.2989688 -1.6549529 -1.0190233

TS20 : S_N2 replacement of NH_3 with CO_2
11
Energy = -271.9305525599
B 0.0018452 -0.3629497 -1.1125846
H -0.9223622 0.3932172 -1.0664822
H 1.1199010 0.0538703 -1.0348684
H -0.1883327 -1.5304538 -1.2830845
N 0.0054557 0.1720387 -4.2667567

H -0.9527425 0.2039729 -4.6140036
H 0.4136878 1.0872835 -4.4552122
H 0.5054073 -0.4959391 -4.8531559
O -0.0841753 -0.6661055 1.1343263
C 0.0084644 0.1611756 1.9599566
O 0.0994600 0.9770508 2.7852973

TS2a$^-$: S_N2 replacement of NH_3 with HCO_3^-
13
Energy = -347.9681988902
B -0.2119162 -0.1874577 -1.3923269
H -0.5969558 0.9494835 -1.3383915
H 0.9571267 -0.4323227 -1.2614374
H -0.9860388 -1.0714502 -1.6544581
O -0.6041916 -0.5206628 0.6148064
C -0.0258731 0.1885341 1.4844422
O 0.7880028 1.1250408 1.3593855
O -0.3906430 -0.1738741 2.8012775
H 0.1023393 0.4304612 3.3853411
N 0.1348487 0.0786999 -3.5998374
H -0.7263744 0.3190894 -4.0903211
H 0.8067059 0.8208689 -3.7939899
H 0.4961728 -0.7722522 -4.0303370

TS2a : S_N2 replacement of NH_3 with H_2O
11
Energy = -159.7293756124
B 0.0061516 -0.0008029 0.1811804
H -0.6034673 1.0292626 0.0823165
H 1.2039597 0.0136698 0.0834155
H -0.5791309 -1.0447557 0.0795256
N 0.0051344 0.0010285 -2.2996575
H -0.9462672 -0.0081478 -2.6660243
H 0.4636292 0.8232381 -2.6915339
H 0.4783977 -0.8137404 -2.6892254
O -0.0623358 -0.0045716 2.1387674
H 0.4474976 -0.7689003 2.4599178
H 0.4256431 0.7720601 2.4632330

TS2b$^-$: S_N2 replacement of NH_3 with HCO_2^-
12
Energy = -272.6783194499
B -1.3248669 0.2097672 0.0712121
H -1.1177632 -0.9050417 -0.3328124
H -1.5025135 1.1105058 -0.7065069
H -1.4220076 0.4143795 1.2526599
H 1.0513185 -1.3232203 -0.1506050
C 1.5196365 -0.3243304 0.0096145
O 0.7064443 0.6456940 0.1272234
O 2.7739865 -0.2641221 0.0547872
N -3.5140642 -0.2323288 0.0058743
H -4.0789702 0.5458046 0.3456007
H -3.7468982 -1.0436116 0.5782397
H -3.8256628 -0.4366200 -0.9434361

TS2b : S_N2 replacement of NH_3 with Dbu
35
Energy = -545.6433033570
C -0.5314694 -2.3471878 -0.2348632
C -0.0373842 -1.3484148 0.8342429
C -2.0561144 -2.5012719 -0.2910330
H -0.1434520 -2.0357996 -1.2134401
H -0.0904301 -3.3274155 -0.0175636
H -0.6112802 -1.4840803 1.7601142
H 1.0129505 -1.5399053 1.0544181
C -0.1074997 0.0888461 0.3762010
C -2.8272757 -1.2034209 -0.5599839
H -2.3992380 -2.9112858 0.6701783
H -2.3153152 -3.2414239 -1.0583599
N -1.3517081 0.6604502 0.3024210
N 1.0106147 0.6758788 0.0645085
C -2.5831976 -0.1156541 0.4986660
H -3.9008278 -1.4299624 -0.5723479
H -2.5731927 -0.7995203 -1.5489106
C -1.4971833 2.0272523 -0.2109819
C 0.9796524 2.0623205 -0.3983025
H -2.5851209 -0.5649384 1.5004132
H -3.3987351 0.6113565 0.4750194
H -2.3776839 2.4710561 0.2643722
H -1.6765060 2.0111433 -1.2964169
C -0.2404359 2.8271930 0.1091616
H 1.9069065 2.5422353 -0.0638176
H 1.0022276 2.0750619 -1.4981308
H -0.3013049 3.8188406 -0.3513502
H -0.1654840 2.9627468 1.1950181
B 3.0647966 -0.1092512 -0.0243768
H 3.2647982 0.3186082 1.0823364
H 2.6905742 -1.2404811 -0.1795105
H 3.2251949 0.6094886 -0.9770702
N 5.1324869 -0.7634904 -0.1632426
H 5.7823857 0.0169785 -0.0691175
H 5.3672995 -1.4380692 0.5647807
H 5.3280076 -1.2098212 -1.0592571

TS2c$^-$: transfer hydrogenation of HCO_3^-
13
Energy = -347.9522490610
B -1.6027663 -0.9368126 -0.4759288
H -1.5959992 -1.9433001 0.1972621
H -1.7555672 -1.0703242 -1.6706276
N -2.2360906 0.2748470 0.1169592
H -2.5926883 0.2175281 1.0653887
H -0.7395631 1.1491224 0.1549794
H -2.8745186 0.8135558 -0.4590691
H -0.2221266 -0.6787247 -0.4627360
O 0.2486168 1.3170874 -0.0310384
O 1.7936507 -0.1657032 -0.8508989
C 0.8239019 0.0512016 -0.0712891
O 0.9514230 -0.3983224 1.2943252
H 1.4900224 -1.2076755 1.2443810

TS2 : transfer hydrogenation of CO_2
11
Energy = -271.9623842486
B -1.6351942 1.1070755 0.0001874
H -1.5903356 1.6663016 -1.0485711
H -1.5906461 1.6660591 1.0490924
N -1.9372560 -0.3472398 -0.0001144
H -2.4102095 -0.7023441 -0.8314223
H -0.8304524 -0.8696639 -0.0000598
H -2.4103403 -0.7028028 0.8309291
H 0.1483851 0.8907648 0.0007228
C 0.9536494 0.0572208 -0.0000896
O 0.4579704 -1.1197913 -0.0002001
O 2.1220941 0.4306904 -0.0005173

TS3a : HCO_2H addition to B=N
11
Energy = -271.9798037064
B 0.4722211 1.2324343 0.1583825
H 1.6231174 1.3316430 -0.1515015
H -0.1423573 -0.9118771 1.0239167
C -0.0491765 -1.5675186 -0.7397205
O -0.2725587 -1.8071976 0.5395775
O 0.2557481 -0.4676441 -1.2001886
H -0.1628951 -2.4595216 -1.3687354
N 0.1612811 0.7292758 1.4735636
H -0.7179367 0.9686941 1.9200761
H 0.8985462 0.5887167 2.1565269
H -0.3813528 1.8164059 -0.4421261

TS3b : cyclic addition of three H_2O to B=N
15
Energy = -311.5476957272
O 1.2438864 -0.1839606 0.9535507
H 1.4219776 -1.1021709 1.2164698
B -0.0181807 0.4322316 1.6489482
H 0.0957702 0.1497817 2.8254133
H 0.0352395 1.6226543 1.4242746
N -1.3018027 -0.1644496 0.9893762
H -2.1236412 0.3425705 1.3242727
H -1.4632764 -1.1390754 1.2517472
H -1.3337041 -0.0621921 -0.3470124
O 1.2284232 -0.0339031 -1.5191721
H 1.2840140 -0.1087835 -0.1338669
H 1.6289557 0.7906454 -1.8400135
O -1.2815505 0.0022360 -1.5460246
H 0.1766076 0.0458330 -1.6563439
H -1.6547337 0.8630068 -1.7959171

TS3 : cyclic addition of two H_2O to B=N
12
Energy = -235.0583426660
O 1.1885566 0.0236235 -0.5245839
H 1.6698727 -0.8158338 -0.6098657
B 0.8064337 0.3336605 1.0058588
H 1.5648308 -0.3396901 1.6687995
H 0.9548574 1.5296057 1.1321866
N -0.6949011 -0.0455344 1.1632655
H -1.2255267 0.6501773 1.6837513
H -0.8559998 -0.9428548 1.6185135
H -1.1549610 -0.1098214 -0.1563943
O -1.1225561 -0.1977633 -1.3110296
H 0.2439912 -0.0656936 -1.0779909
H -1.4920554 0.6191001 -1.6861915

TS4a : CO_2 hydrogenation with $HOBH_2NH_3$
12
Energy = -347.2906460178
B -1.2430143 0.2821559 -0.5198741
H -1.2671077 0.4068615 -1.7203195
N -1.4517595 -1.2340725 -0.0861088
H -2.2214921 -1.6847939 -0.5860535
H -0.6024988 -1.7811448 -0.2665615
H -1.6577775 -1.3162951 0.9131924
H 0.0383149 0.4426605 -0.2021184
C 1.4386934 0.0401951 0.0232683
O 1.4907599 -1.1572792 -0.1233135
O 2.0187372 1.0641124 0.2686878
O -2.0750544 1.1026618 0.2877200
H -2.2288537 1.9684128 -0.1181205

TS4b : CO_2 hydrogenation with $MeOBH_2NH_3$
15
Energy = -386.6125443858
B -0.8646816 -0.4962636 -0.4452136
H -0.9820719 -0.5227207 -1.6481614
N -0.4378182 -1.9047948 0.1463600
H -0.8992368 -2.6895450 -0.3185317
H 0.5768369 -2.0364919 0.0457613
H -0.6566824 -1.9756625 1.1436389
H 0.2530187 0.2084155 -0.2515422
C 1.7018811 0.4013151 -0.0765146
O 2.2047121 -0.6970908 -0.0262138
O 1.8611189 1.5928255 -0.0503154
O -1.9221977 0.0230817 0.3354490
C -2.5789904 1.1943227 -0.1640963
H -3.4641386 1.3684159 0.4526542
H -1.9174883 2.0676698 -0.0984483
H -2.8818741 1.0537783 -1.2096675

TS4c : CO_2 hydrogenation with BH_3NHMe_2
17
Energy = -350.6174272048
B -0.6644311 1.5070918 -0.0088142
H -0.5035005 2.0370674 -1.0613870
H -0.5088870 2.0507996 1.0375453
N -1.2432530 0.1404399 -0.0012576
H -0.2173863 -0.5280298 0.0068273
H 1.0849442 0.9711979 -0.0013134

C 1.7070170 -0.0031793 0.0081530
O 0.9819311 -1.0569475 0.0143453
O 2.9273965 0.1202315 0.0106921
C -1.9587300 -0.3006208 -1.2399670
H -1.3782864 0.0063533 -2.1101056
H -2.0606154 -1.3877346 -1.2233533
H -2.9480136 0.1601174 -1.2722250
C -1.9666719 -0.2835219 1.2388277
H -1.3908720 0.0338232 2.1083376
H -2.9555072 0.1788703 1.2594097
H -2.0699495 -1.3706205 1.2356948

TS4$^-$: S_N2 replacement of NH_3 with HCO_2^-
13
Energy = -347.9960022732
B -1.0396905 0.3229355 -0.1089298
H -0.7286658 -0.6268678 -0.7689524
O -1.3223445 0.0808812 1.2323130
H -1.1206643 1.4284667 -0.5667458
H -1.5946112 0.8887859 1.6927405
H -4.0416522 0.5926248 -0.4927026
N -3.3914975 -0.0428655 -0.9556077
H -3.6634628 -0.9876613 -0.6840394
H -3.5655686 0.0373578 -1.9578425
O 1.3120212 0.7651713 0.0935843
C 2.0342838 -0.2397694 -0.1671550
H 1.4913456 -1.1417331 -0.5436495
O 3.2873090 -0.3354694 -0.0530308

TS4 : S_N2 replacement of NH_3 with H_2O
12
Energy = -235.0521851088
B -0.0469257 0.4237462 0.1656374
H -1.1948112 0.7622466 0.1373341
H 0.8541294 1.2112890 0.1819089
O 0.3059120 -0.9049988 0.0391467
H -0.4629902 -1.4936869 -0.0183068
O -0.1201090 0.5124425 2.5744656
H 0.1475178 -0.4086774 2.7329813
H 0.6708080 1.0299962 2.8004119
N -0.0821242 0.5926214 -2.6575927
H -0.9559963 0.0896763 -2.8148050
H 0.1312809 1.0719518 -3.5338225
H 0.6378123 -0.1196072 -2.5363662

TS5a$^-$: S_N2 replacement of HCO_2^- with H_2O
12
Energy = -367.8745094730
B -1.2210830 0.1886245 -0.3574740
H -1.0326371 -0.9511266 -0.6718806
O -1.1849351 0.4638726 0.9988111
H -1.3058821 1.0728868 -1.1623605
H -1.2755820 1.4108896 1.1848935
H -3.6422684 -0.9079551 0.0207911
O -3.4710774 -0.2061403 -0.6298248
H -3.9228349 0.5727745 -0.2632126
O 1.4300855 0.4653687 -0.7901815
C 1.9549557 -0.3523983 0.0150604
H 1.2659871 -1.1174564 0.4517639
O 3.1627816 -0.4057268 0.3843722

TS5a : H_2-release from BH_2OH and three H_2O
14
Energy = -331.4177858025
B 1.1339807 0.3808125 -0.1818816
H 0.4623696 -0.2050322 -1.2206096
H 0.9137200 1.5714868 -0.3150669
O 0.5634476 -0.1066981 1.0790064
H -0.5871897 -0.1324688 -1.3238698
H 0.8470014 -1.0193297 1.2538068
O -1.7507858 -0.0179804 -1.3611022
H -2.1206670 -0.8284074 -1.7572304
H -2.0243271 0.0159739 -0.3379686
O -2.0475007 0.0536276 1.1316518
H -2.3574027 0.9038041 1.4851032
H -1.0415174 0.0261904 1.2670403
O 2.4982204 -0.0685901 -0.3282513
H 2.9262896 0.3408167 -1.0951470

TS5b$^-$: H_2-release: $BH_2(OH)_2^-$ and HCO_2H
12
Energy = -367.8859637618
B -0.4670910 -1.8250013 0.0910811
H -1.0456777 -0.4781673 -0.0137410
O 0.1813208 -2.1183419 -1.1455412
H 1.0535357 -1.6937012 -1.1860531
H -0.5114526 0.2243498 -0.3180319
C 0.2070887 2.2715127 -0.1186850
O 0.2627184 1.1901734 -0.8252019
O -0.4877802 2.4764408 0.8877525
H 0.8727515 3.0753254 -0.4992029
H -1.5304797 -2.4023022 0.2142120
O 0.4172927 -1.7837285 1.2161373
H -0.0678385 -1.6891966 2.0493802

TS5b : H_2-release from BH_2OH and two H_2O
11
Energy = -254.9235852237
B -0.7787323 -0.2101105 0.5470906
H 0.0005648 0.8125575 1.0039873
O 0.1214897 -1.0312957 -0.3256030
H 0.9956933 0.8214949 0.6483938
H 0.1815966 -1.9442463 -0.0060990
H -1.1265316 -0.7752119 1.5602624
O 2.0106161 0.4809123 0.1369099
H 2.2482247 1.1150215 -0.5649183
H 1.4770167 -0.3122918 -0.2857504
O -1.8841761 0.3825742 -0.1491072
H -1.6171463 0.7405532 -1.0106943

TS5ca : H_2-release from BH_2NH_2 and two H_2O
12
Energy = -235.0270592557
O 0.6913394 -1.1127874 -0.4361376
H 1.0295036 -1.6311901 0.3125175
B 1.4354128 0.2045143 -0.4957430
H 2.0738298 0.3420909 -1.5203391
H 0.4319096 1.1197864 -0.6856546
N 2.2118436 0.4636290 0.7419903
H 1.6778979 0.6079250 1.5966719
H 2.9102365 1.1990055 0.6760339
H -0.5638716 0.7646213 -0.5493642
O -1.4574274 0.0269793 -0.3075229
H -0.7252118 -0.7478845 -0.3257017
H -2.0187250 -0.0498600 -1.1009547

TS5cn : H_2-release: BH_3OH^- and $NH_4^+.OH_2$
14
Energy = -236.2265672529
B -0.3414341 -1.5046605 0.9873379
H 0.2960237 -0.4953978 1.9936378
O 0.2967525 -1.3964166 -0.2690102
H -1.4827318 -1.1341358 0.9985165
H 0.0002049 -2.3906467 1.7291869
H 1.1625084 -1.8318371 -0.2950095
H 0.0825286 -0.0156456 -1.3502169
O -0.0081935 0.8213003 -1.8721545
H -0.9004053 0.7839798 -2.2519265
H 0.1501577 0.2500515 1.6620852
N 0.0128157 1.8516181 1.0388250
H 0.8103108 2.4494422 1.2539978
H -0.8244287 2.3339229 1.3643938
H -0.0495856 1.7619631 0.0186291

TS5c : H_2-release from BH_2NH_2 and three H_2O
15
Energy = -311.5189617652
O 0.6844773 -1.1617268 -0.5592209
H 1.2496263 -1.8494859 -0.1706819
B 1.4440827 0.1270216 -0.5654772
H 2.3199004 0.1906010 -1.4128861
H 0.5417643 0.9655166 -1.1317115
N 1.9187262 0.5347407 0.7845136
H 1.2069756 0.6525687 1.5034537
H 2.5314883 1.3462489 0.8090262
H -0.3887396 1.1618787 -0.7395572
O -1.6177736 -0.9889858 0.6065345
H -0.7196543 -1.2013999 0.1607848
H -2.2787438 -1.5722685 0.1981931
O -1.4696052 1.3489934 -0.2614794
H -1.7089198 0.3792459 0.1064054
H -2.0763727 1.5602593 -0.9943389

TS5d : H_2-release:$HOBH_2NH_3$ and HCO_2H
14
Energy = -348.4631191798
B -0.5064197 -1.8972402 0.0419059
H -1.4028637 -0.6407669 -0.0318711
O 0.1365032 -2.1105235 -1.1622441
H 0.8933594 -1.5204842 -1.3191049
H -0.7795611 -0.1082243 -0.1396629
C 0.4038668 1.9926267 0.0786045
O 0.6073469 0.7817035 -0.3048935
O -0.6592302 2.4671805 0.5177050
H 1.2914358 2.6575986 -0.0089727
H -1.4345165 -2.5926507 0.3162898
H 0.9005099 -0.6101372 1.0262085
H -0.1145105 -1.3493895 2.1231302
H 1.1107052 -2.2117466 1.4497465
N 0.4086750 -1.4920129 1.2557408

TS6a : H_2-release from $BH(OH)_2$ and two H_2O
12
Energy = -330.2455505490
B -0.4364114 0.1389099 -0.0229420
H 0.3093334 1.2821649 0.0882655
O 0.4071209 -0.9987217 0.4321429
H 1.3539784 1.0603991 0.0514657
H 0.2253010 -1.2075823 1.3633609
O 2.3810967 0.4933520 0.1672872
H 2.8433410 0.4751152 -0.6916816
H 1.8563168 -0.3939175 0.2841370
O -0.6647251 0.1200199 -1.4451248
H -1.1993631 -0.6543171 -1.6872999
O -1.5565114 0.2801101 0.8652970
H -2.1765980 0.9488244 0.5364928

TS6 : H_2-release from $BH(OH)_2$ and three H_2O
15
Energy = -406.7399537750
B 1.0056830 0.1305802 -0.1147786
H 0.3770714 -0.1831109 -1.2890441
O 0.4098254 -0.7138972 0.9332544
H -0.7049820 -0.1826998 -1.4195439
H 0.6387485 -1.6478205 0.8020180
O -1.8481862 -0.1452180 -1.4621957
H -2.1613145 -0.9141115 -1.9729403
H -2.1425099 -0.2524724 -0.4437793
O -2.1636705 -0.2300298 1.0134801
H -2.7341053 -0.9070694 1.4132140
H -1.2045508 -0.5170365 1.1662074
O 2.3847414 -0.2107841 -0.3350646
H 2.7798152 0.3589298 -1.0129964
O 0.7936772 1.5347321 0.1356882
H -0.1176227 1.7401837 0.3936984

TS7$^-$: hydride from $HCO_2BH_2OH^-$ to CO_2
12
Energy = -480.1142724652
B -0.2305491 0.8770976 0.9317782

H -0.3160855 1.2391396 2.0858555
O -0.2189802 1.9416749 -0.0196866
O -1.2516200 -0.2298439 0.7047252
H 0.9055778 0.2292330 0.8373040
H 0.2436254 1.6634540 -0.8305928
C -2.0240037 -0.2849583 -0.3584399
O -2.8178704 -1.2005629 -0.5606976
H -1.9177425 0.5606868 -1.0557010
C 1.9602840 -0.3441145 -0.1288572
O 2.5552348 -1.1392432 0.5423898
O 1.7918924 0.2171747 -1.1781827

TS8⁻ : hydride from $BH_2(OH)_2^-$ to CO_2
10
Energy = -366.6994415390
B -1.4347463 -0.0269955 0.7327671
H -1.7887509 0.1516759 1.8968161
H -0.1722515 0.2188795 0.6707929
O -2.1543235 0.9450932 -0.1157558
H -1.8767571 0.8560296 -1.0411082
C 1.3624538 -0.0779804 -0.1798402
O 2.0652490 0.6838923 0.3969292
O 1.0467356 -0.9079765 -0.9681367
O -1.6218944 -1.4424330 0.3663260
H -1.0332966 -1.6639844 -0.3732944

TS9⁻ : hydride from $BH(OH)_3^-$ to CO_2
11
Energy = -442.0204700882
B -1.1429054 0.1395943 0.1094778
H 0.1421637 0.2048432 0.0384536
O -1.5622800 1.5165229 0.3953210
H -2.5044631 1.6062296 0.1761005
C 1.8029880 -0.2219724 -0.0196358
O 2.2199515 0.5730593 -0.7995998
O 1.8462783 -1.1354326 0.7390638
O -1.6577049 -0.3983824 -1.1627579
H -1.3449283 0.1494777 -1.8989979
O -1.5126122 -0.7566468 1.2055763
H -1.1706894 -1.6465509 1.0294625

aTS1⁻ : hydride from BH_4^- to CO_2
8
Energy = -216.0723164995
B -2.2519746 -0.2576793 0.0197277
H -2.4373911 -0.3044514 1.2161629
H -2.4731109 -1.2857440 -0.5819361
H -2.6317904 0.7591350 -0.5194576
H -0.9293402 -0.1500012 -0.0744471
C 0.4379496 -0.0065558 -0.0425386
O 0.6913197 1.0929854 0.3980876
O 0.9231898 -1.0306364 -0.4713039

aTS1 : H_2-release from BH_4^- and $H_5O_2^+$
12
Energy = -180.7861950137
B -1.5234407 -0.1477017 -1.0340667
H -0.7084587 0.5075441 -1.7981617
H -1.2776793 -1.3300074 -1.1047170
H 0.1184013 0.2056639 -1.3861821
H -2.5391260 0.1733771 -1.6123793
O 1.3715382 -0.0116074 -1.0686968
H 1.8959691 0.7734201 -1.3079402
H 1.3959558 -0.0902270 -0.0546320
O 1.2561543 -0.2111383 1.5394546
H 1.5301952 -1.0772102 1.8862505
H 0.3083947 -0.1438974 1.7497361
H -1.4426246 0.3077197 0.0867062

aTS2⁻ : S_N2 replacement of HCO_2^- with H_2O
11
Energy = -292.5511162673
B -1.4595878 0.2071790 0.0762117
H -1.2606664 -0.3255186 -0.9805226
H -1.2593327 -0.4010282 1.0913945
H -1.6473069 1.3918174 0.1221750
H -3.5077076 -1.1593524 -0.1775182
O -3.4316513 -0.2076988 0.0096065
H -3.7842746 -0.1065017 0.9106752
O 0.8553485 0.7190262 0.1031733
C 1.5373897 -0.3409898 -0.0098756
H 0.9544717 -1.2724365 -0.2130195
O 2.7896529 -0.4580619 0.0793611

aTS3⁻ : hydride from BH_3OH^- to CO_2
9
Energy = -291.3812104879
B -1.5401674 -0.8158710 0.2413894
H -1.5075302 -0.9998963 1.4610558
H -1.9789607 -1.7940989 -0.3569576
H -0.3062228 -0.7382249 -0.1131326
O -2.2654941 0.3934391 -0.1838336
H -1.8980648 1.1687696 0.2665192
C 1.1332597 0.1671802 0.0844673
O 0.7540988 1.2904161 -0.0082469
O 1.9311713 -0.7046241 0.2294815

aTS4a : H_2-release from BH_3 and two H_2O
10
Energy = -179.6057091388
B -1.2254521 0.6469949 0.0040645
H -0.2053807 1.4435283 0.3619662
H -1.4930444 1.0344835 -1.1115724
O -0.7913390 -0.7766578 -0.0124470
H 0.6753775 0.9524016 0.1695868
H -0.9704118 -1.2025011 0.8399240
H -2.0355593 0.9159116 0.8629985
O 1.5484883 0.1216804 0.0042502
H 1.9860858 0.2819776 -0.8521691
H 0.8143387 -0.5842850 -0.1319921

aTS4b : H_2-release from BH_3 and one H_2O

7

Energy = -103.0984294935

B	-0.1029653	0.5687326	-0.0502280
H	0.1217294	1.1001648	1.1425602
H	-0.1118820	1.4728309	-0.8332552
O	1.2833459	-0.2153936	-0.1170235
H	0.9238175	0.4948446	0.8931019
H	1.1455956	-1.1418431	0.1463395
H	-1.0573132	-0.1439310	0.0574312

aTS4 : H_2-release from BH_3 and three H_2O

13

Energy = -256.1005394798

B	-1.5150319	-0.1944183	-0.8533925
H	-0.6242767	0.4670542	-1.6120299
H	-1.2893631	-1.3706197	-1.0268767
O	-1.3722249	0.1665042	0.5640858
H	0.3075958	0.2245231	-1.3896252
H	-1.7397157	1.0441200	0.7478301
H	-2.5184543	0.2263623	-1.3919649
O	1.5107469	0.0130761	-1.1090341
H	2.0142380	0.8161199	-1.3354725
H	1.4951501	-0.0698047	-0.0723420
O	1.0937654	-0.1573997	1.4026529
H	1.2092690	-1.0508905	1.7657332
H	0.1020114	-0.0434358	1.2330136