Electronic Supplementary Material (ESI) for ChemComm.


# Electronic Supplementary Information

# A Novel Strategy for Reversible Hydrogen Storage in $Ca(BH_4)_2$

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## Methods

**Experimental.** The samples of $Ca(BH_4)_2$ (purity, 95%) and $CaB_6$ (purity, 95%) were purchased from Sigma-Aldrich and $CaB_{12}H_{12}$ from Katchem. The $H_2$ desorption of $Ca(BH_4)_2$ was performed using a custom made pressure-composition-temperature (*pcT*) apparatus under dynamic vacuum (lower than $10^{-4}$ mbar). The samples were heated to the target temperatures with a ramp of 10 ºC/min. The $H_2$ desorption amount was recorded by a flow meter connected. After $H_2$ desorption, the samples were cooled rapidly to room temperature for further characterization. The rehydrogenation was carried out at 300 to 350ºC under 130 to 185 bar $H_2$ for 80 h.

XRD measurements were performed using a Bruker D8 diffractometer equipped with a Goebel mirror selecting Cu Kα radiation (λ = 1.5418 Å) and a linear detector system (Vantec). Samples for XRD measurements were filled and sealed under an argon atmosphere into glass capillaries (diameter 0.7 mm; wall thickness 0.01 mm).

Solid state $^{11}B$ magic angle spinning (MAS) NMR experiments were performed on a Bruker Avance-400 NMR spectrometer using a 4 mm CP-MAS probe. The $^{11}B$ NMR spectra were recorded at 128.38 MHz at 12 kHz sample rotation applying a Hahn echo pulse sequence to suppress the broad background resonance of boron nitride in the probe. Pulse lengths of 1.5 μs (π/12 pulse) and 3.0 μs were applied for the excitation and echo pulses, respectively. For selected samples, $^{11}B$ cross polarization magic angle spinning (CP-MAS) NMR experiments were performed using weak radio-frequency powers for spin locking of the $^{11}B$ nucleus on resonance. Solution-state NMR experiments were carried out using a 5 mm inverse broadband probe at 25 °C. $^{11}B$ NMR chemical shifts are reported in parts per million (ppm) externally referenced to a 1M $B(OH)_3$ aqueous solution at 19.6 ppm as external standard sample.

Fourier transform infrared spectroscopy (FT-IR) measurements were carried out at room temperature under protective Ar atmosphere using a Bruker Alpha spectrometer equipped with a platinum ATR single reflection diamond ATR module. The calculation of IR spectrum was generated from GaussView 05 after calculating the vibrational frequency and IR intensities during optimization process.[1]

**Theoretical calculations.** First principles calculations were carried out using density functional theory (DFT) with B3LYP hybrid functional for exchange-correlation potential.[2, 3] All calculations were performed using Gaussian 09 code with 6-311+G(d) basis sets.[4] Since the bonding in $Ca(BH_4)_2$ is primarily covalent between B and H atoms and ionic between $Ca^{2+}$ and $(BH_4)^-$ ions, we used a cluster approach to study the relative stability of various moieties that can form during the dehydrogenation process. Past studies have shown that this is a valid approach.[5]

We calculated the structures of $BH_4^-$, $B_2H_6^q$ (q=0, -1, -2), $B_3H_8^-$, and $B_{12}H_{12}^{2-}$ moieties as well their corresponding salts, namely $Ca(BH_4)_2$, $Ca(B_2H_6)$, $Ca(B_3H_8)_2$, and $Ca(B_{12}H_{12})$. The geometries of the above clusters were optimized without any symmetry constraint. The forces and total energies were converged to 1 x $10^{-2}$ eV/Å and 1 x $10^{-6}$ eV, respectively.

**Figure S1**

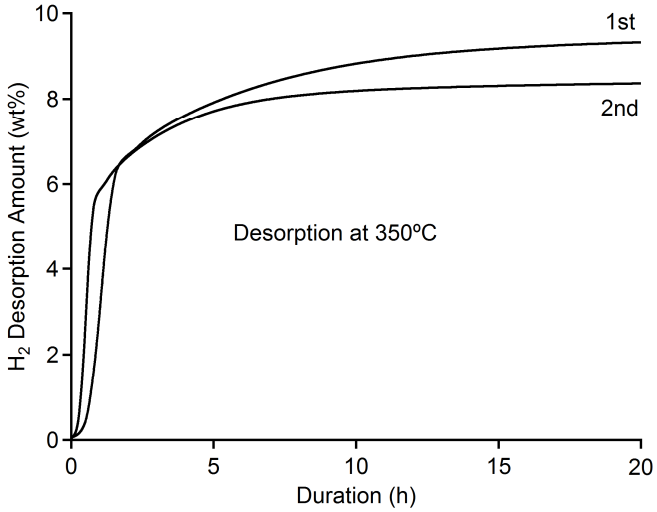


Fig. S1 Temperature-programmed-desorption (TPD) profiles of $Ca(BH_4)_2$ in the first two cycles. Desorption: 350°C, vacuum, 20h; resorption: 350°C, 185 bar $H_2$, 80h

**Figure S2**

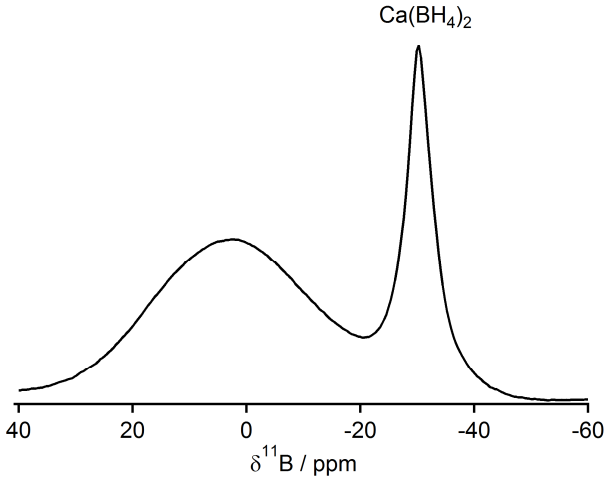


**Fig. S2** $^{11}B$ MAS NMR spectra of rehydrogenated $Ca(BH_4)_2$ at 350ºC under 185 bar $H_2$. Before rehydrogenation, $Ca(BH_4)_2$ was fully dehydrogenated at 450 ºC for 0.5 h. A small amount of boron atom (approximately 33 %) was converted back to $Ca(BH_4)_2$.

**Figure S3**

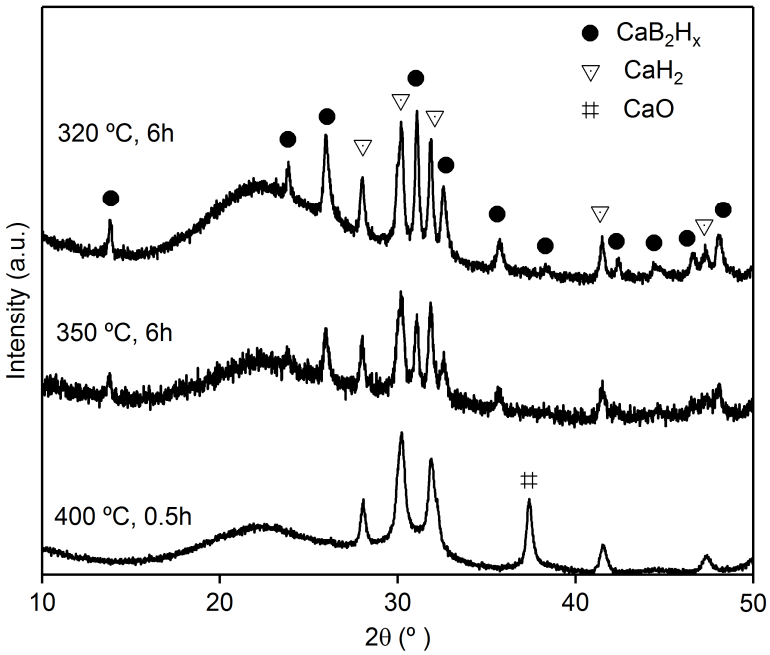


**Figure S3.** XRD patterns of $Ca(BH_4)_2$ after decomposition under vacuum at 320ºC (6 h), 350ºC (6 h) and at 400 ºC (0.5 h), respectively.

**Figure S4**

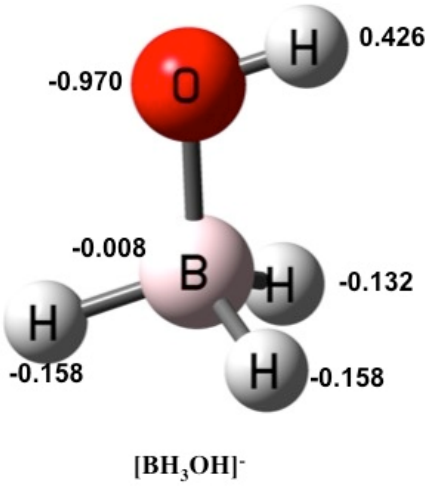


**Figure S4.** Optimized Geometries of $[BH_3{\bullet}OH]^-$ with NBO charges. The coordinates are shown in Table S1.

**Table S1**

***Table S1.*** Optimized cartesian coordinates of $[BH_3{\bullet}OH]^-$.

| Center Number | Atomic Number | Coordinates (Angstroms) | | |
|---|---|---|---|---|
| | | X | Y | Z |
| 1 | 5 | -0.743092 | 0.013874 | 0.000046 |
| 2 | 1 | -1.150902 | 0.628925 | -1.008664 |
| 3 | 1 | -1.150576 | 0.630559 | 1.007799 |
| 4 | 1 | -1.231547 | -1.118939 | 0.000767 |
| 5 | 8 | 0.764162 | -0.121675 | 0.000021 |
| 6 | 1 | 1.135187 | 0.763481 | -0.000298 |

**Figure S5**

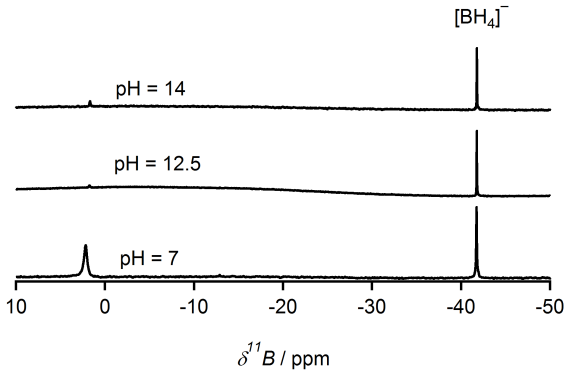


**Figure S5.** $^{11}B$ NMR spectra recorded in $D_2O$ of $Ca(BH_4)_2$ hydrolyzed in aqueous solutions with pH value from 7 to 14.

**Figure S6**

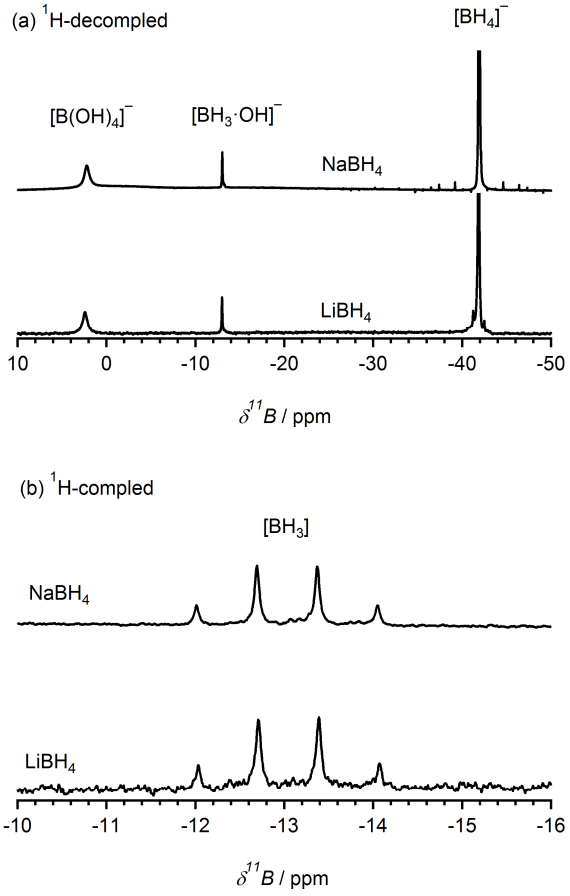


**Figure S6.** Hydrolysis products of $NaBH_4$ and $LiBH_4$ in $D_2O$ observed by $^{11}B$ NMR spectra: (a) $^1H$-coupled, (b) $^1H$-decoupled. The $[BH_3]$ species show the typical quartet splitting with a $^1H$, $^{11}B$ coupling constant of 87 Hz.

**Figure S7**

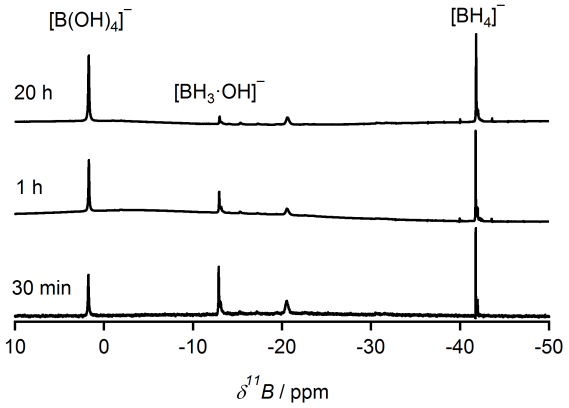


**Figure S7.** Decay of $[BH_3{\bullet}OH]^-$ observed in partially decomposed $Ca(BH_4)_2$ (350 ºC, vacuum, 6 h) in alkaline solution (pH = 14, at room temperature), monitored by $^{11}B$ NMR spectroscopy.

**Figure S8**

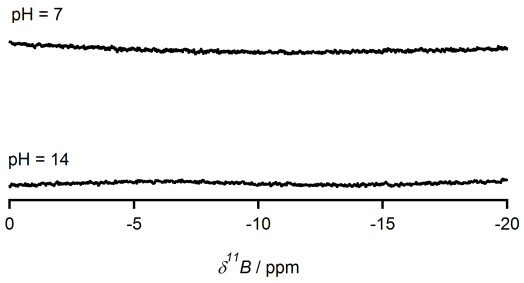


**Figure S8.** $^{11}$B NMR spectra of $CaB_6$ hydrolyzed in aqueous solutions with pH value from 7 to 14.

### *First principles cluster calculations*

First principles calculations were carried out using density functional theory (DFT) with B3LYP hybrid functional for exchange-correlation potential.[2, 3] All calculations were performed using Gaussian 09 code with 6-311+G(d) basis sets.[4] Since the bonding in $Ca(BH_4)_2$ is primarily covalent between B and H atoms and ionic between $Ca^{2+}$ and $(BH_4)^-$ ions, we used a cluster approach to study the relative stability of various moieties that can form during the dehydrogenation process. Past studies have shown that this is a valid approach.[5]

We calculated the structures of $BH_4^-$, $B_2H_6^q$ (q=0, -1, -2), $B_3H_8^-$, and $B_{12}H_{12}^{2-}$ moieties as well their corresponding salts, namely $Ca(BH_4)_2$, $Ca(B_2H_6)$, $Ca(B_3H_8)_2$, and $Ca(B_{12}H_{12})$. The structural details were shown in Table S4. All calculations were performed using Gaussian 09 code with 6-311+G(d) basis sets. The geometries of the above clusters were optimized without any symmetry constraint. The forces and total energies were converged to 1 x $10^{-2}$ eV/Å and,1 x $10^{-6}$ eV, respectively.

We begin with the results on $B_2H_6^q$ (q=0, -1, -2) moieties. The geometries of these clusters as well as Natural Bond Orbital (NBO) charges on the atoms and some representative interatomic distances are given in Fig. S9. The neutral $B_2H_6$ is composed of four radially bonded hydrogen atoms each carrying a charge of -0.001e while each of the bridge bonded H atoms carry a charge of +0.10e. Each of the B atoms carries a charge of -0.10e. As an electron is attached the bridge bonded hydrogen atoms become radially bonded and the bond between the B atoms become weaker as seen by an in increase in the B-B bond from 1.77 Å in neutral $B_2H_6$ to 2.14 Å in $B_2H_6^-$. The anion is only 0.13 eV lower in energy than it's neutral. This is consistent with the fact that $BH_3$ is a stable molecule with closed electronic shells. $B_2H_6^{2-}$ dianion is metastable lying 3.69 eV above the neutral state and can only be stabilized with the help of a counter cation, in this case $Ca^{2+}$. The extra electron(s) in $B_2H_6^-$ ($B_2H_6^{2-}$) is shared between the B and H atoms. $BH_4^-$ has a perfect tetrahedral symmetry with each hydrogen atom carrying a charge of -0.08e and the majority of the extra electron being located on the B atom. $B_3H_8^-$ is composed of a triangular B network with each B atom bound to two radially bonded H atoms. Two more H atoms are bridge bonded. As in neutral $B_2H_6$, the radially bonded H atoms in $B_3H_8^-$ carry a negative charge (ranging between -0.02e and -0.03e) while each of the bridge bonded H atoms carries a charge of +0.11e. In $B_{12}H_{12}^{2-}$ the B atoms remain negatively charged while the H atoms are positively charged each carrying a small charge of +0.007e.

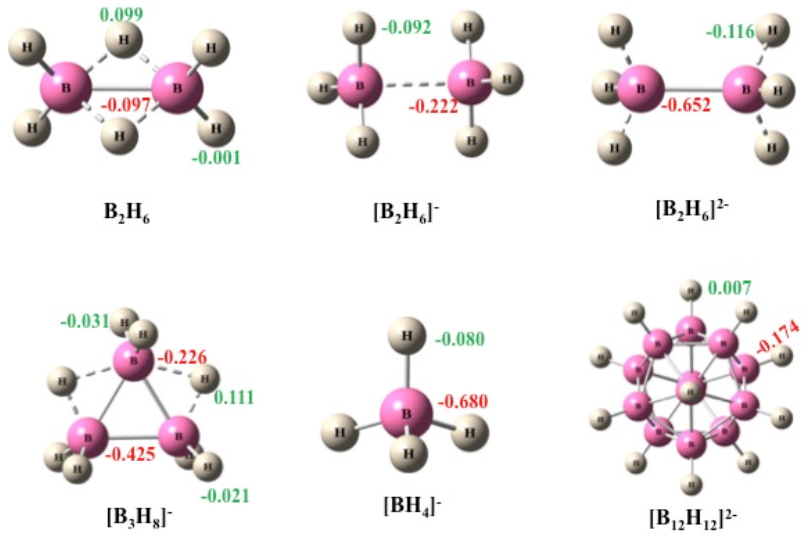


***Figure S9.*** Optimized Geometries of Different Boranes with Representative Bond Distances (Å) and NBO charges (Red: Boron; Green: Hydrogen)

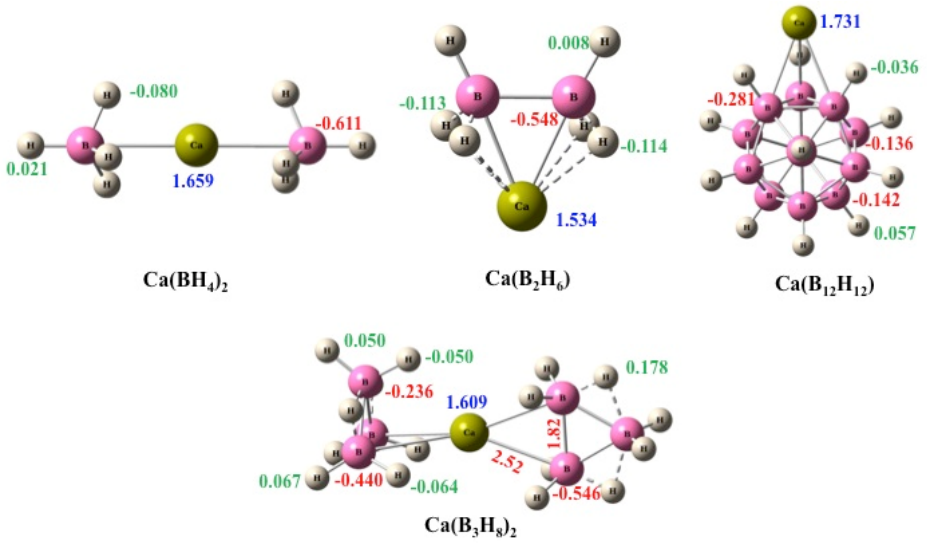


***Figure S10.*** Optimized Geometries of Different Ca- Borane Complexes with Representative Bond Distances (Å) and NBO Charges (Red: Boron; Blue: Calcium; Green: Hydrogen)

In Fig. S10 we plot the geometries of the Ca salts made of the above anionic components. In the gas phase $Ca(BH_4)_2$ cluster forms a linear chain with the $Ca^{2+}$ being inserted between two $BH_4^-$ units. Here, there are two kinds of H atoms, one type carrying a charge of -0.08 while the other charged positively with a charge of +0.21e. As we will see later the two H atoms, one charged positively and the charged negatively, combine and desorb as $H_2$, leaving behind $Ca(B_2H_6)$. In $Ca(B_2H_6)$ four of the H atoms carry a charge of -0.11e each while the other two carry a charge of +0.008e. The Ca atom in $Ca(B_{12}H_{12})$ is bonded to two B and one H atoms and the $B_{12}H_{12}$ unit retains the same structure as the isolated $B_{12}H_{12}^{2-}$. Structure of $Ca(B_3H_8)_2$ also exhibit similar structure where the $B_3H_8$ units retain the isolated geometry of $B_3H_8^-$ discussed in the above. There are two kinds of H atoms, one carrying a positive charge while another carrying a negative charge. It is important to note that in $CaB_xH_y$ salts, there are two different types of H atoms, one being positive while the other being negative. As in $Ca(BH_4)_2$, it is expected that in all other Ca salts the two oppositely charged H atom will combine to and desorb as a $H_2$ molecule.

We now discuss the relative stability of the various salts to predict the preferred intermediate phase during dehydrogenation. To accomplish this we list the total energies in Hartree atomic units of different Ca-Borane complexes and all possible products given in Table S2. Two quantities are of interest, the binding energy (Table S2), $E_b$ and the dissociation energy, ΔE (Table S3). The binding energy of different Ca salts are defined as,

$$E_b(1) = E(Ca^{2+}) + 2E(BH_4^-) - E[Ca(BH_4)_2]$$
$$E_b(2) = E(Ca^{2+}) + E(B_2H_6^{2-}) - E(CaB_2H_6)$$
$$E_b(3) = E(Ca^{2+}) + 2E(B_3H_8^-) - E[Ca(B_3H_8)_2]$$
$$E_b(4) = E(Ca^{2+}) + E(B12H_{12}^{2-}) - E(CaB_{12}H_{12})$$

We note that among all the Ca salts, $CaB_2H_6$ is most strongly bound salt followed by $Ca(BH_4)_2$, $Ca(B_3H_8)_2$ and $Ca(B_{12}H_{12})$. This would suggest that during dehydrogenation of $Ca(BH_4)_2$, the most preferred intermediate phase is $Ca(B_2H_6)$. One can also arrive at the same conclusion by calculating the dissociation energy, i.e. the energy needed to dissociate the parent salt, namely, $Ca(BH_4)_2$ into possible products. We note that the least energy needed to dissociate $Ca(BH_4)_2$ is 2.45 eV where the product is $CaB_2H_6$ and $H_2$.

**Table S2.** Binding energy measured against decomposition into ions ($E_b$ in eV) of different calcium salts.

| Ca-B-H compounds | Binding Energy ($E_b$ in eV) |
|---|---|
| $Ca(BH_4)_2$ | 19.85 |
| $CaB_2H_6$ | 23.07 |
| $Ca(B_3H_8)_2$ | 18.71 |
| $CaB_{12}H_{12}$ | 18.22 |

**Table S3.** Dissociation energy (ΔE in eV) of $Ca(BH_4)_2$ to different compounds.

| Dissociation Pathways | Dissociation Energy (ΔE in eV) |
|---|---|
| $Ca(BH_4)_2 \rightarrow CaB_2H_6 + H_2$ | 2.34 |
| $Ca(BH_4)_2 \rightarrow [Ca(B_3H_8)_2 + 2\ CaH_2 + 2H_2]/3$ | 2.45 |
| $Ca(BH_4)_2 \rightarrow [CaB_{12}H_{12} + CaB_2H_6 + 5\ CaH_2 + 14H_2]/7$ | 3.10 |
| $Ca(BH_4)_2 \rightarrow [CaB_{12}H_{12} + 5\ CaH_2 + 13H_2]/6$ | 3.23 |
| $Ca(BH_4)_2 \rightarrow B_2H_6 + CaH_2$ | 3.69 |
| $CaB_2H_6 + H_2 \rightarrow [CaB_6 + 2\ CaH_2 + 10\ H_2]/3$ | 4.63 |

**Table S4.** Number of imaginary frequency (NImag), Energy and optimized cartesian coordinates of different Boranes and Ca-Borane complexes.

| System | NImag | Energy (au) | Coordinate (Cartesian) | | | | |
|---|---|---|---|---|---|---|---|
| | | | Center Number | Atomic Number | Coordinates (Angstroms) | | |
| | | | | | X | Y | Z |
| $BH_4^-$ | 0 | -27.27045 | 1 | 5 | 0.000000 | 0.000000 | 0.000000 |
| | | | 2 | 1 | 0.715752 | 0.715752 | 0.715752 |
| | | | 3 | 1 | -0.715752 | -0.715752 | 0.715752 |
| | | | 4 | 1 | -0.715752 | 0.715752 | -0.715752 |
| | | | 5 | 1 | 0.715752 | -0.715752 | -0.715752 |
| $B_2H_6$ | 0 | -53.29544 | 1 | 5 | 0.883360 | 0.000025 | 0.000067 |
| | | | 2 | 1 | 1.458587 | 1.039216 | 0.000388 |
| | | | 3 | 1 | 1.459882 | -1.038423 | -0.000613 |
| | | | 4 | 5 | -0.883401 | 0.000016 | -0.000040 |
| | | | 5 | 1 | -1.458884 | 1.039032 | 0.000169 |
| | | | 6 | 1 | -1.459516 | -1.038683 | -0.000132 |
| | | | 7 | 1 | 0.000022 | -0.001364 | 0.977491 |
| | | | 8 | 1 | 0.000118 | 0.000021 | -0.977437 |
| $B_2H_6^-$ | 0 | -53.29049 | 1 | 5 | -1.072025 | 0.001947 | -0.001003 |
| | | | 2 | 1 | -1.309140 | -1.154406 | -0.278679 |
| | | | 3 | 1 | -1.280405 | 0.826173 | -0.865670 |
| | | | 4 | 5 | 1.070331 | -0.001779 | 0.000848 |
| | | | 5 | 1 | 1.277561 | -0.809848 | 0.881242 |
| | | | 6 | 1 | 1.315252 | 1.157597 | 0.258389 |
| | | | 7 | 1 | -1.293929 | 0.345128 | 1.139957 |
| | | | 8 | 1 | 1.299132 | -0.365487 | -1.134465 |
| $B_2H_6^{2-}$ | 0 | -53.15968 | 1 | 5 | 0.000000 | 0.000000 | 0.912542 |
| | | | 2 | 1 | -0.587405 | 1.017916 | 1.395174 |
| | | | 3 | 1 | 1.175244 | -0.000250 | 1.395174 |
| | | | 4 | 1 | -0.587839 | -1.017666 | 1.395174 |
| | | | 5 | 5 | 0.000000 | 0.000000 | -0.912542 |
| | | | 6 | 1 | 0.587405 | 1.017916 | -1.395174 |
| | | | 7 | 1 | 0.587839 | -1.017666 | -1.395174 |
| | | | 8 | 1 | -1.175244 | -0.000250 | -1.395174 |
| $B_3H_8^-$ | 0 | -79.41069 | 1 | 5 | 0.920687 | -0.537943 | -0.000042 |
| | | | 2 | 5 | -0.921645 | -0.536448 | 0.000040 |
| | | | 3 | 5 | 0.000943 | 0.999066 | 0.000003 |
| | | | 4 | 1 | 1.446641 | 0.610333 | -0.000042 |
| | | | 5 | 1 | -1.446090 | 0.612369 | 0.000045 |
| | | | 6 | 1 | -1.324024 | -1.035491 | -1.026289 |
| | | | 7 | 1 | -1.323959 | -1.035479 | 1.026400 |
| | | | 8 | 1 | 1.322449 | -1.037405 | -1.026395 |
| | | | 9 | 1 | 1.322518 | -1.037430 | 1.026272 |
| | | | 10 | 1 | 0.001244 | 1.649866 | -1.018276 |
| | | | 11 | 1 | 0.001299 | 1.649864 | 1.018283 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $B_{12}H_{12}^{2-}$ | 0 | -305.74722 | 1 | 5 | -0.317174 | -1.667062 | -0.087783 |
| | | | 2 | 5 | -0.627051 | -0.577987 | -1.469450 |
| | | | 3 | 5 | 0.579397 | 0.738976 | -1.416116 |
| | | | 4 | 5 | 1.635187 | 0.463616 | -0.001322 |
| | | | 5 | 5 | 1.051450 | -0.923799 | -0.963658 |
| | | | 6 | 5 | 0.317145 | 1.667144 | 0.087788 |
| | | | 7 | 5 | -1.080962 | 1.023242 | -0.820096 |
| | | | 8 | 5 | -0.579411 | -0.738944 | 1.416031 |
| | | | 9 | 5 | -1.051428 | 0.923732 | 0.963602 |
| | | | 10 | 5 | 0.627048 | 0.578011 | 1.469535 |
| | | | 11 | 5 | 1.080974 | -1.023318 | 0.820149 |
| | | | 12 | 1 | 2.794528 | 0.792577 | -0.001599 |
| | | | 13 | 1 | 1.796641 | -1.579163 | -1.647315 |
| | | | 14 | 1 | 0.990507 | 1.262501 | -2.420711 |
| | | | 15 | 1 | -1.071228 | -0.987977 | -2.511980 |
| | | | 16 | 1 | -1.846948 | 1.749136 | -1.402009 |
| | | | 17 | 1 | -0.541896 | -2.849372 | -0.150363 |
| | | | 18 | 1 | -1.796635 | 1.579095 | 1.647259 |
| | | | 19 | 1 | -0.990527 | -1.262468 | 2.420635 |
| | | | 20 | 1 | 1.071212 | 0.987992 | 2.512063 |
| | | | 21 | 1 | 1.846953 | -1.749205 | 1.402059 |
| | | | 22 | 1 | 0.541862 | 2.849446 | 0.150364 |
| | | | 23 | 5 | -1.635171 | -0.463610 | 0.001319 |
| | | | 24 | 1 | -2.794489 | -0.792566 | 0.001605 |
| $Ca(BH_4)_2$ | 0 | -732.17599 | 1 | 5 | 2.420552 | -0.002942 | 0.005255 |
| | | | 2 | 1 | 1.946286 | -0.947950 | -0.653432 |
| | | | 3 | 1 | 1.942720 | 1.037574 | -0.486611 |
| | | | 4 | 1 | 1.936197 | -0.099824 | 1.149050 |
| | | | 5 | 1 | 3.612988 | -0.000302 | 0.010753 |
| | | | 6 | 20 | 0.000092 | 0.002535 | -0.004532 |
| | | | 7 | 5 | -2.420820 | -0.003129 | 0.004842 |
| | | | 8 | 1 | -1.946716 | 0.968429 | -0.614480 |
| | | | 9 | 1 | -1.943727 | -1.022011 | -0.530414 |
| | | | 10 | 1 | -1.934894 | 0.046563 | 1.151003 |
| | | | 11 | 1 | -3.613352 | 0.002824 | 0.014289 |
| $Ca(B_3H_8)_2$ | 0 | -836.41470 | 1 | 5 | 2.201580 | 0.928791 | -0.011185 |
| | | | 2 | 5 | 2.282066 | -0.895703 | 0.014249 |
| | | | 3 | 5 | 3.783152 | 0.085176 | 0.005182 |
| | | | 4 | 1 | 3.277572 | 1.531022 | -0.016519 |
| | | | 5 | 1 | 3.404904 | -1.403318 | 0.025416 |
| | | | 6 | 1 | 1.731992 | -1.288028 | 1.028699 |
| | | | 7 | 1 | 1.739866 | -1.315426 | -0.993965 |
| | | | 8 | 1 | 1.619693 | 1.300888 | 0.992921 |
| | | | 9 | 1 | 1.627010 | 1.271620 | -1.030336 |
| | | | 10 | 1 | 4.388902 | 0.125143 | 1.030401 |
| | | | 11 | 1 | 4.394760 | 0.096411 | -1.017286 |
| | | | 12 | 5 | -2.650928 | -0.365006 | 0.983542 |
| | | | 13 | 5 | -2.679423 | -0.612236 | -0.822881 |
| | | | 14 | 5 | -2.680532 | 1.033369 | -0.128043 |
| | | | 15 | 1 | -2.757305 | 0.837817 | 1.341753 |
| | | | 16 | 1 | -2.804016 | 0.450194 | -1.487759 |
| | | | 17 | 1 | -1.632803 | -1.090279 | -1.251204 |
| | | | 18 | 1 | -3.629232 | -1.257478 | -1.131439 |
| | | | 19 | 1 | -1.589646 | -0.715355 | 1.491431 |
| | | | 20 | 1 | -3.588671 | -0.898253 | 1.483476 |
| | | | 21 | 1 | -1.621080 | 1.634378 | -0.228123 |
| | | | 22 | 1 | -3.619102 | 1.759986 | -0.212324 |
| | | | 23 | 20 | -0.111121 | -0.095564 | -0.011473 |
| $Ca(B_2H_6)$ | 0 | -730.91341 | 1 | 5 | 1.184050 | 0.922869 | 0.002429 |
| | | | 2 | 1 | 2.244868 | 1.479725 | -0.017607 |
| | | | 3 | 1 | 0.488402 | 1.329511 | 0.991409 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | 4 | 1 | 0.473869 | 1.327463 | -0.979906 |
| | | | 5 | 5 | 1.181297 | -0.924100 | 0.000849 |
| | | | 6 | 1 | 0.477079 | -1.329112 | 0.985924 |
| | | | 7 | 1 | 0.474748 | -1.326137 | -0.984465 |
| | | | 8 | 1 | 2.238632 | -1.487767 | -0.004263 |
| | | | 9 | 20 | -0.911217 | 0.000624 | -0.000374 |
| $Ca(B_{12}H_{12})$ | 0 | -983.32252 | 1 | 5 | 0.537591 | -0.281676 | -1.004502 |
| | | | 2 | 5 | -0.459576 | 1.181080 | -1.208124 |
| | | | 3 | 5 | -1.093483 | 1.626914 | 0.415991 |
| | | | 4 | 5 | 0.537579 | 1.010183 | 0.258825 |
| | | | 5 | 5 | -2.113168 | 0.279061 | 0.995139 |
| | | | 6 | 5 | -2.114068 | 0.722896 | -0.739085 |
| | | | 7 | 5 | -0.460086 | -1.637536 | -0.418489 |
| | | | 8 | 5 | -2.113120 | -1.000913 | -0.256392 |
| | | | 9 | 5 | -1.093902 | -1.173568 | 1.200716 |
| | | | 10 | 5 | 0.538486 | -0.729944 | 0.745933 |
| | | | 11 | 1 | 1.539184 | 1.713983 | 0.438335 |
| | | | 12 | 1 | -1.269413 | 2.766430 | 0.707345 |
| | | | 13 | 1 | -0.180644 | 1.990121 | -2.036092 |
| | | | 14 | 1 | -3.052863 | 1.232124 | -1.260145 |
| | | | 15 | 1 | 1.538960 | -0.477172 | -1.704343 |
| | | | 16 | 1 | -3.052212 | -1.706693 | -0.436423 |
| | | | 17 | 1 | -0.182007 | -2.759275 | -0.705223 |
| | | | 18 | 1 | -1.270717 | -1.995398 | 2.041919 |
| | | | 19 | 1 | 1.539817 | -1.237705 | 1.265346 |
| | | | 20 | 1 | -3.051828 | 0.475616 | 1.697025 |
| | | | 21 | 5 | -1.093558 | -0.453079 | -1.616838 |
| | | | 22 | 5 | -0.459952 | 0.455604 | 1.627126 |
| | | | 23 | 1 | -1.270110 | -0.770945 | -2.749115 |
| | | | 24 | 1 | -0.181229 | 0.768538 | 2.741705 |
| | | | 25 | 20 | 2.791467 | 0.000263 | -0.000091 |


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