

Borane-Aluminum Surface Interactions: Enhanced Fracturing and Generation of Boron-Aluminum Core-Shell Nanoparticles

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Supporting Information

Mass Spectral Sensitivity Calibration

Each time before leaking the analyte gas mixture into the mass spectrometry chamber, a spectrum of the chamber background gas was taken, and these background spectra were subtracted from the raw spectra of the analyte mixtures. Next, each peak in the background-subtracted spectra were fit to Gaussians, and fits were used to determine the integrated peak area for each mass. Because the peak widths varied systematically with mass, the peak areas were corrected by dividing by the full width at half maximum (FWHM) values. Finally, to compensate for gas loss by sampling, and to correct for any variation in instrument sensitivity, all spectra were normalized to the mass 20 (Ar^{2+}) peak.

Qualitative interpretation of the mass spectra in Figs. 1, and S1-S5 is unambiguous. Milling Al balls in either diborane or pentaborane results in consumption of the borane, with H_2 as the only gaseous product. The question which requires more quantitative analysis is how much H_2 was present in the diborane/argon gas mixture. To answer this question, we need to know what contribution to the mass signal is made by dissociative ionization of diborane, and this analysis requires understanding the electron impact ionization cross sections for diborane, Ar, and H_2 , and also the transmission efficiency vs. mass for our mass spectrometer.

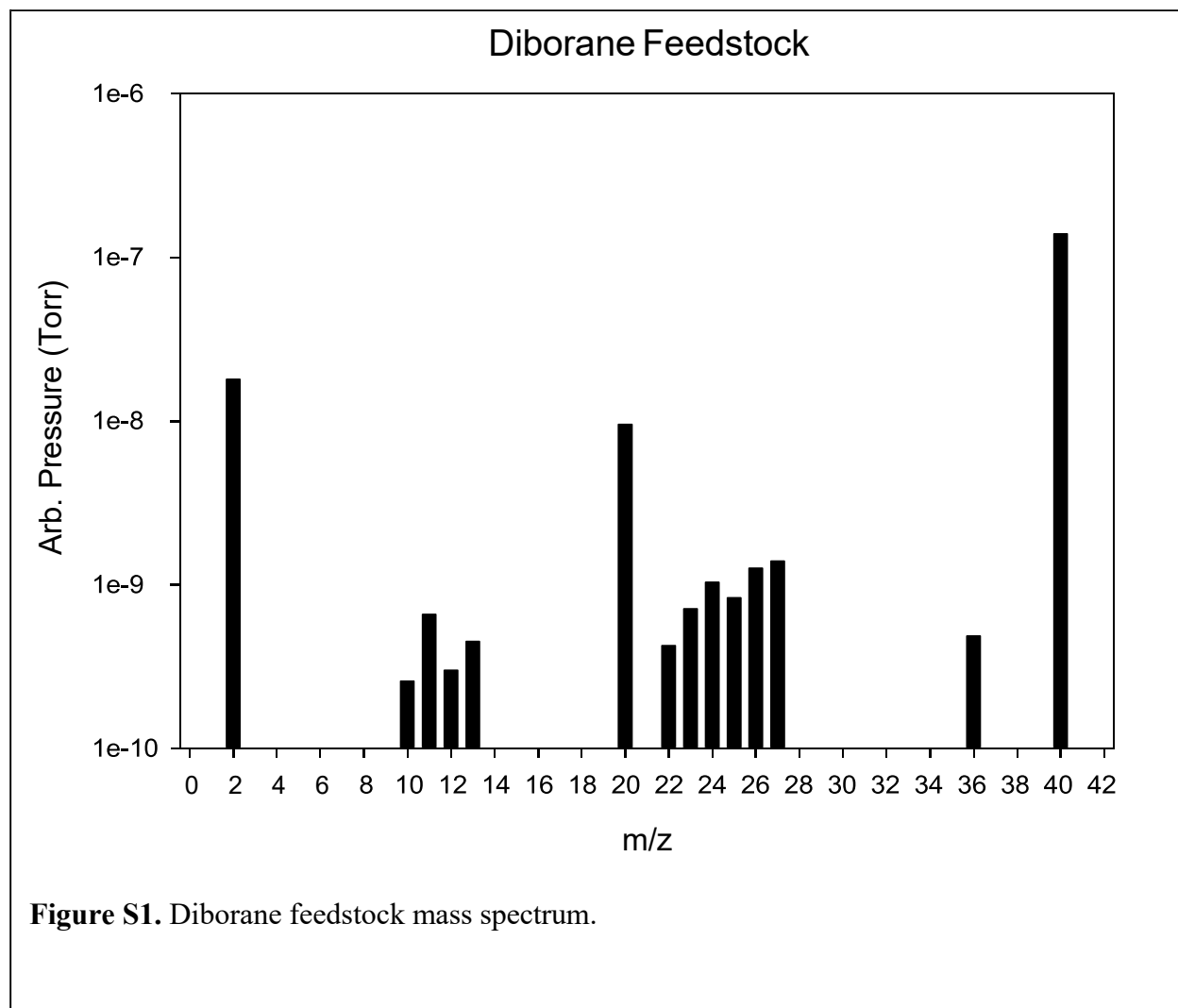
The transmission efficiencies vs. mass were determined by leaking a 1×10^{-7} Torr of several pure gases into the mass spectrometry chamber, then measuring the mass spectra using identical conditions and analysis procedures to those described above for the analyte spectra. The pressure was monitored by an ionization gauge, and corrected for the sensitivity factors for each gas reported by the manufacturer: 0.43, 1.55, 2.3, 2.63, and 1.2, for H_2 , CH_4 , C_2H_4 ,

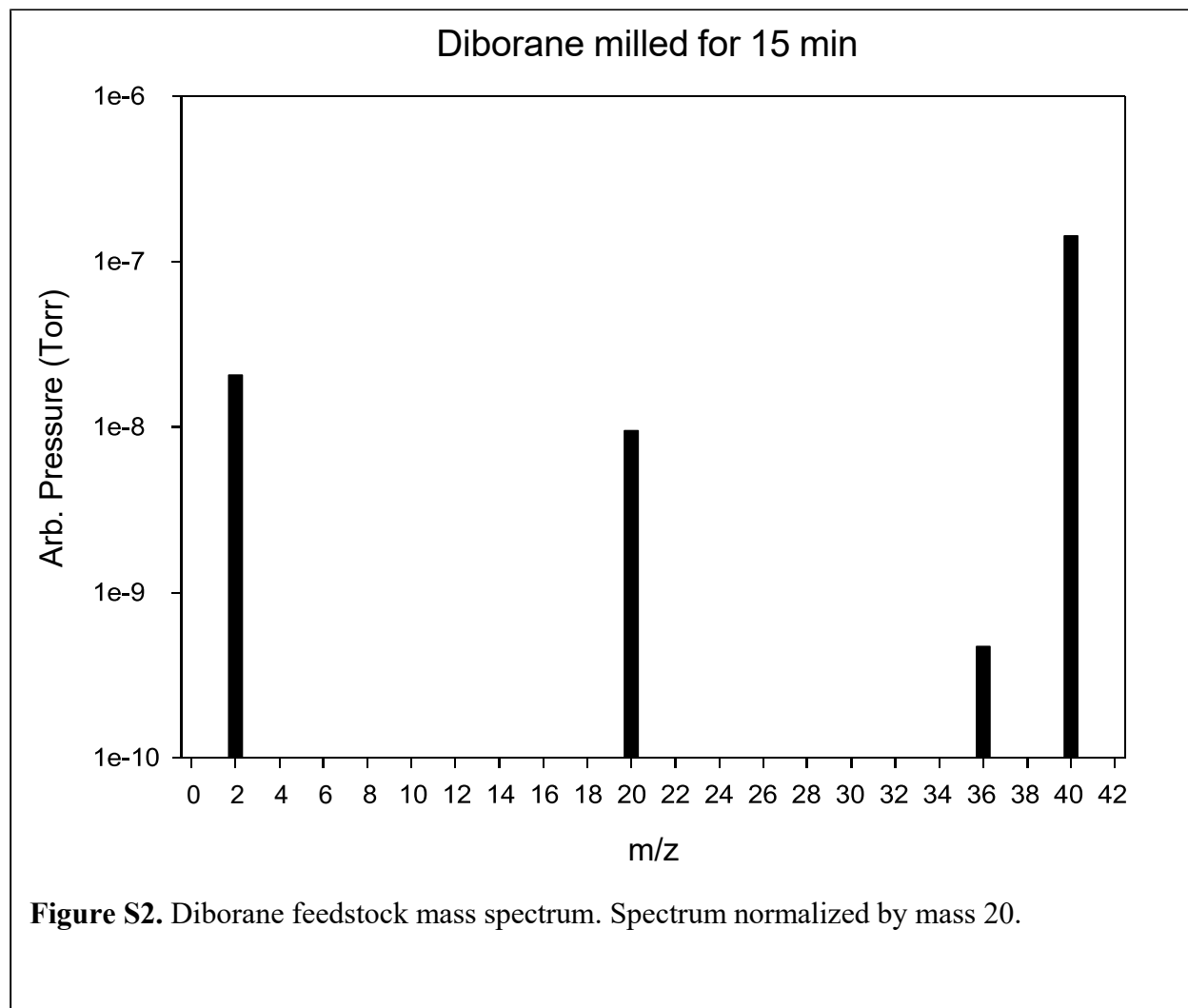
C₂H₆, and Ar, respectively. These gases were chosen because they give major peaks in the mass ranges of interest for diborane mass analysis. Relative to the transmission at mass 40, the transmission efficiencies were estimated to be 1.17 for mass 2, 1.08 for masses 10-13, and 1.5 for masses 20-27.

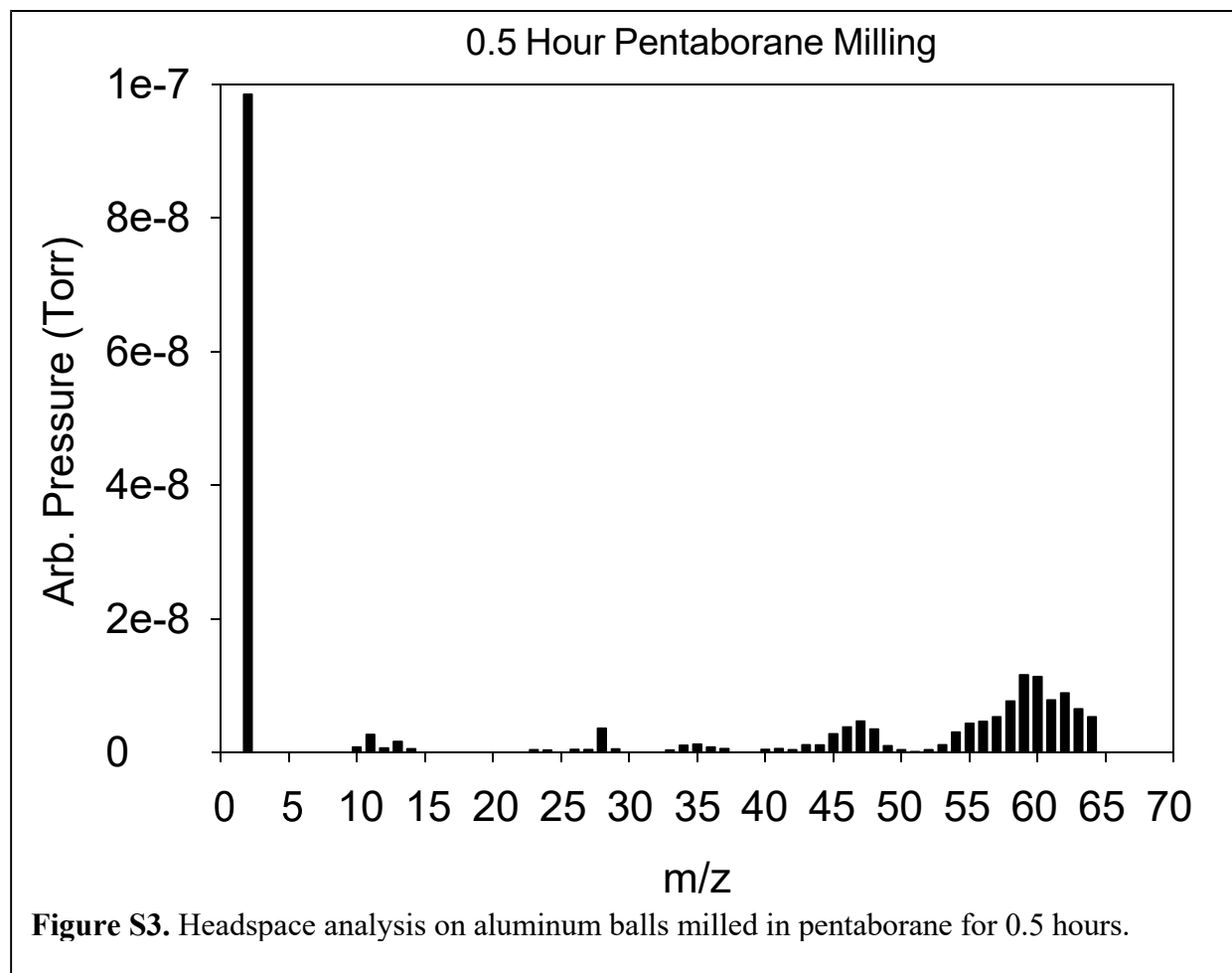
Absolute electron impact ionization cross sections and fragmentation patterns for hydrogen,² diborane,^{1, 3-4} and Ar⁵ have been reported, including results for both natural abundance and ¹⁰B₂H₆. The ionization cross sections reported in Table S1 under each fragment ion molecular formula are 70 eV electron impact values from the work of Basner *et al.*¹ and the “predicted intensities” listed for each mass number are calculated from the cross sections, taking into account all species that contribute to each mass for natural isotope abundance diborane. The predicted intensities are in reasonable agreement with the measured intensities for the diborane-derived peaks in Fig. S1, with the obvious exception that the measured mass 2 intensity is far higher than expected from dissociative ionization of B₂H₆. It is, thus, clear that there must be substantial H₂ contamination of the gas mixture. The experimental spectrum was fit by a linear combination of predicted spectra for diborane, H₂, and Ar, taking transmission efficiency into account. The best fit gas mixture composition was found to be 4.75% B₂H₆, 10.2% H₂, with the balance Ar.

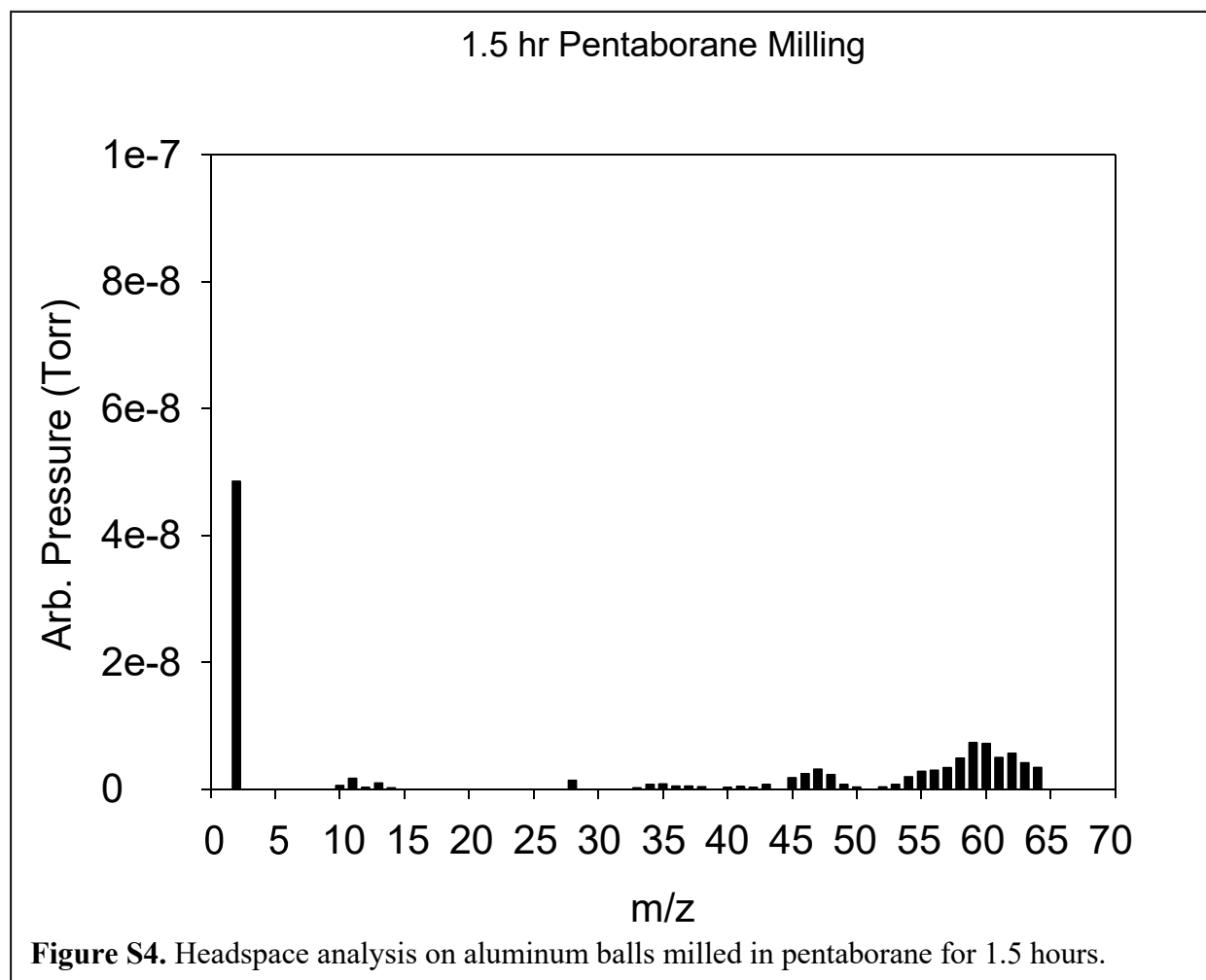
<i>Fragments</i>	<i>H⁺</i>	<i>H₂⁺</i>	<i>H₃⁺</i>	<i>B⁺</i>	<i>BH⁺</i>	<i>BH₂⁺</i>	<i>BH₃⁺</i>	<i>B₂⁺</i>
<i>Ionization cross section</i>	0.416	0.08	0.02	0.672	0.554	1.07	0.06	0.114
<i>Fragments</i>	<i>B₂H⁺</i>	<i>B₂H₂⁺</i>	<i>B₂H₃⁺</i>	<i>B₂H₄⁺</i>	<i>B₂H₅⁺</i>	<i>B₂H₆⁺</i>		
<i>Ionization cross section</i>	0.3	2.18	0.737	1.59	2.87	0.077		
<i>M/Z</i>	1	2	3	10	11	12	13	14
<i>Predicted intensity</i>	0.416	0.080	0.020	0.134	0.649	0.657	0.869	0.048
<i>M/Z</i>	21	22	23	24	25	26	27	28
<i>Predicted intensity</i>	0.036	0.169	0.917	1.697	1.093	1.938	1.866	0.049

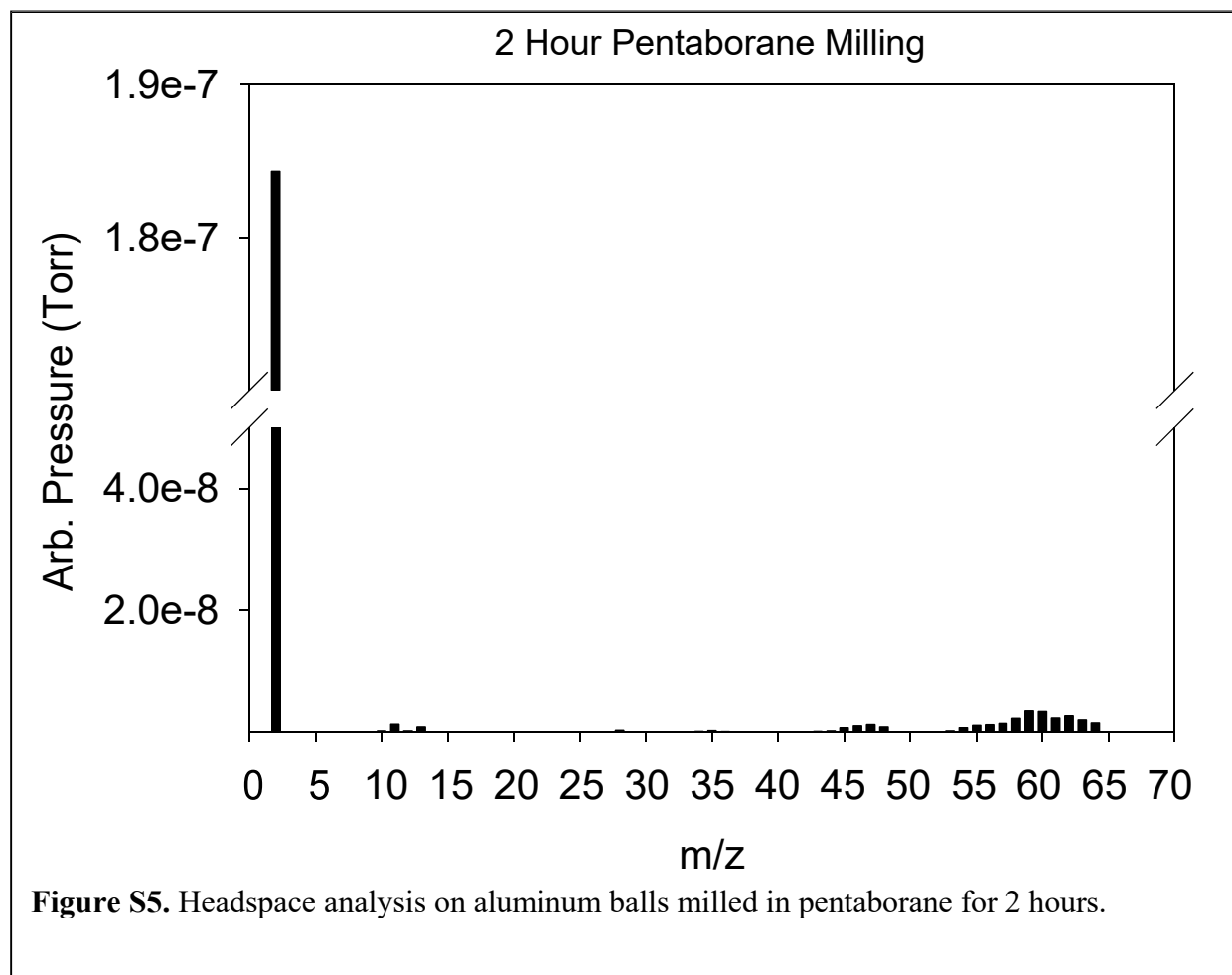
Table S1. Electron impact ionization cross section for diborane species. Ionization cross section data from Basner *et al.*¹

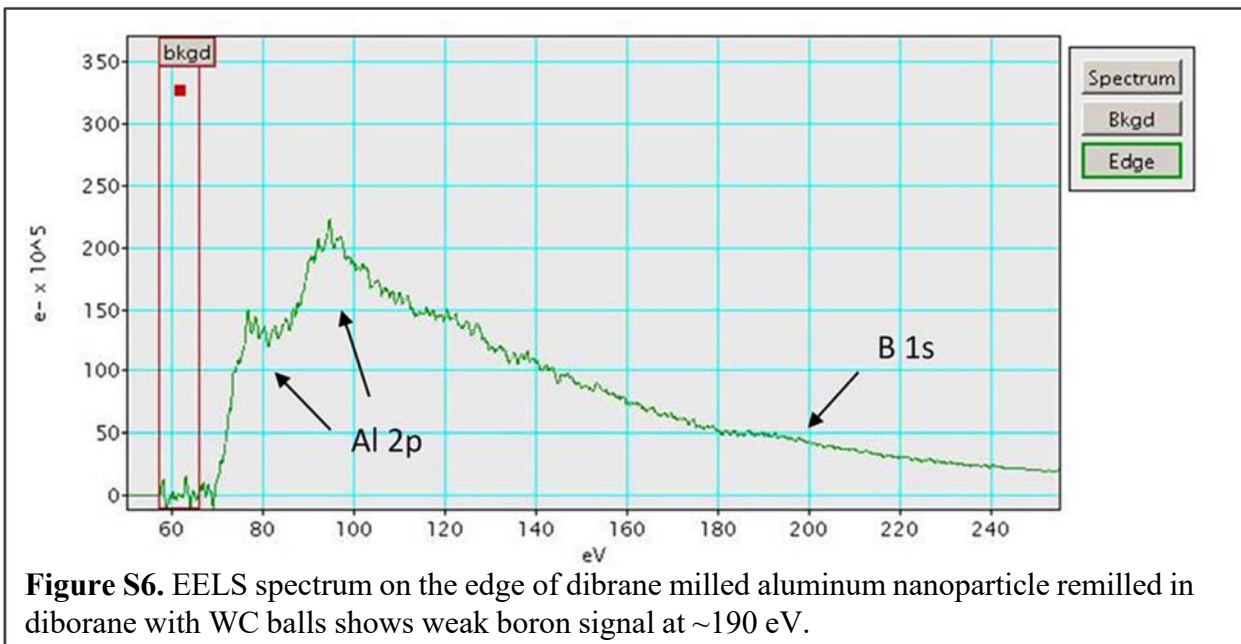
Diborane mass spectra

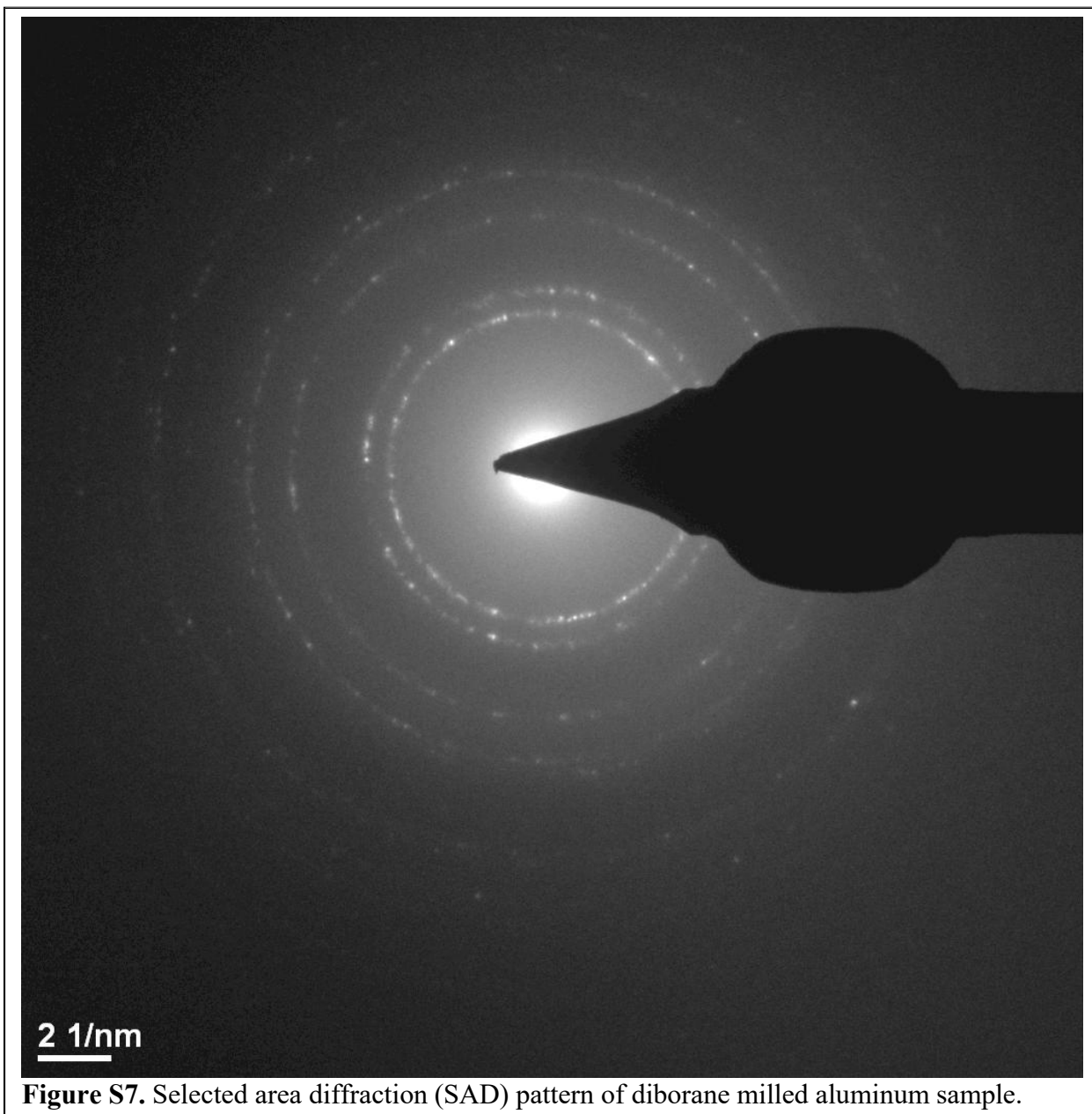


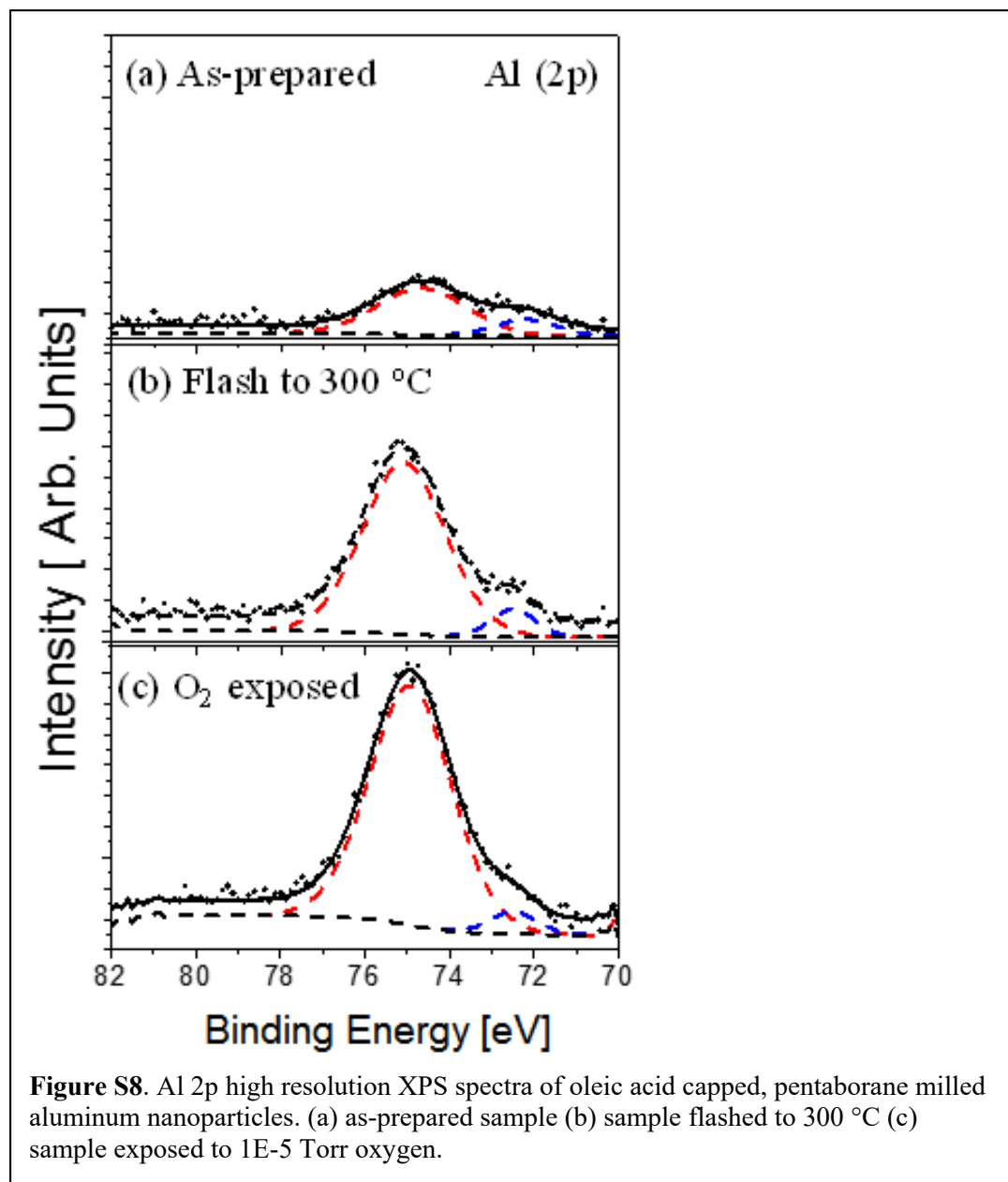
Pentaborane mass spectra

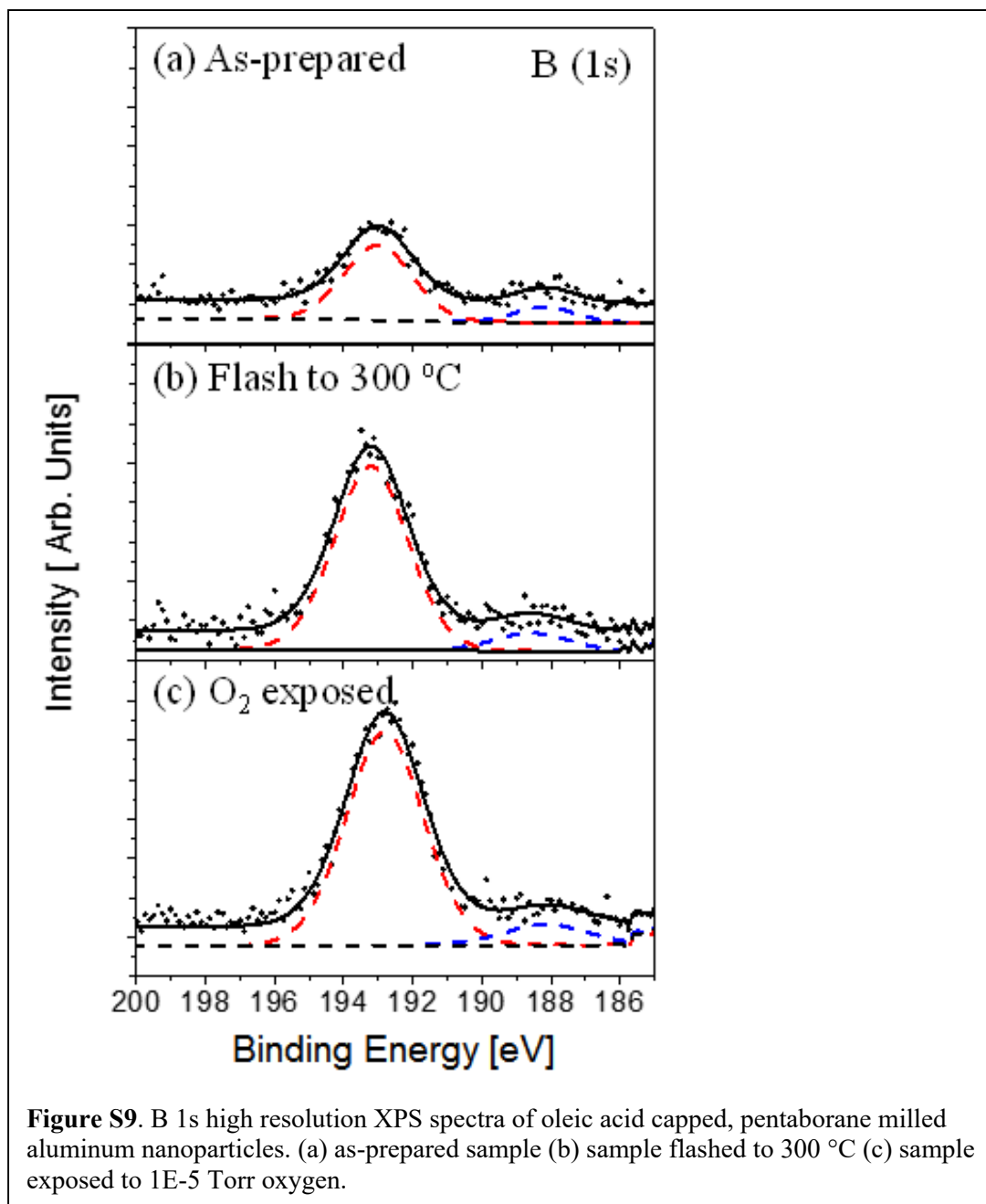












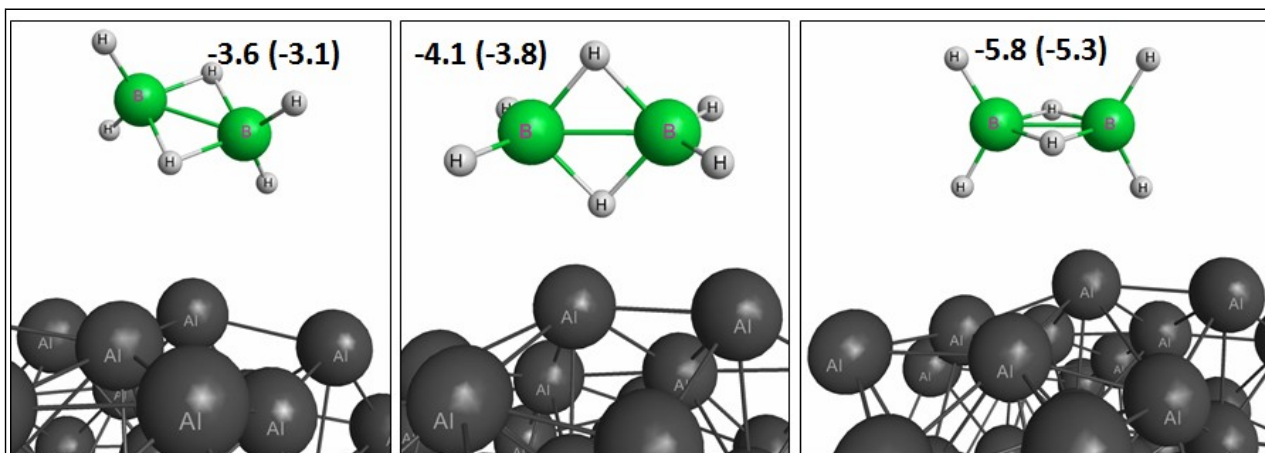


Fig. S10. M06/6-311++G(d,p) structures and binding energies of physisorbed diborane. Energies are in kcal mol⁻¹ and are relative to separated $Al_{80} + B_2H_6$. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al_{80} cluster has been cropped to show the physisorbed species in greater detail.

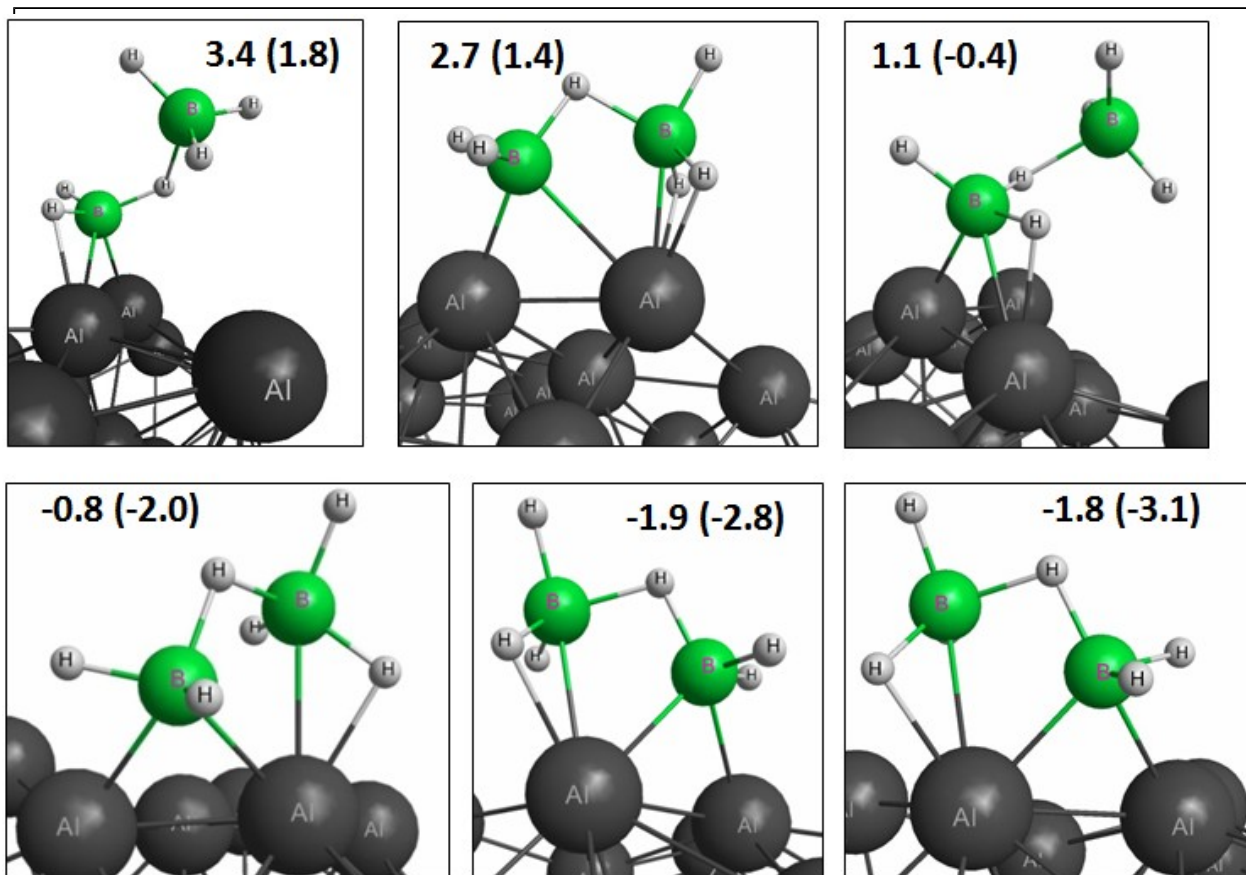
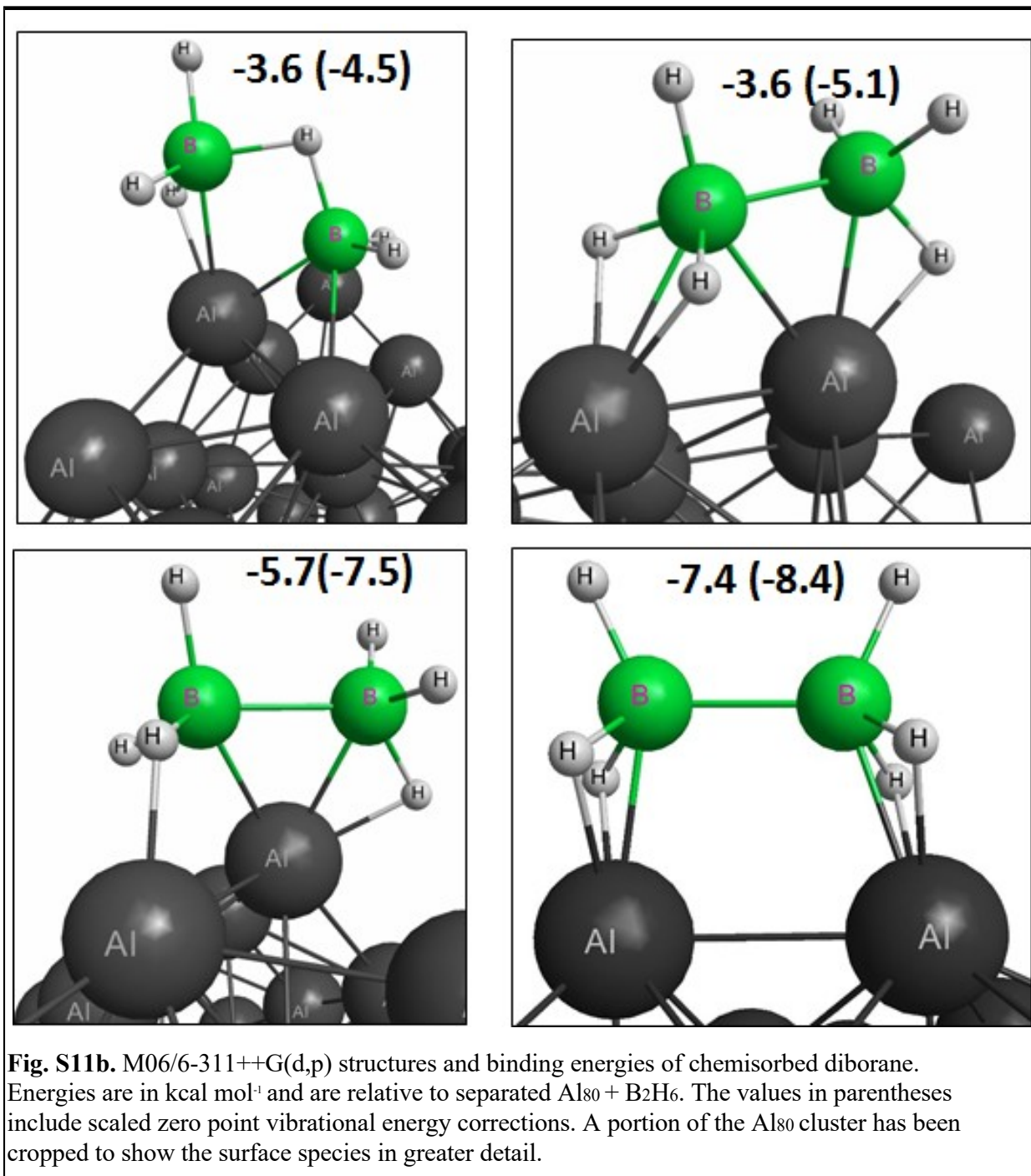
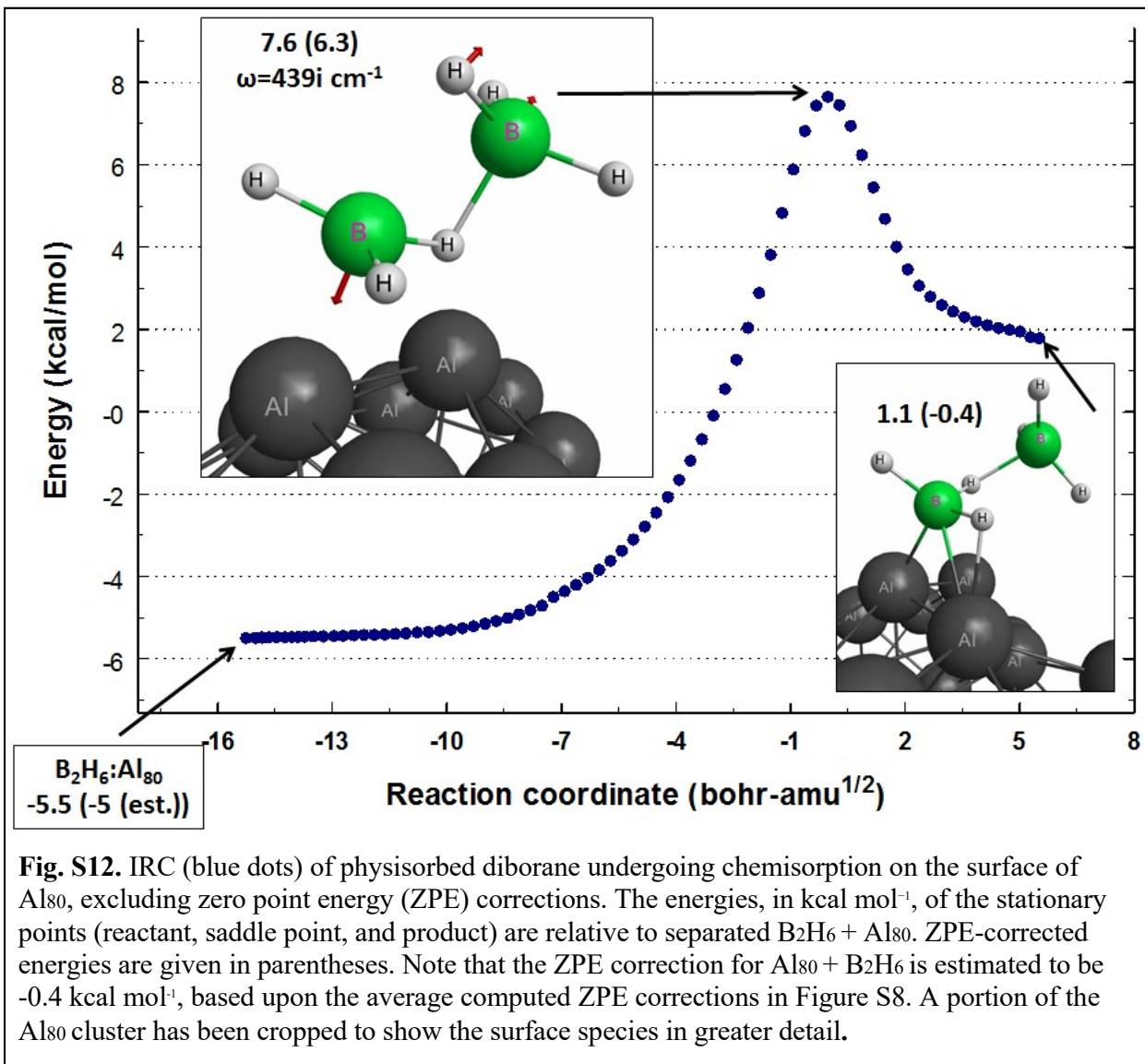
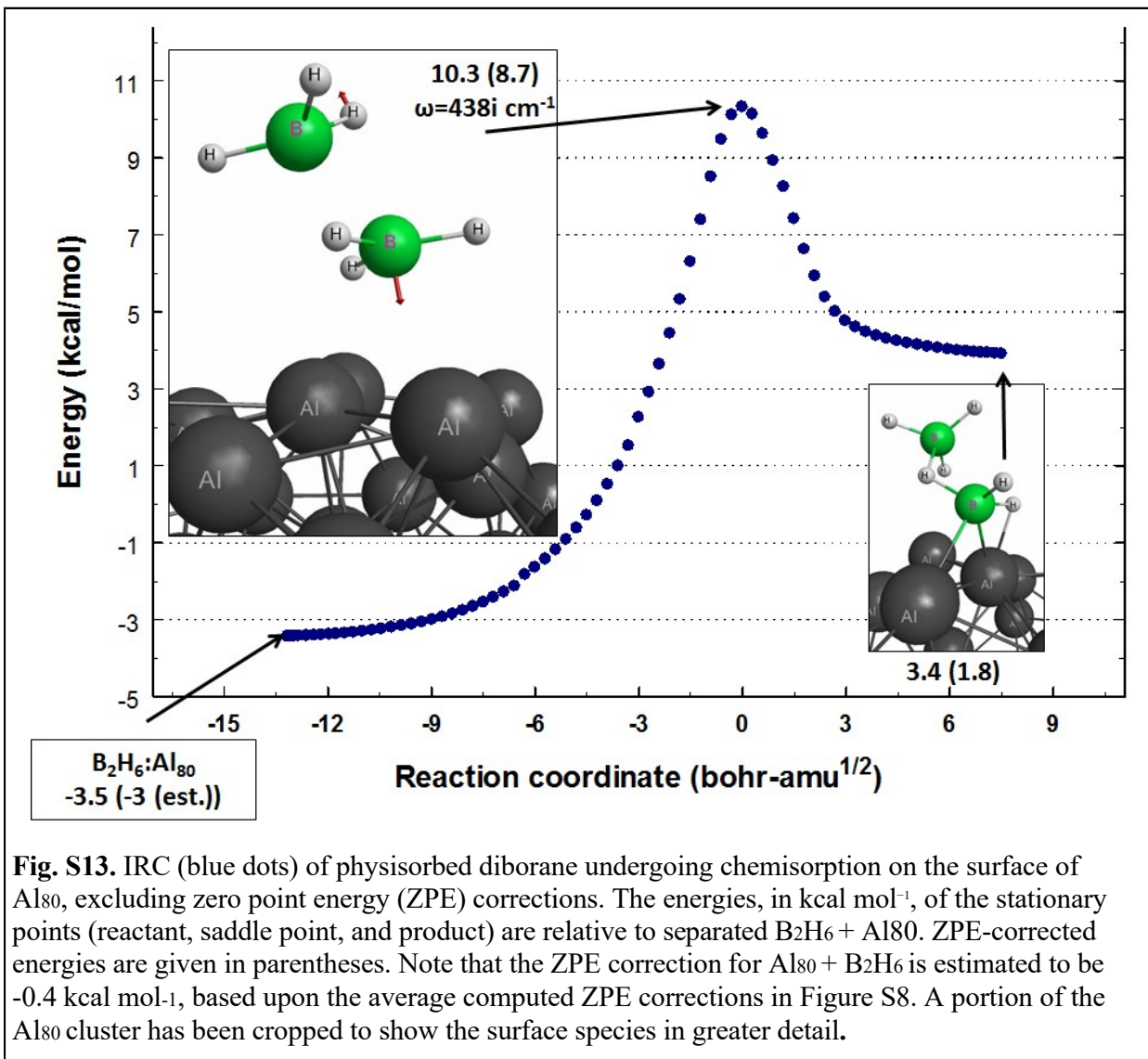
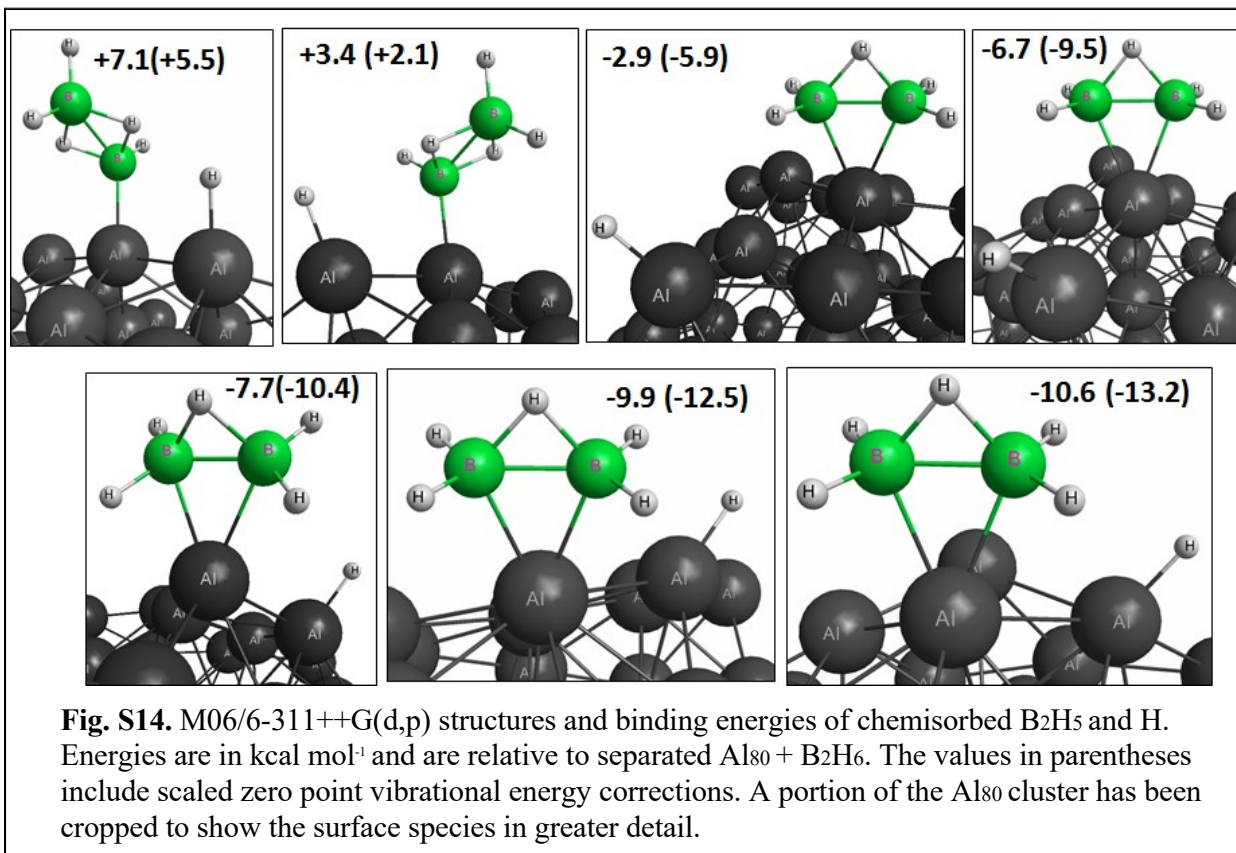


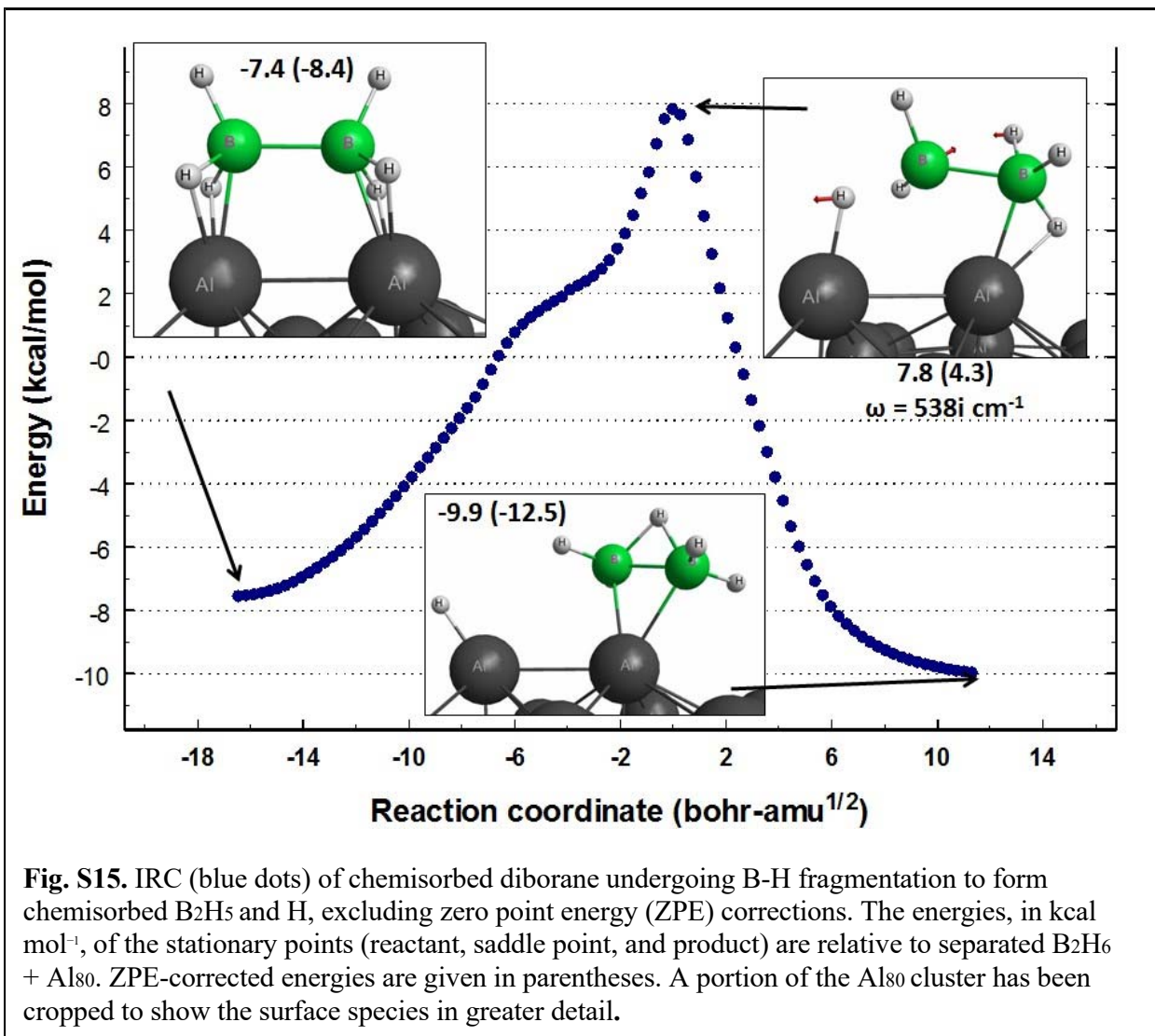
Fig. S11a. M06/6-311++G(d,p) structures and binding energies of chemisorbed diborane. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₂H₆. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the surface species in greater detail.











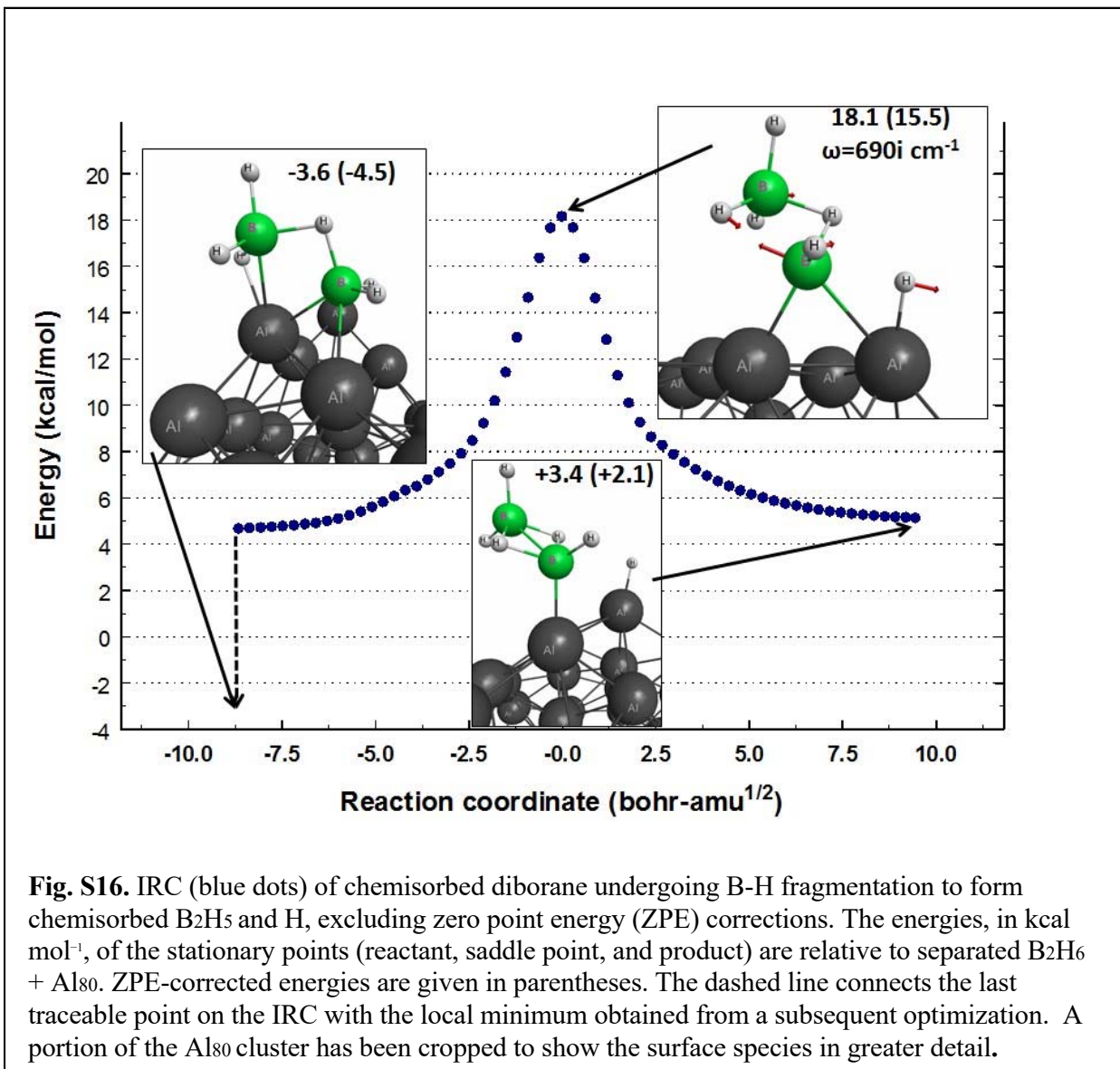


Fig. S16. IRC (blue dots) of chemisorbed diborane undergoing B-H fragmentation to form chemisorbed B₂H₅ and H, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated B₂H₆ + Al₈₀. ZPE-corrected energies are given in parentheses. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al₈₀ cluster has been cropped to show the surface species in greater detail.

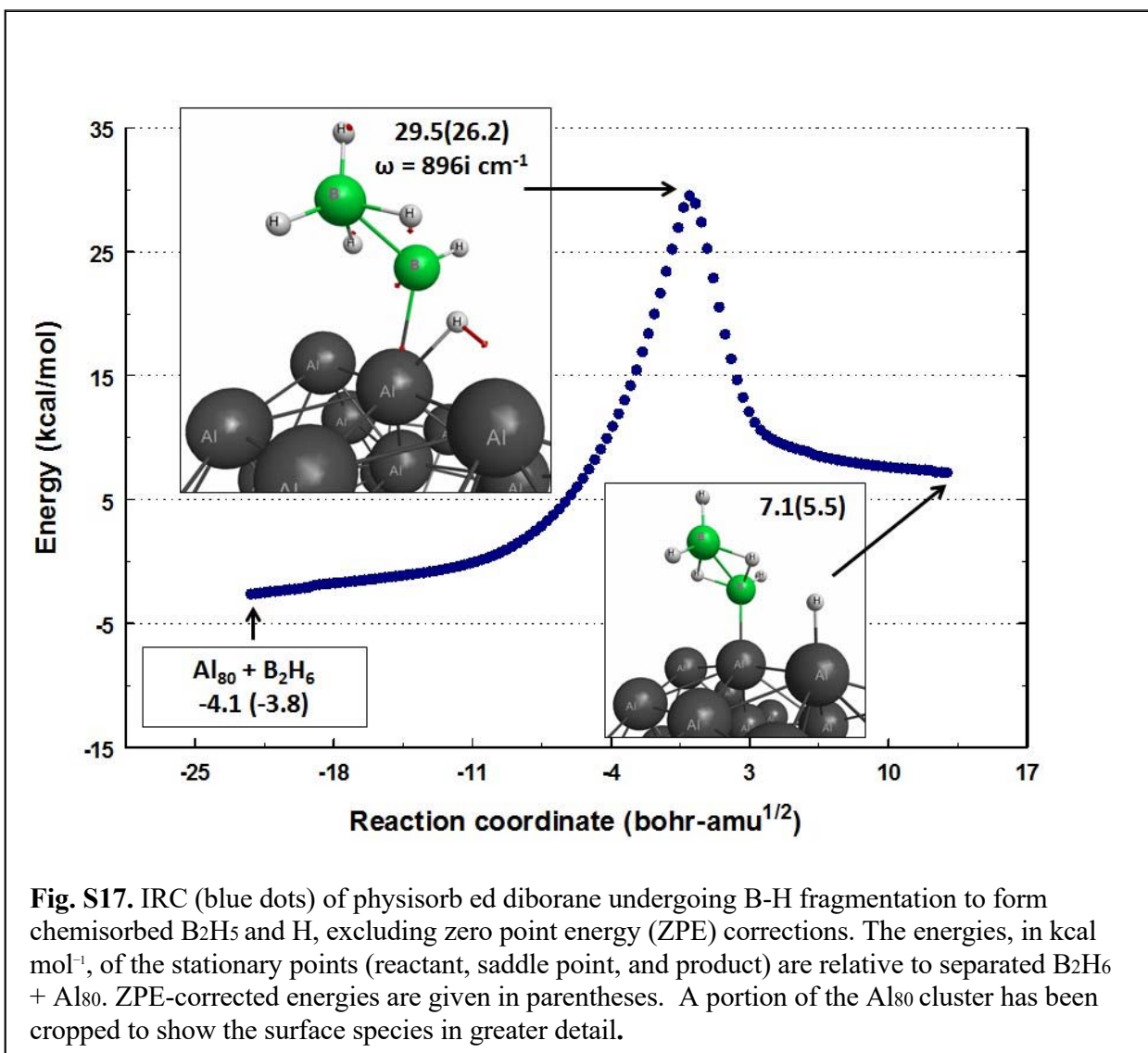
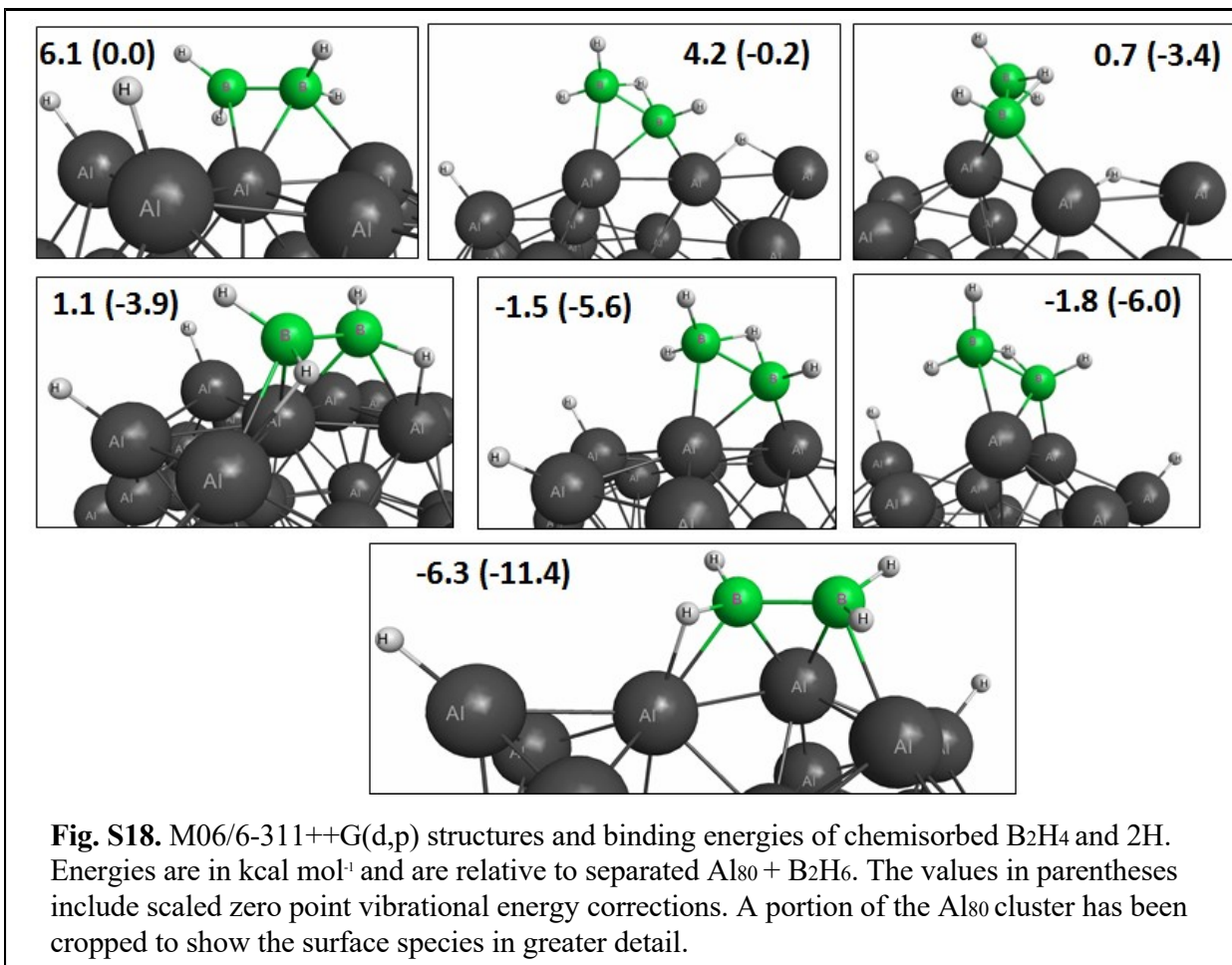


Fig. S17. IRC (blue dots) of physisorbed diborane undergoing B-H fragmentation to form chemisorbed B_2H_5 and H, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. ZPE-corrected energies are given in parentheses. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.



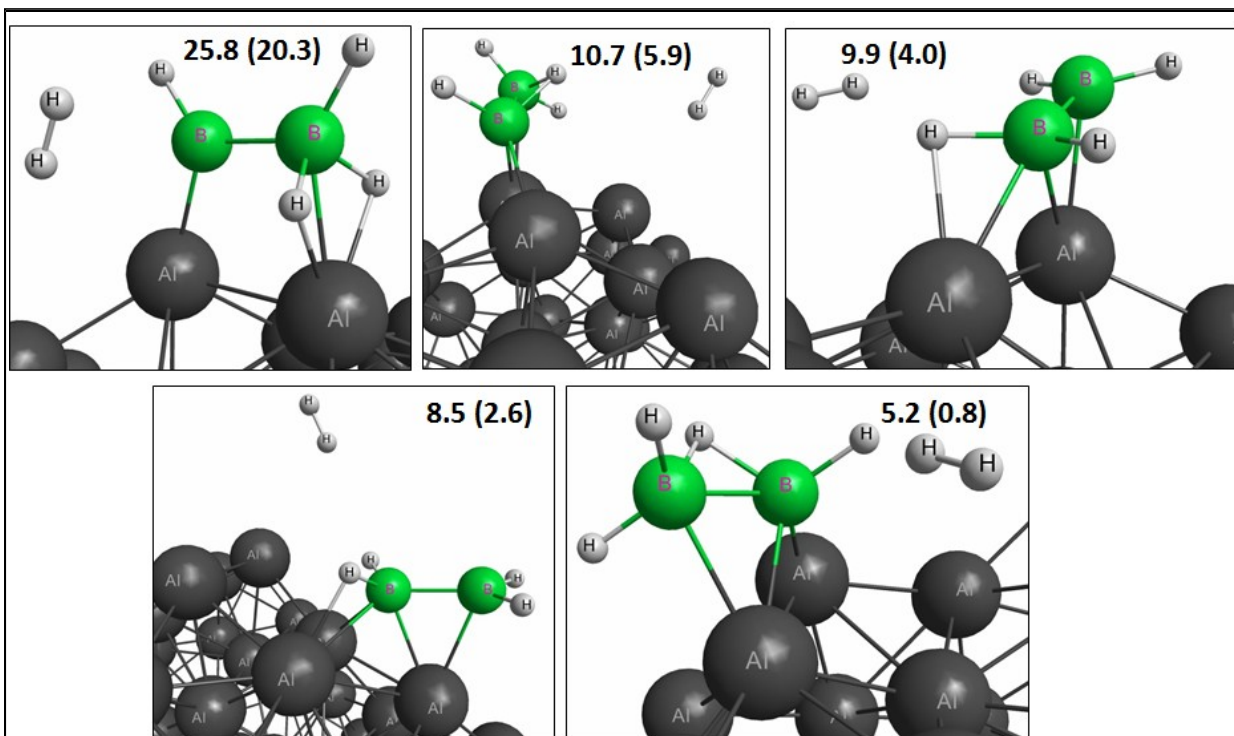


Fig. S19. M06/6-311++G(d,p) structures and binding energies of chemisorbed B₂H₄ and gaseous H₂. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₂H₆. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the surface species in greater detail.

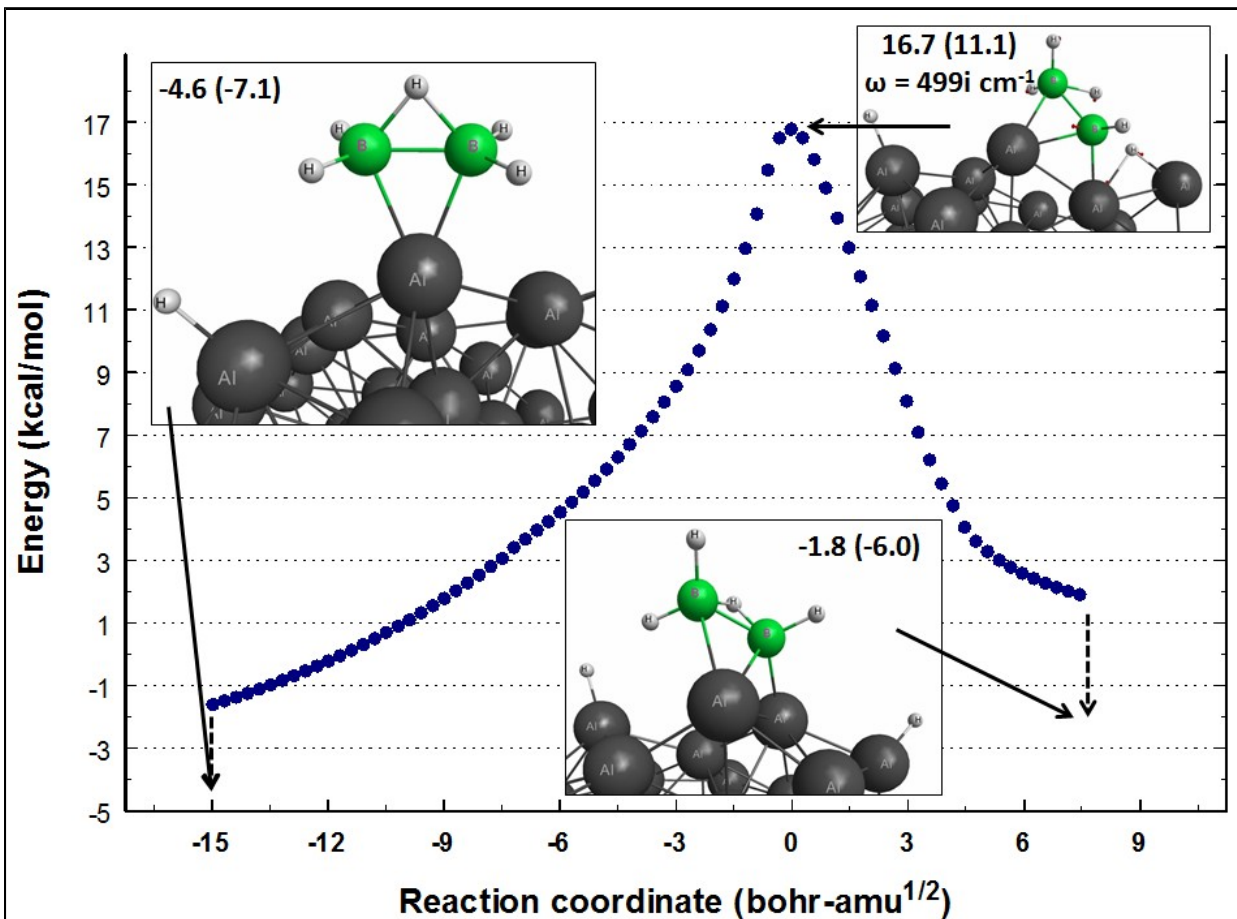


Fig. S20. IRC (blue dots) of B₂H₅-Al₈₀-H undergoing B-H fragmentation to form B₂H₄-Al₈₀-2H, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated B₂H₆ + Al₈₀. ZPE-corrected energies are given in parentheses. The dashed lines connect the last traceable points on the IRC with the local minima obtained from subsequent optimizations. A portion of the Al₈₀ cluster has been cropped to show the surface species in greater detail.

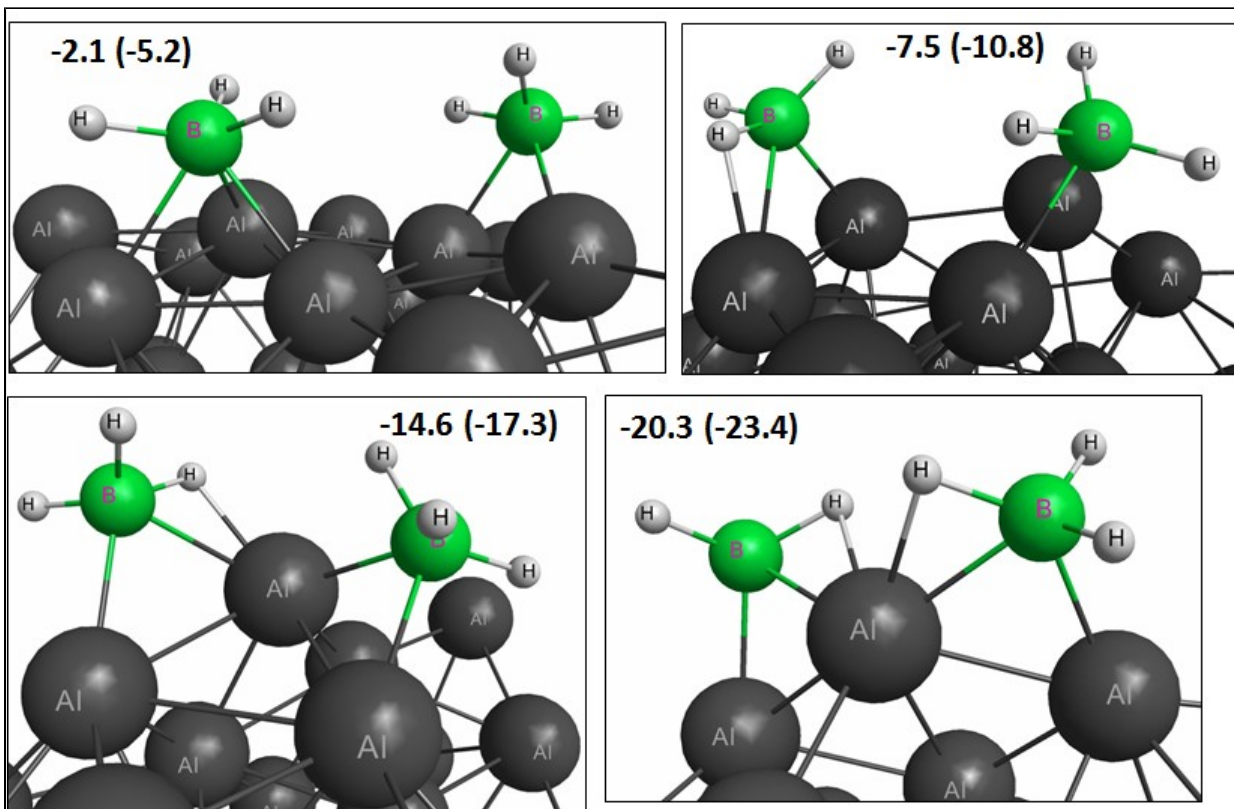


Fig. S21. M06/6-311++G(d,p) structures and binding energies of chemisorbed $\text{H}_3\text{B}-\text{Al}_{80}-\text{BH}_3$. Energies are in kcal mol^{-1} and are relative to separated $\text{Al}_{80} + \text{B}_2\text{H}_6$. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al_{80} cluster has been cropped to show the physisorbed species in greater detail.

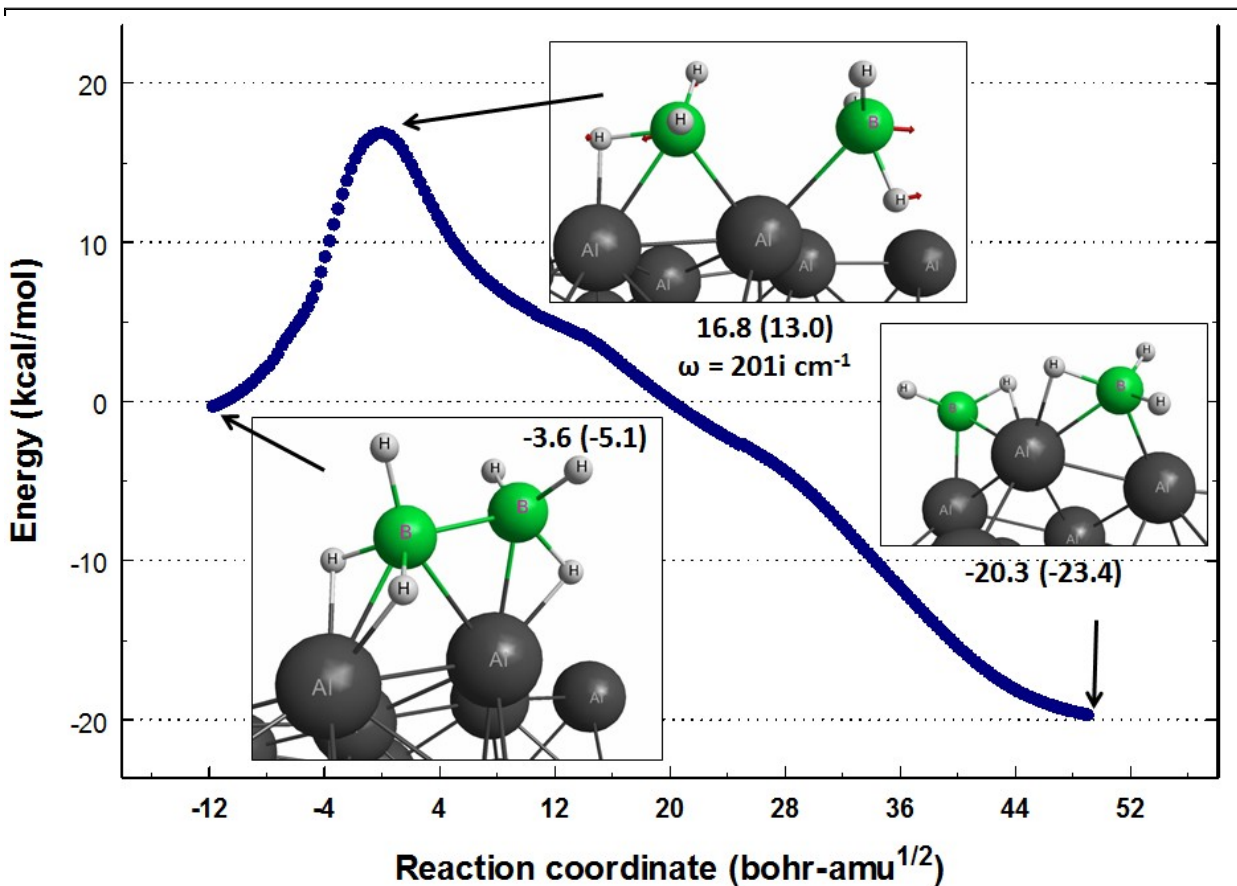


Fig. S22. IRC (blue dots) of $\text{B}_2\text{H}_6\text{-Al}_{80}$ undergoing B-B fragmentation to form $\text{H}_3\text{B-Al}_{80}\text{-BH}_3$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

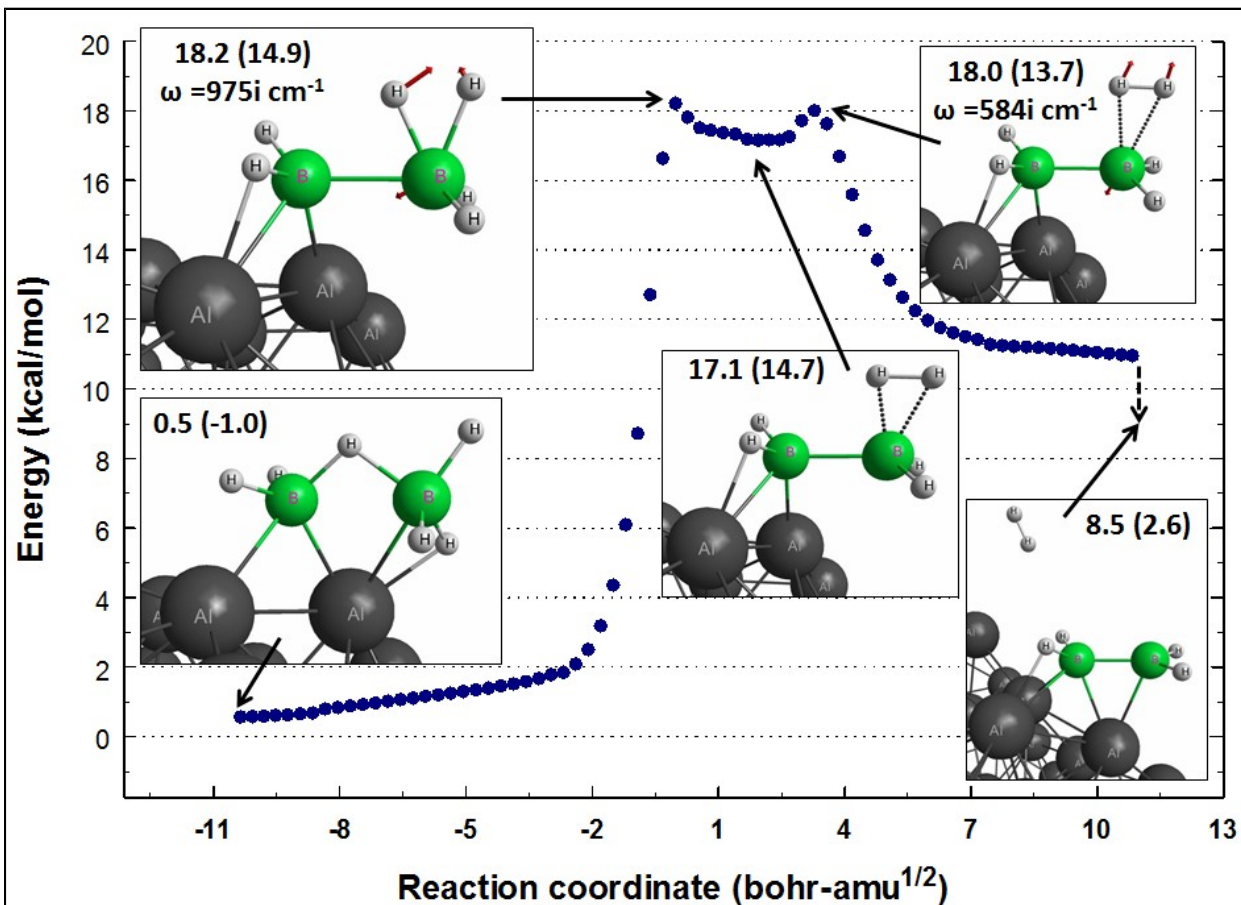


Fig. S23. IRC (blue dots) of $\text{B}_2\text{H}_6\text{-Al}_{80}$ undergoing H_2 elimination to form $\text{B}_2\text{H}_4\text{-Al}_{80} + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol^{-1} , of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

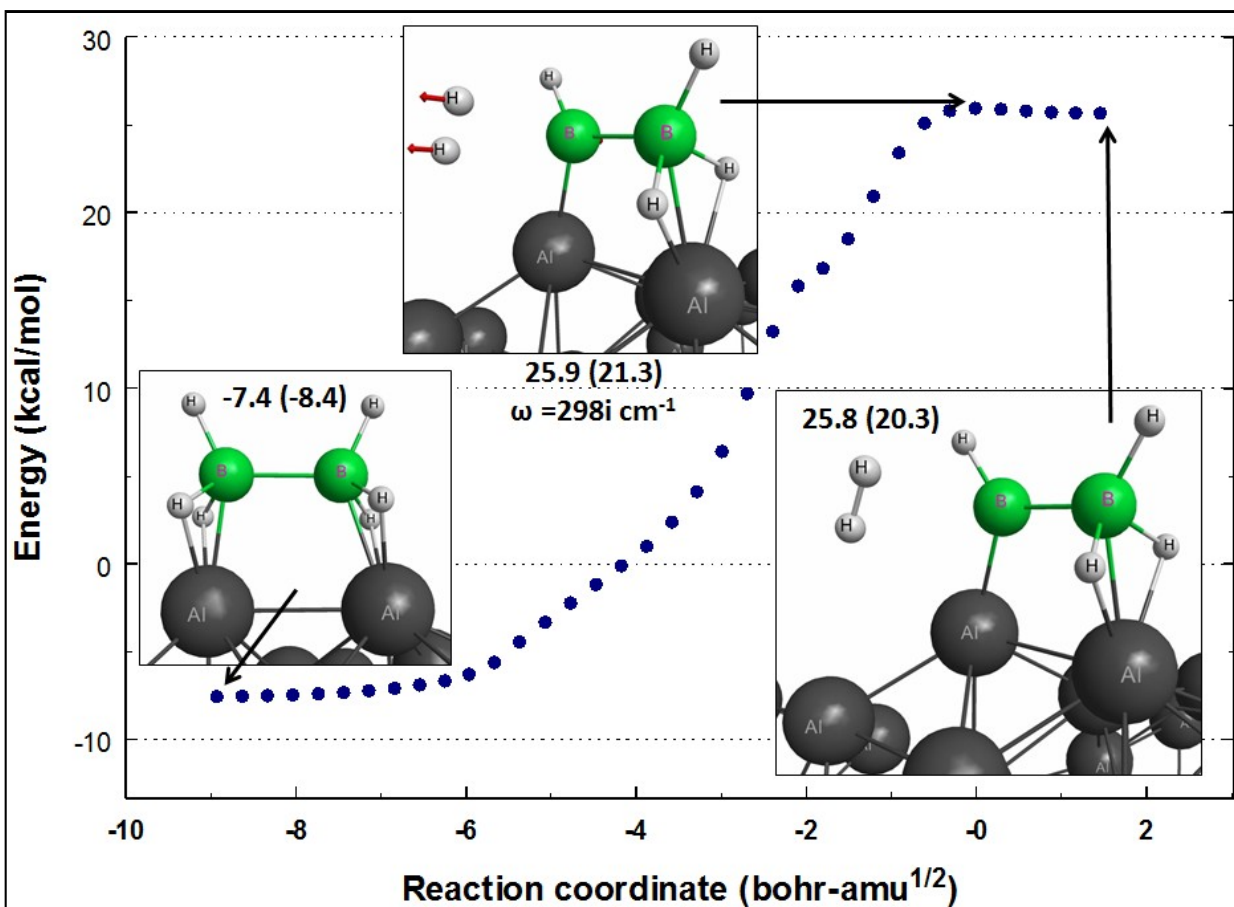


Fig. S24. IRC (blue dots) of $\text{B}_2\text{H}_6\text{-Al}_{80}$ undergoing H_2 elimination to form $\text{BHBH}_3\text{-Al}_{80} + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

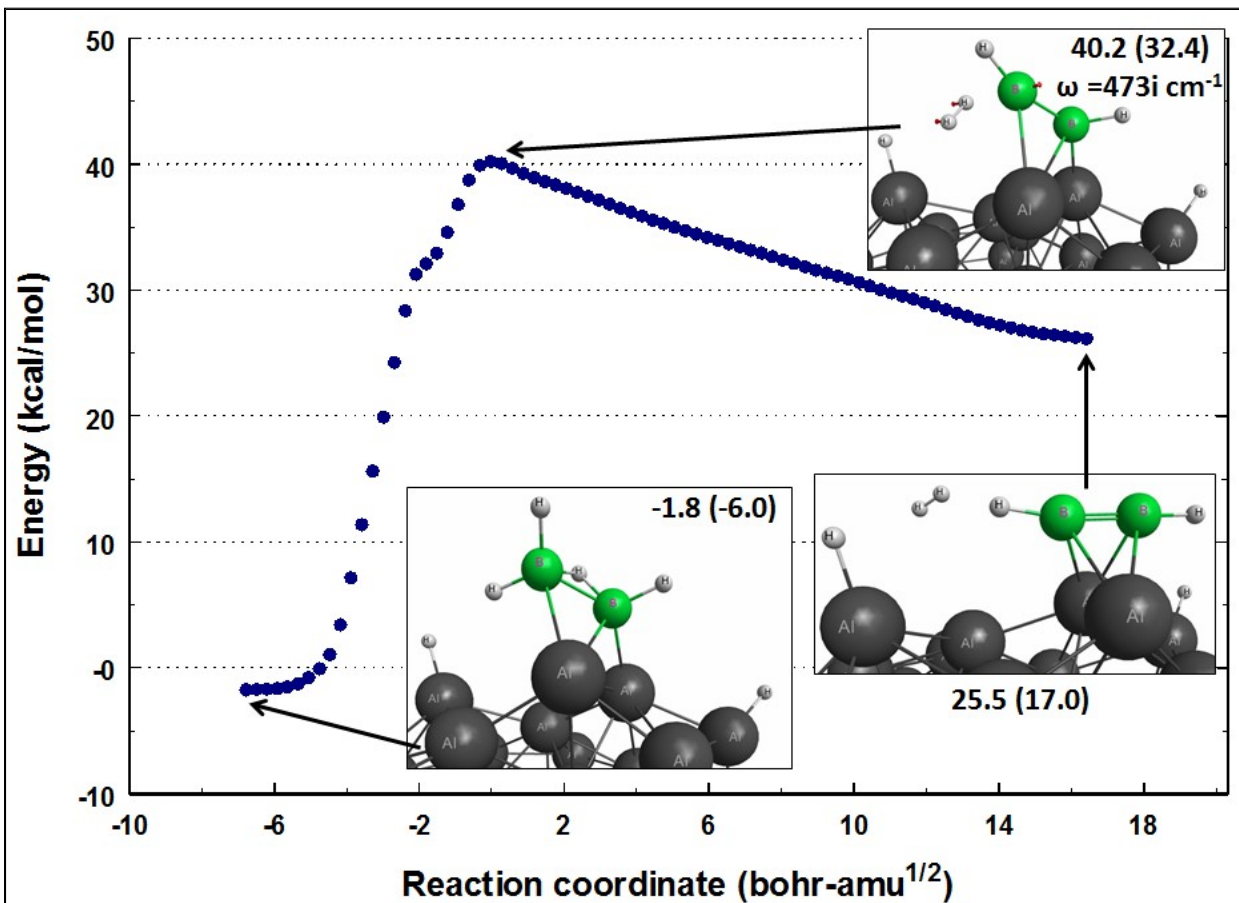


Fig. S25. IRC (blue dots) of $\text{B}_2\text{H}_4\text{-Al}_{80}\text{-2H}$ undergoing H_2 elimination to form $\text{B}_2\text{H}_2\text{-Al}_{80}\text{-2H} + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

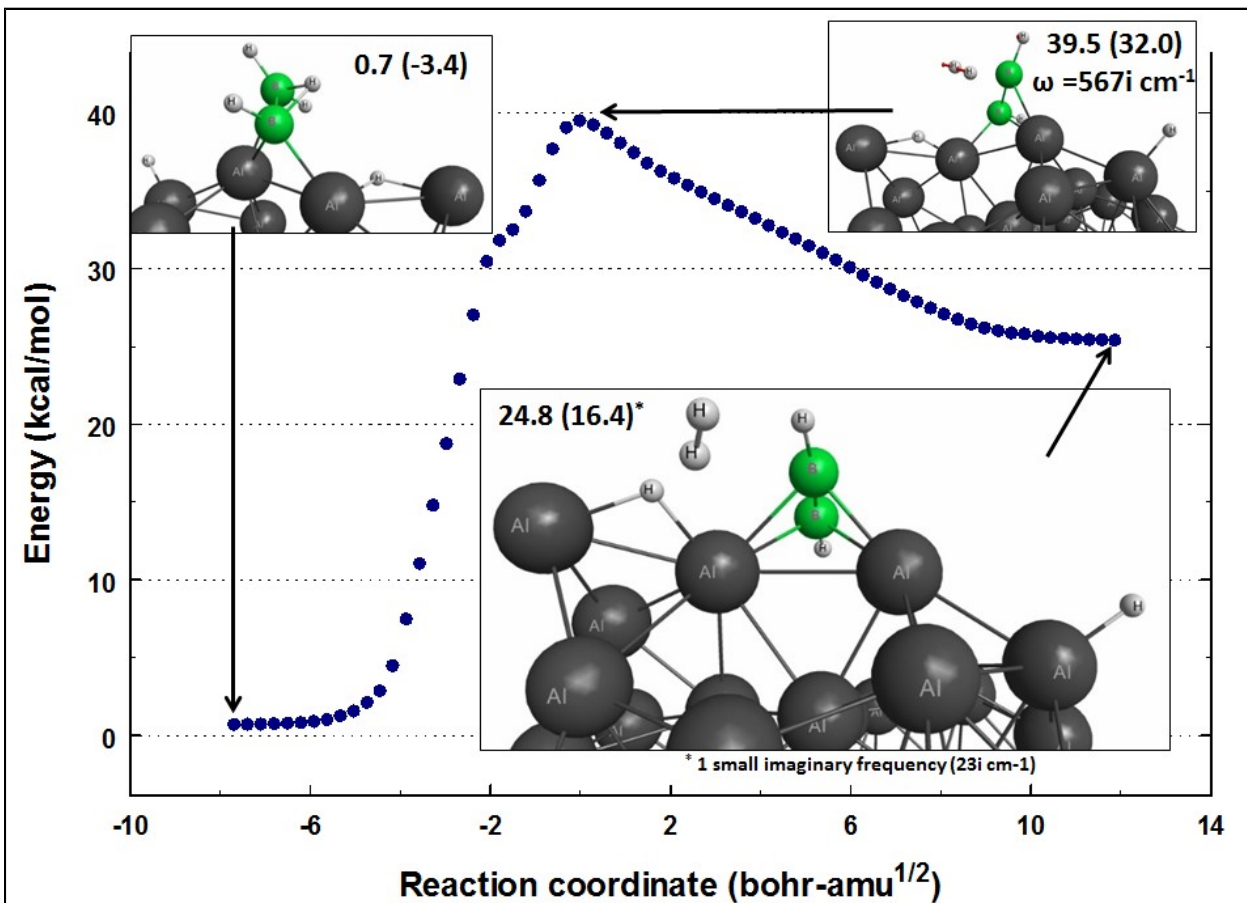


Fig. S26. IRC (blue dots) of $\text{B}_2\text{H}_4\text{-Al}_{80}\text{-2H}$ undergoing H_2 elimination to form $\text{B}_2\text{H}_2\text{-Al}_{80}\text{-2H} + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

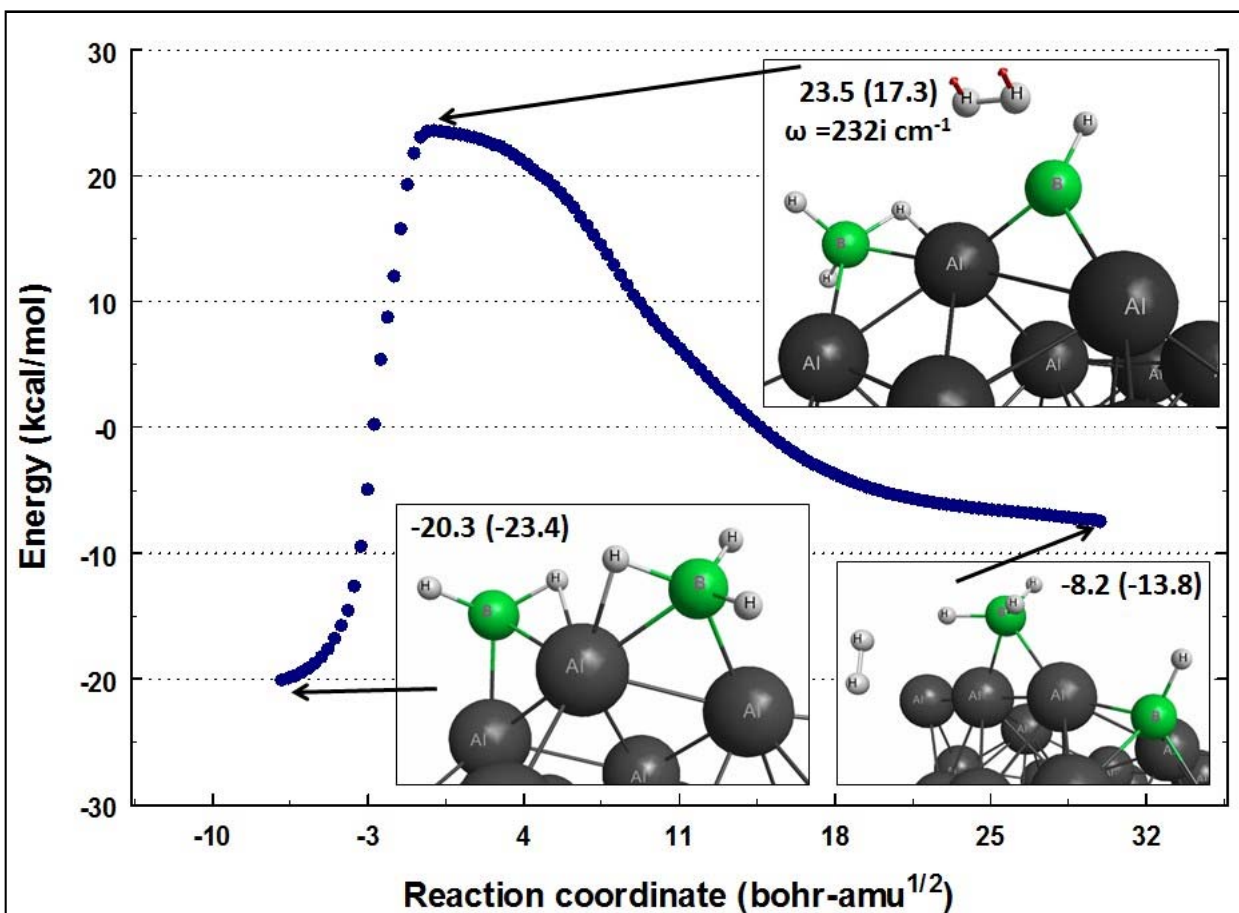


Fig. S27. IRC (blue dots) of $\text{H}_3\text{B}-\text{Al}_{80}-\text{BH}_3$ undergoing H_2 elimination to form $\text{HB}-\text{Al}_{80}-\text{BH}_3 + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

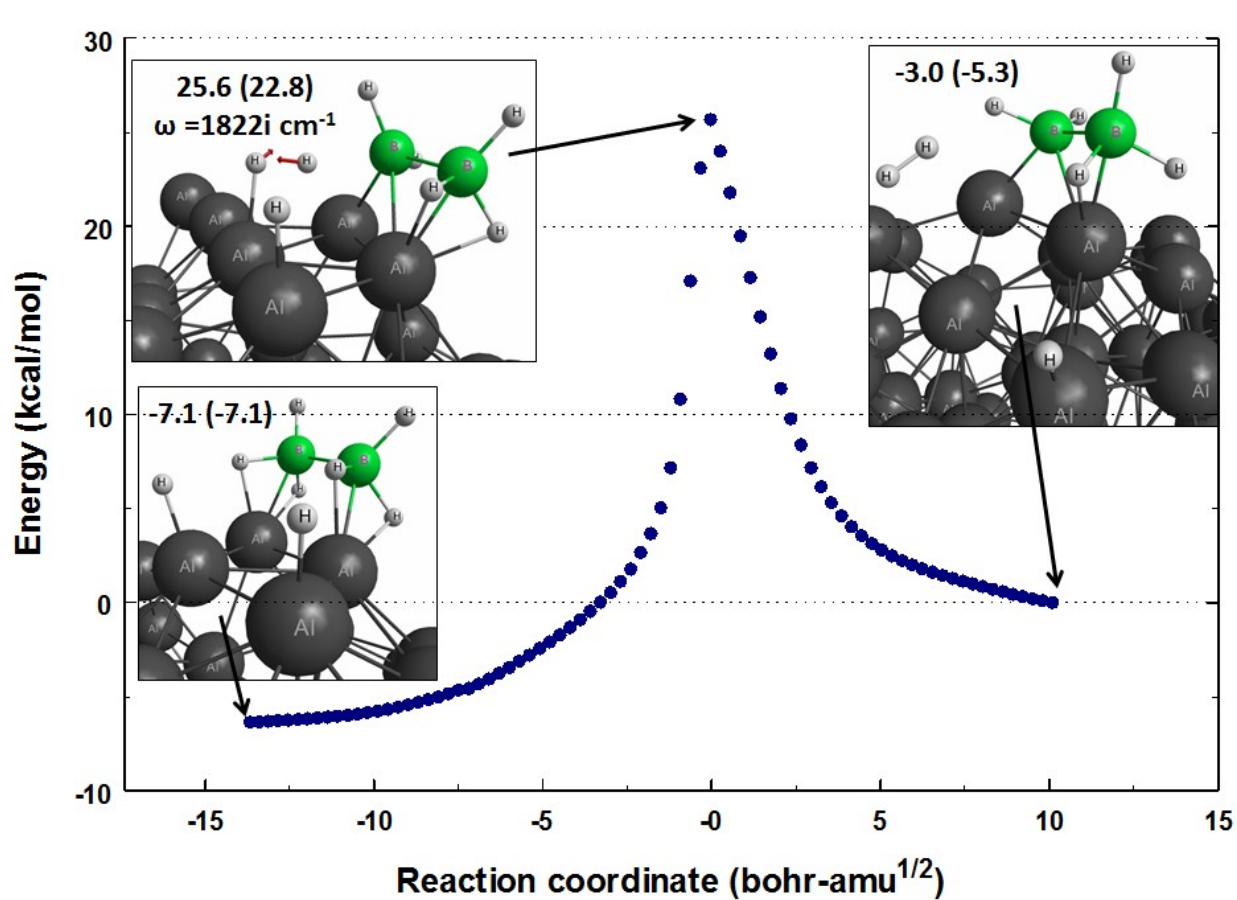
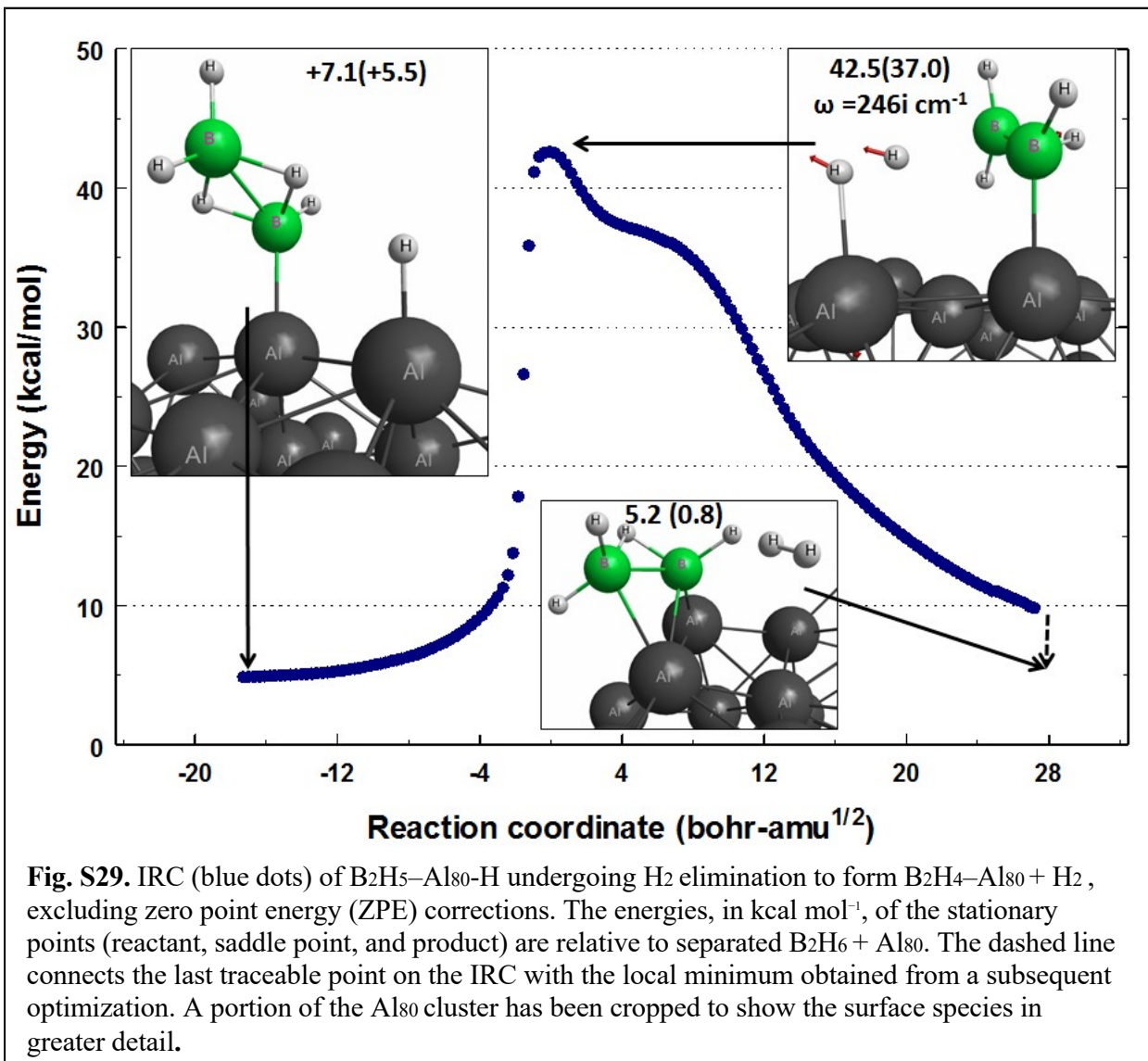
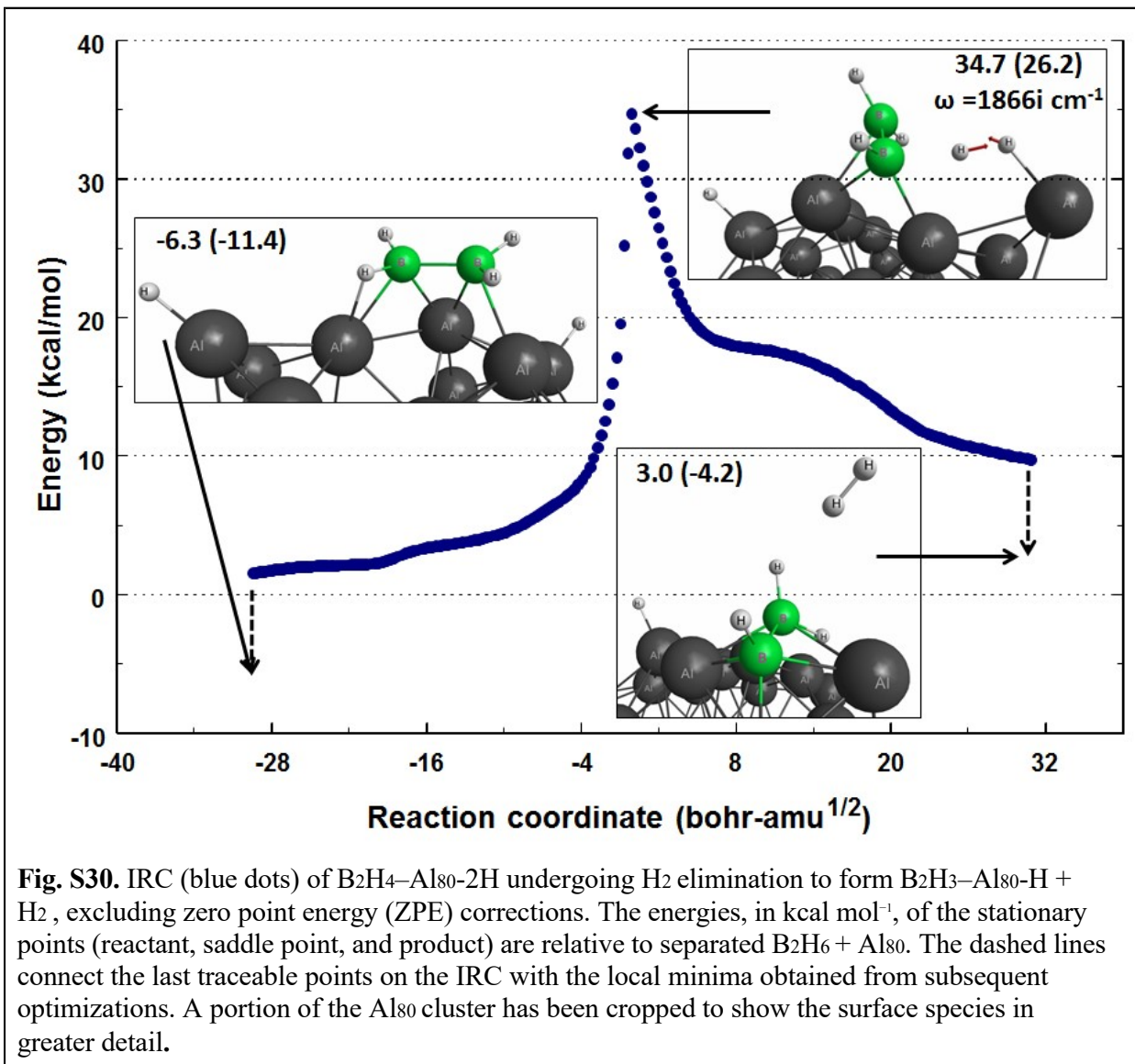


Fig. S28. IRC (blue dots) of $\text{B}_2\text{H}_6\text{-Al}_{80}\text{-2H}$ undergoing H_2 elimination to form $\text{B}_2\text{H}_5\text{-Al}_{80}\text{-H} + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{H}_2 + \text{Al}_{80}$. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.





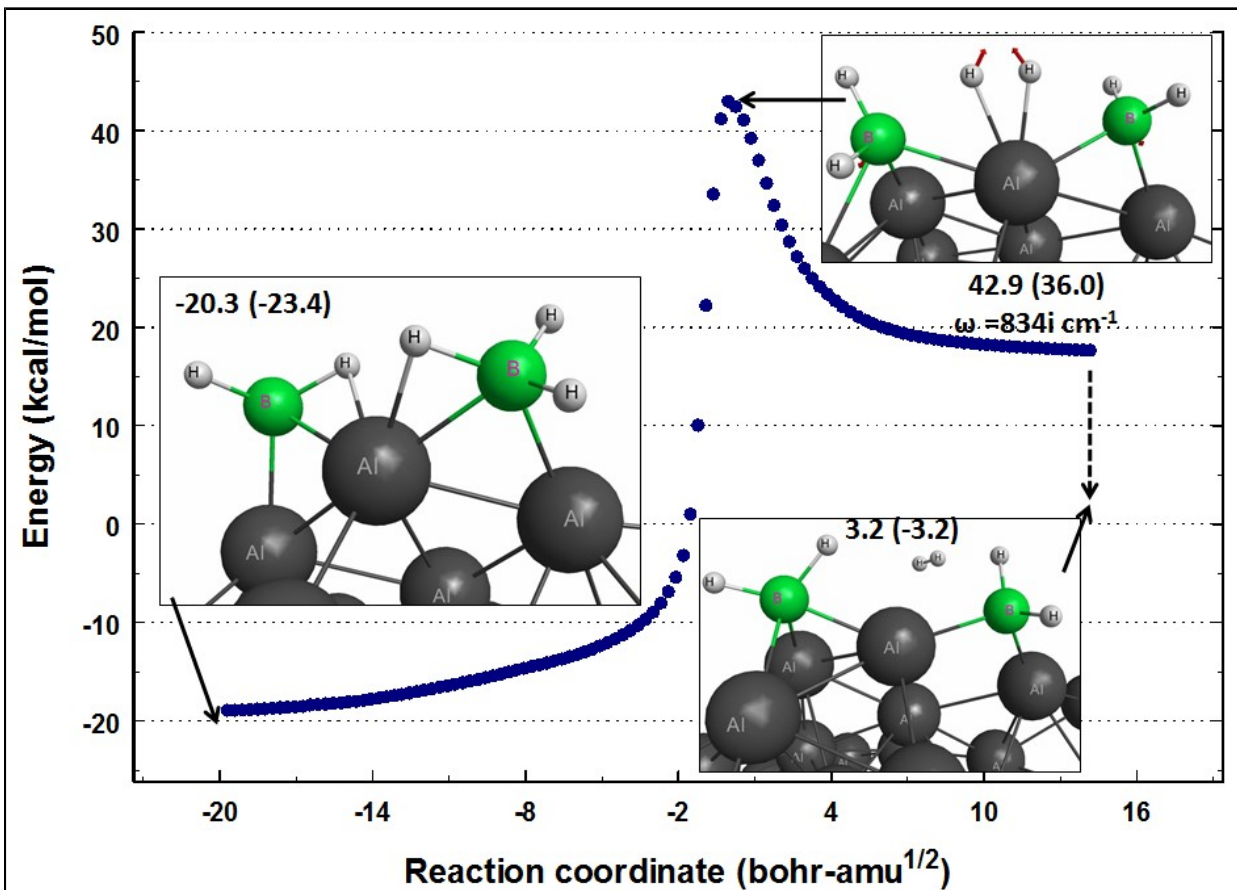


Fig. S31. IRC (blue dots) of $\text{BH}_3\text{-Al}_{80}\text{-BH}_3$ undergoing H_2 elimination to form $\text{BH}_2\text{-Al}_{80}\text{-BH}_2 + \text{H}_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_2\text{H}_6 + \text{Al}_{80}$. The dashed line connects the last traceable point on the IRC with the local minima obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

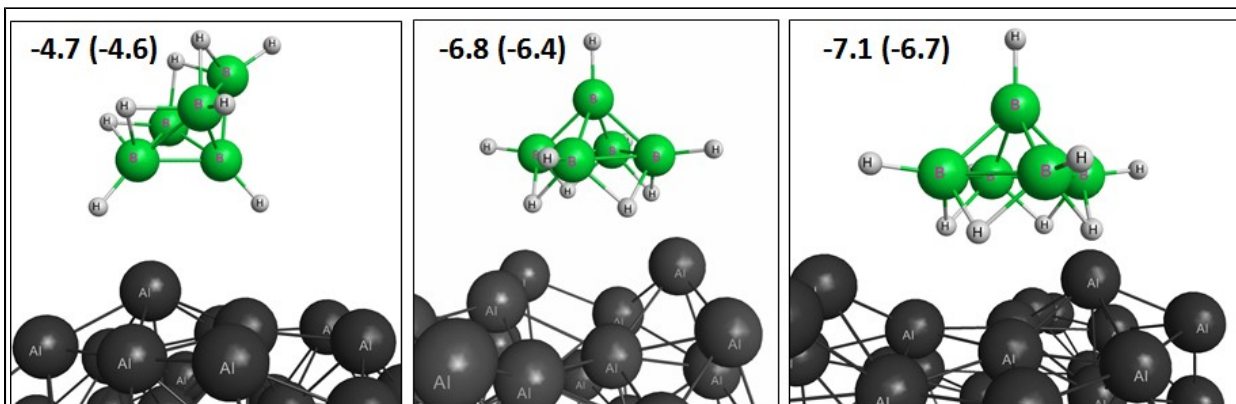
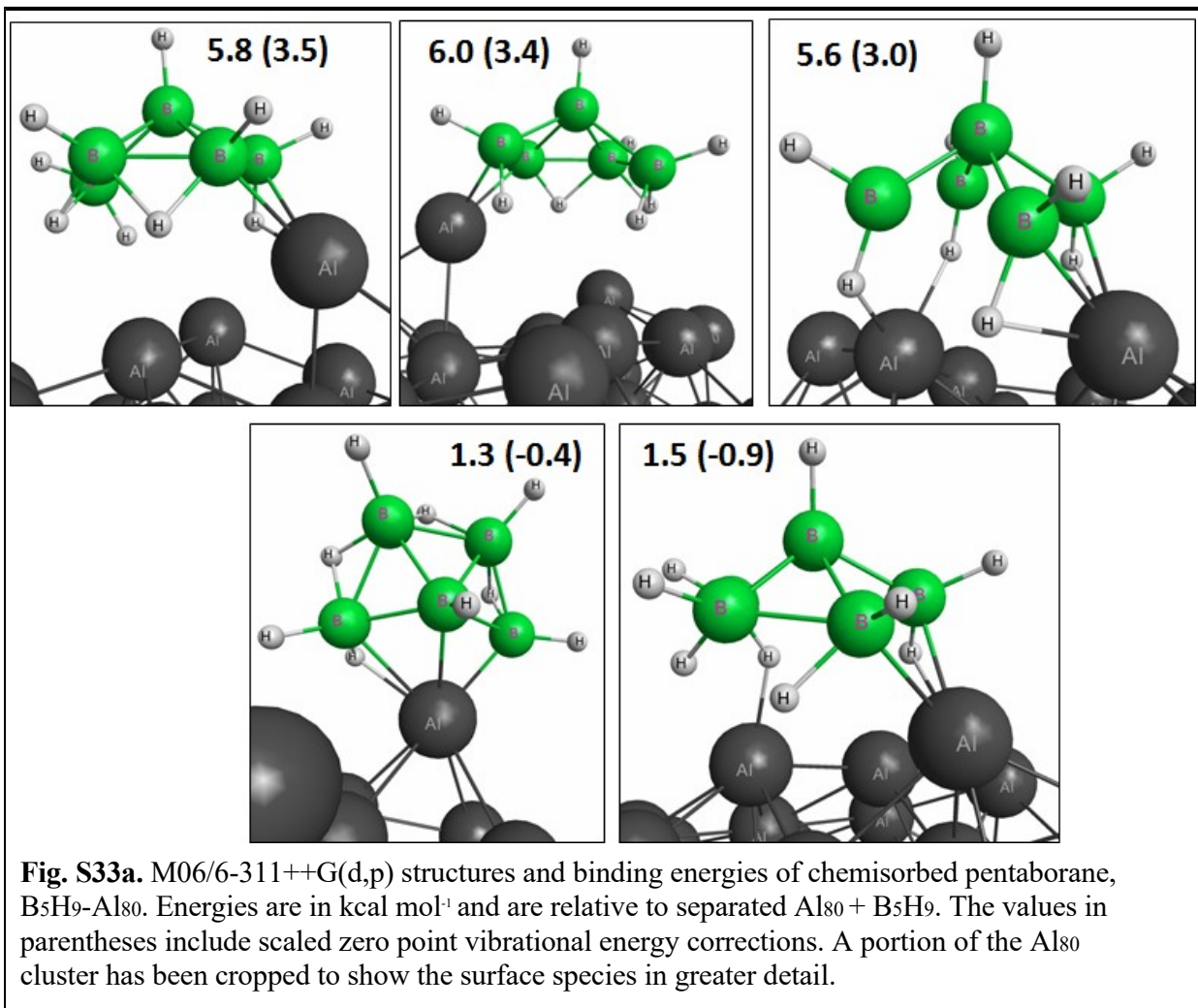


Fig. S32. M06/6-311++G(d,p) structures and binding energies of physisorbed pentaborane, $B_5H_9:Al_{80}$. Energies are in kcal mol⁻¹ and are relative to separated $Al_{80} + B_5H_9$. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al_{80} cluster has been cropped to show the physisorbed species in greater detail.



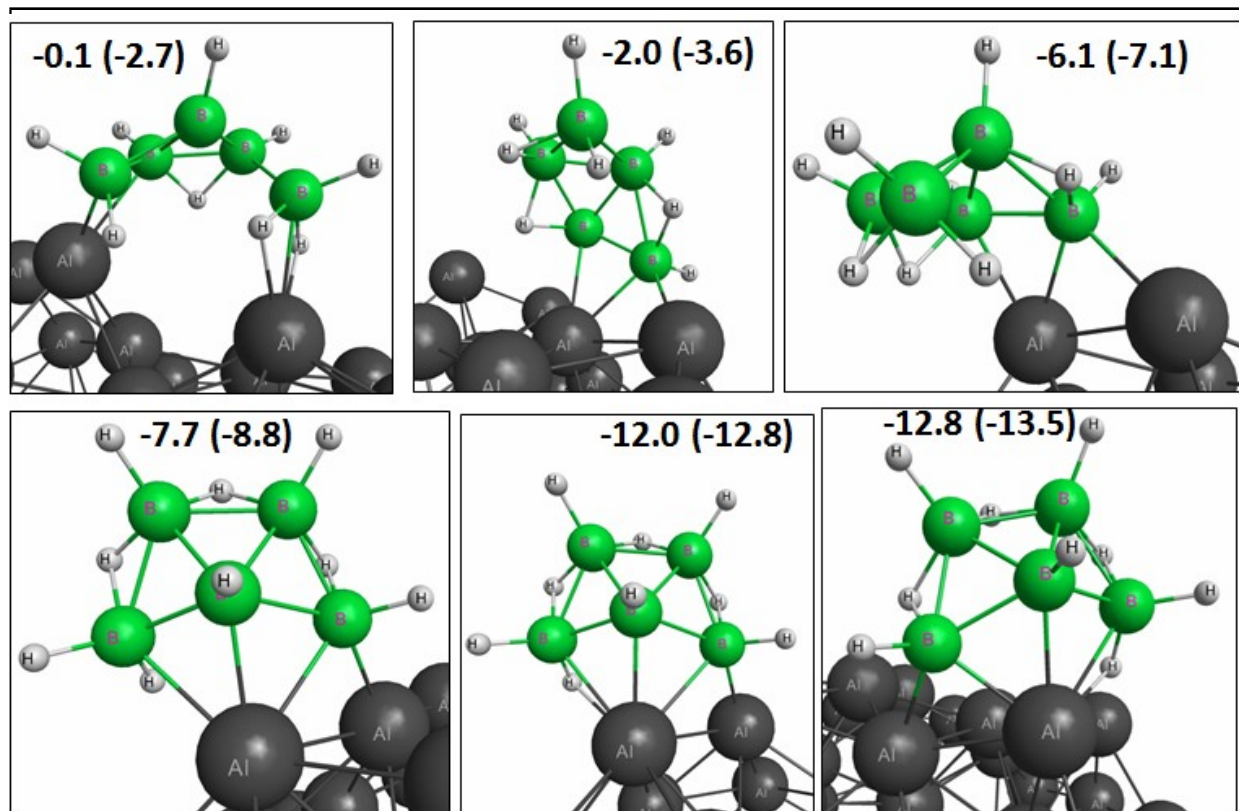


Fig. S33b. M06/6-311++G(d,p) structures and binding energies of chemisorbed pentaborane, B₅H₉-Al₈₀. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₅H₉. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the surface species in greater detail.

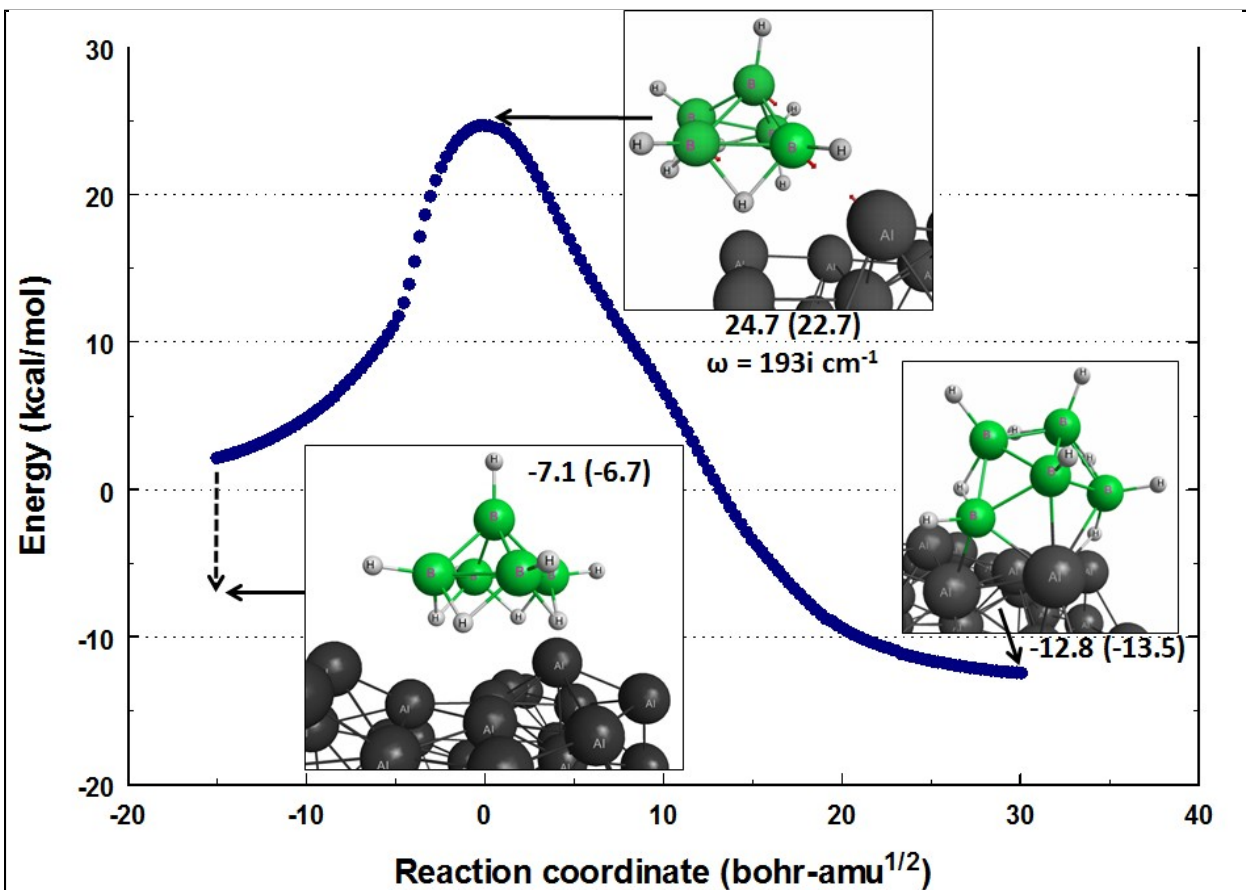


Fig. S34. IRC (blue dots) of physisorbed pentaborane undergoing chemisorption, $\text{B}_5\text{H}_9:\text{Al}_{80} \rightarrow \text{B}_5\text{H}_9\text{-Al}_{80}$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $\text{B}_5\text{H}_9 + \text{Al}_{80}$. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

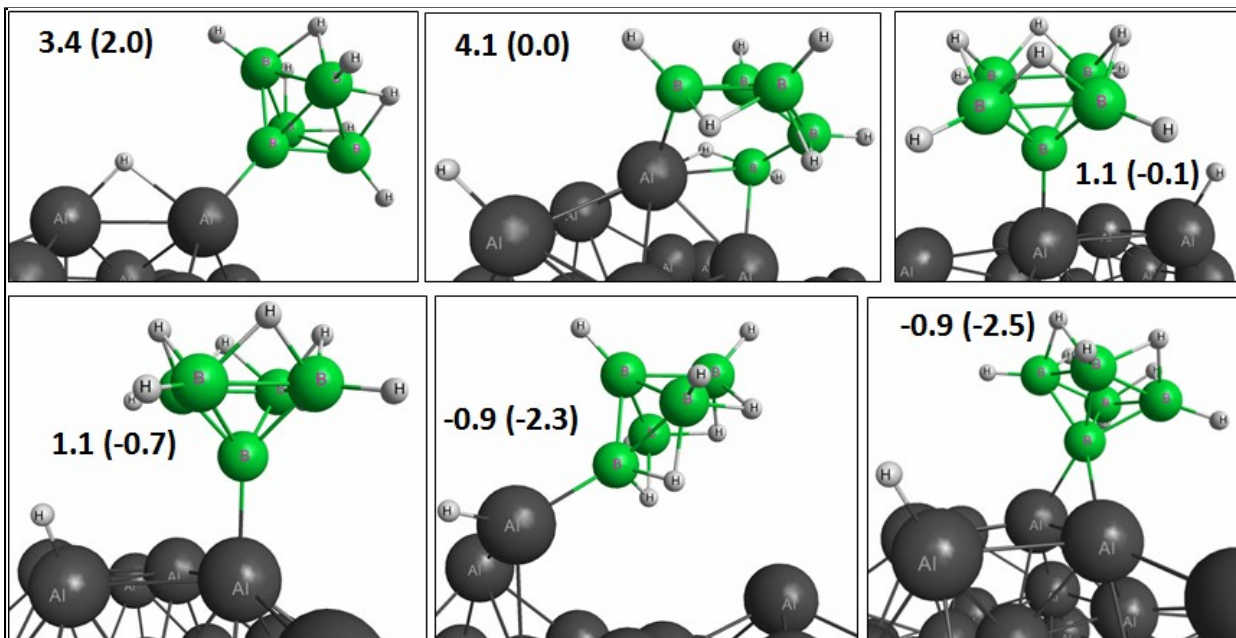


Fig. S35a. M06/6-311++G(d,p) structures and binding energies of chemisorbed B₅H₈ and H. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₅H₉. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the chemisorbed species in greater detail.

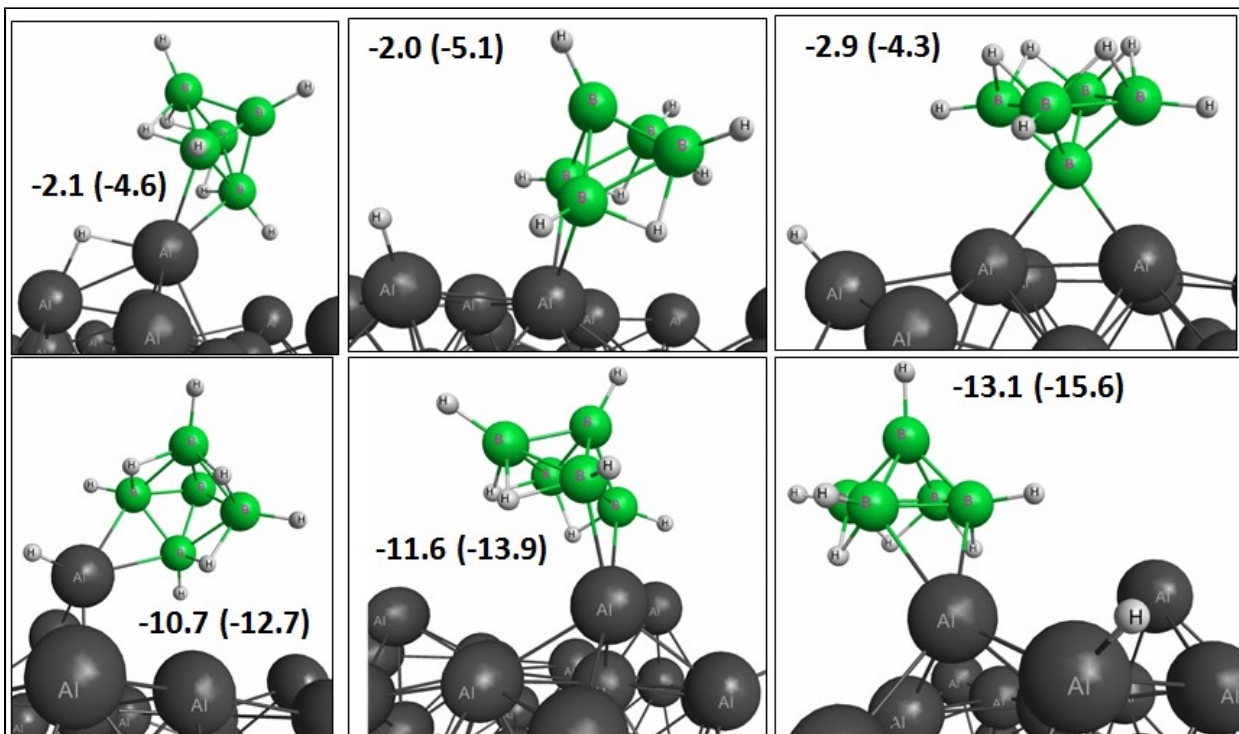


Fig. S35b. M06/6-311++G(d,p) structures and binding energies of chemisorbed B₅H₈ and H. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₅H₉. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the chemisorbed species in greater detail.

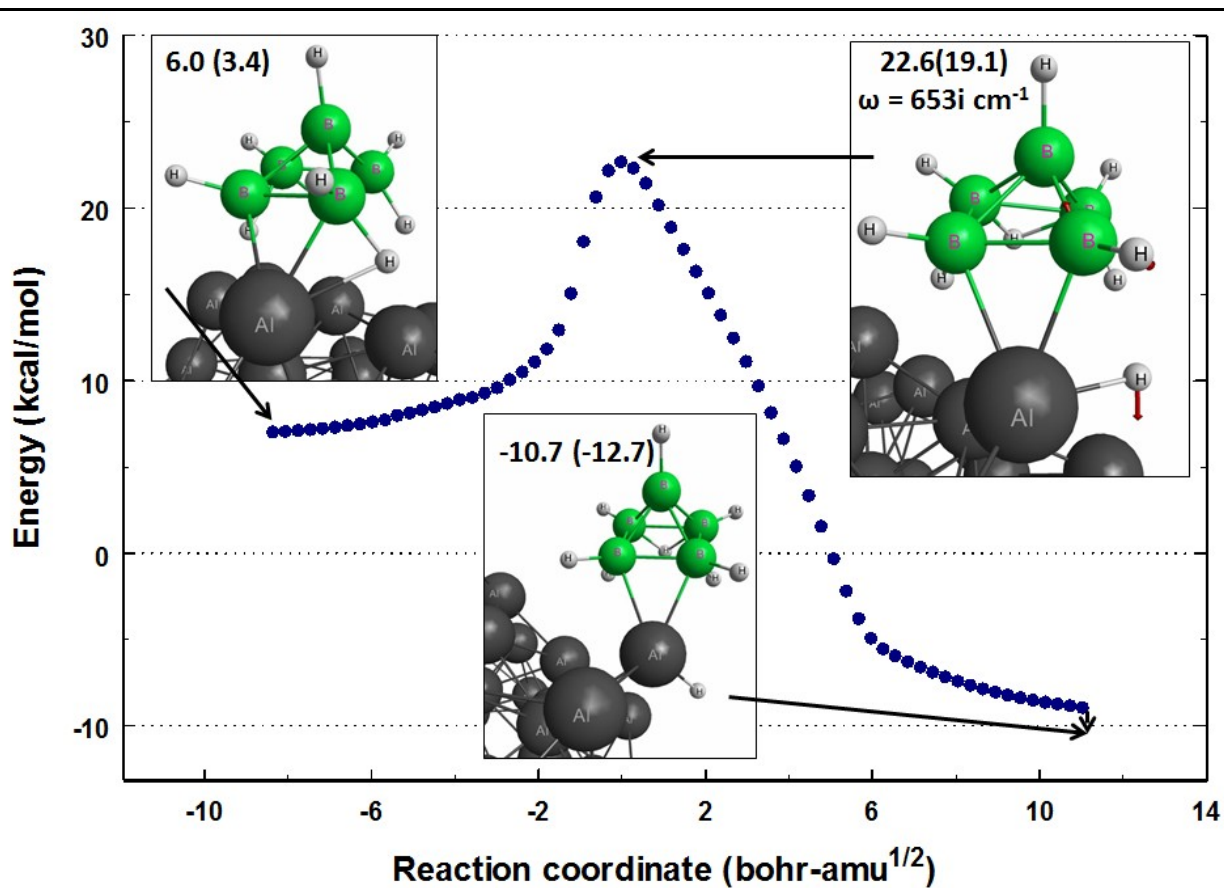


Fig. S36. IRC (blue dots) of chemisorbed pentaborane undergoing B-H fragmentation, $B_5H_9-Al_{80} \rightarrow B_5H_8-Al_{80}-H$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $B_5H_9 + Al_{80}$. The short dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

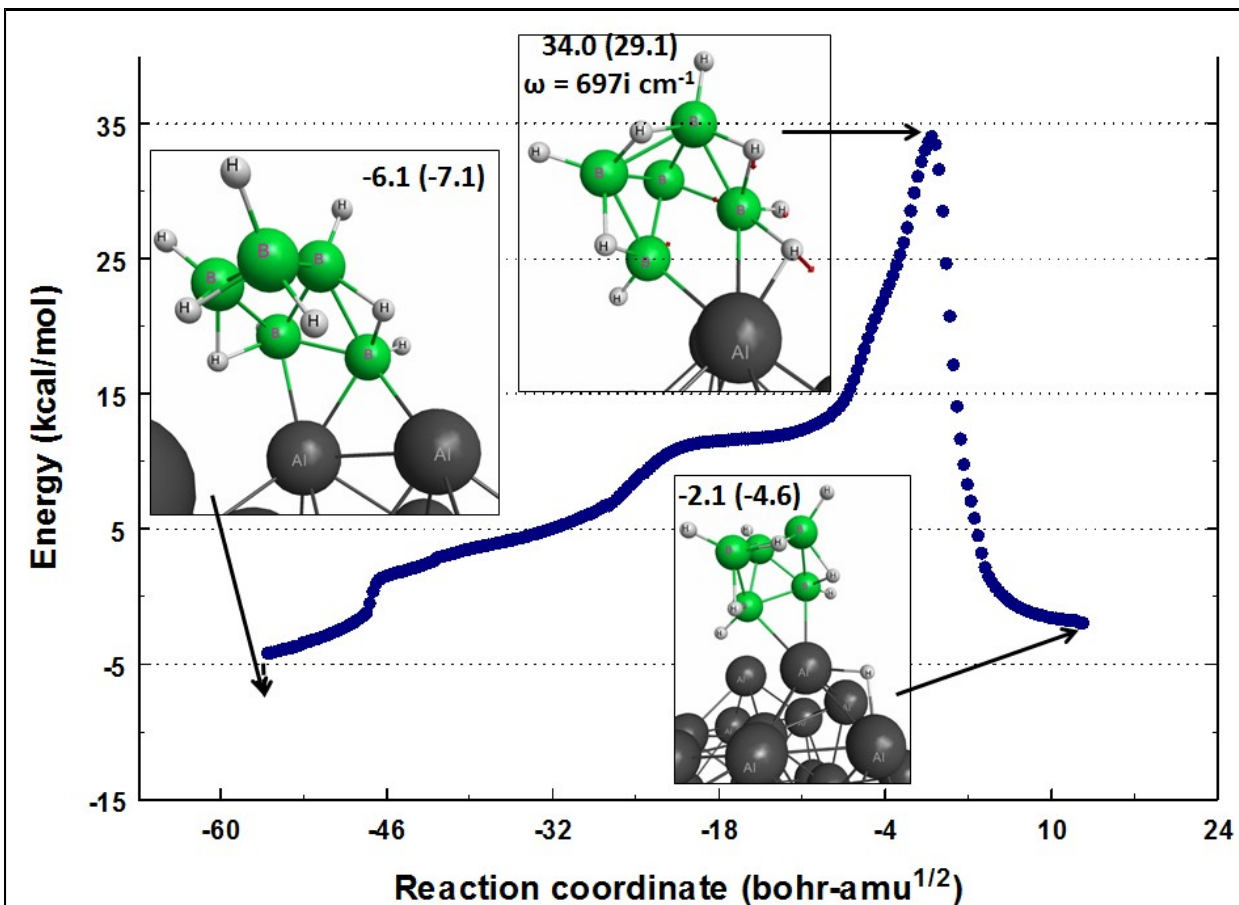
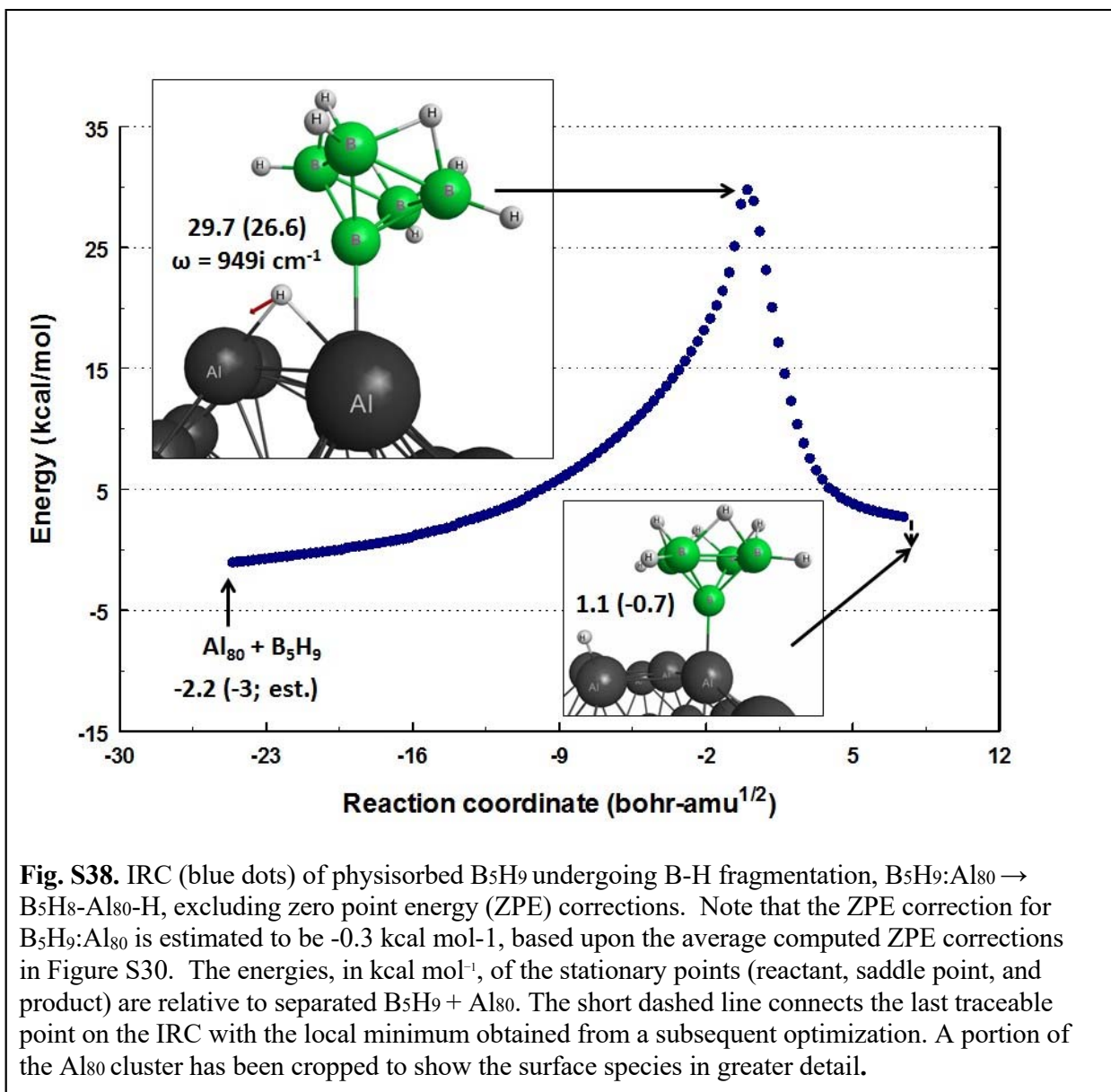
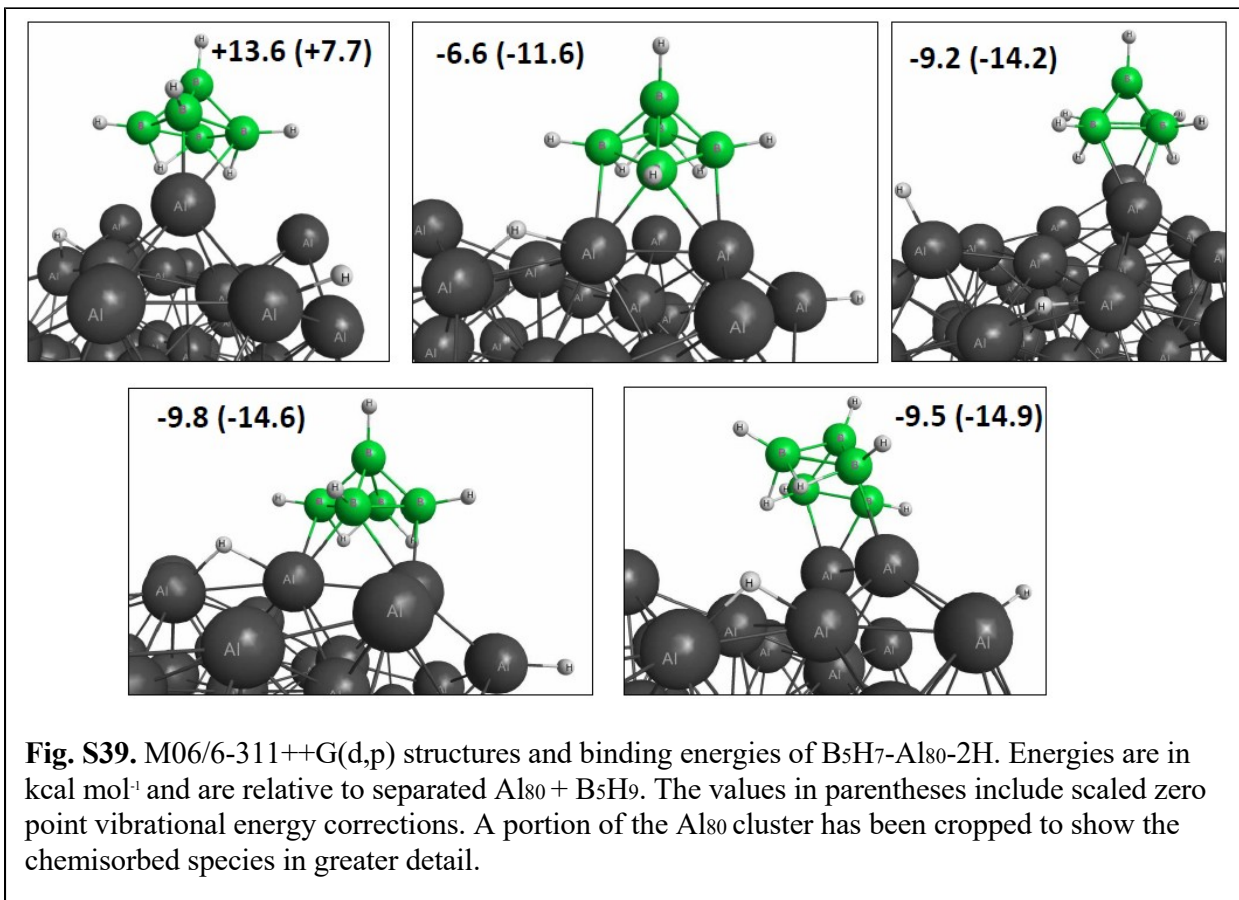
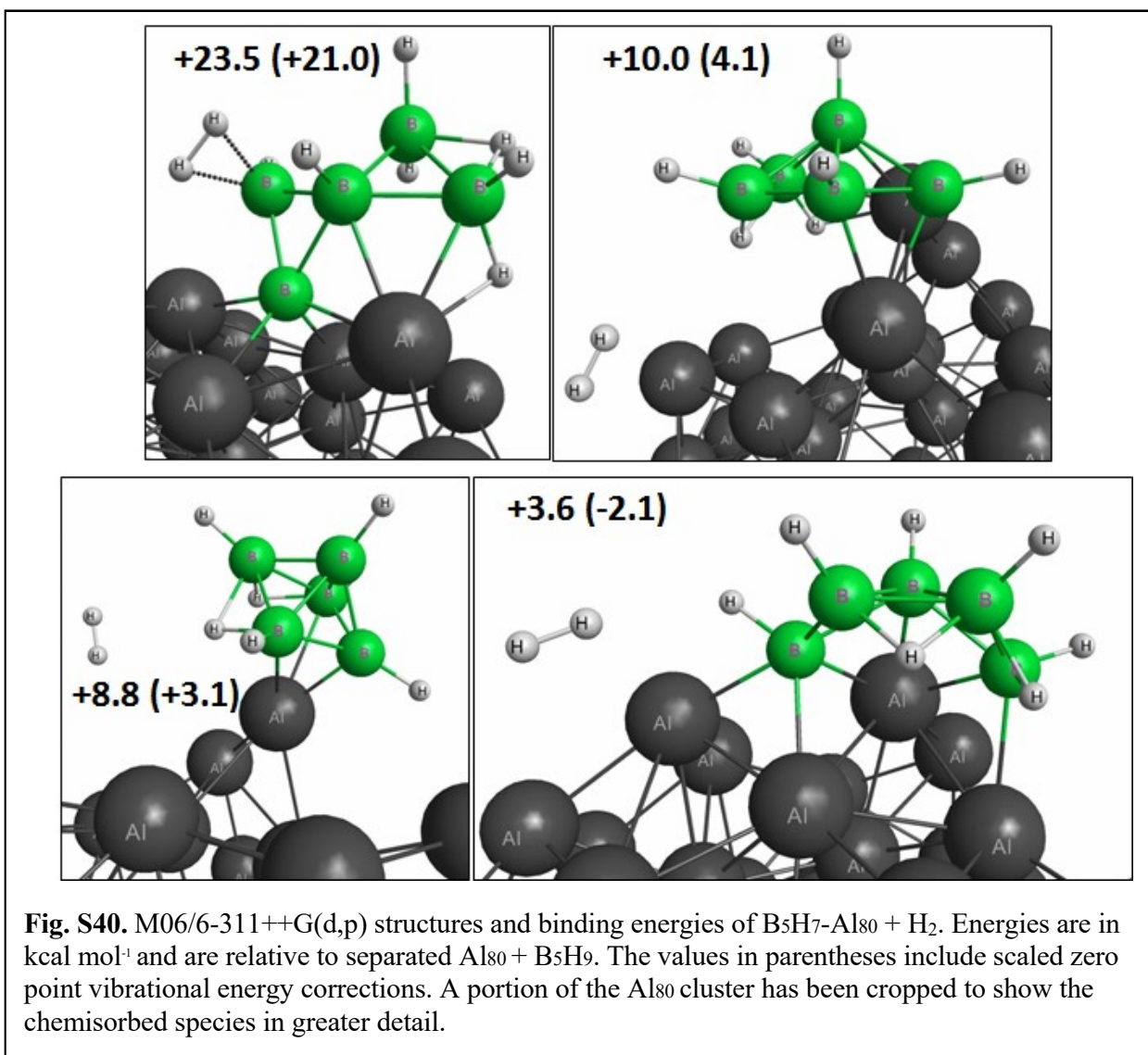


Fig. S37. IRC (blue dots) of chemisorbed pentaborane undergoing B-H fragmentation, $B_5H_9-Al_{80} \rightarrow B_5H_8-Al_{80}-H$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $B_5H_9 + Al_{80}$. The short dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.







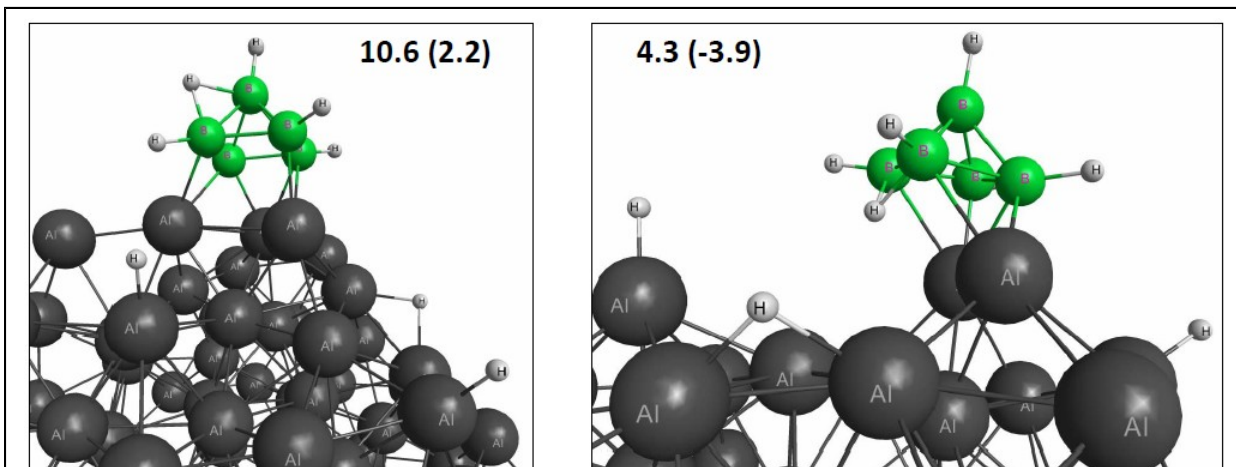
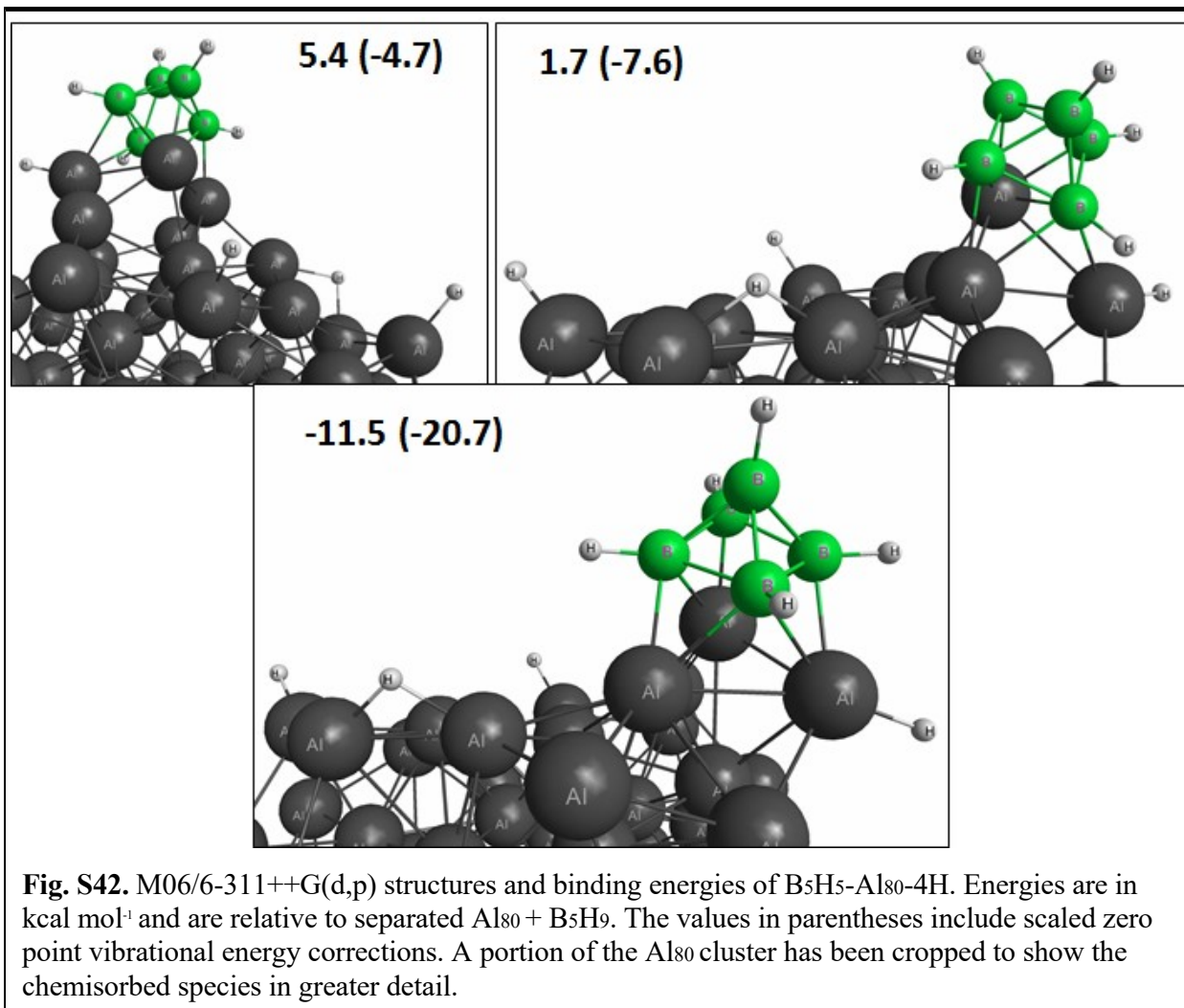


Fig. S41. M06/6-311++G(d,p) structures and binding energies of B₅H₆-Al₈₀-3H. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₅H₉. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the chemisorbed species in greater detail.



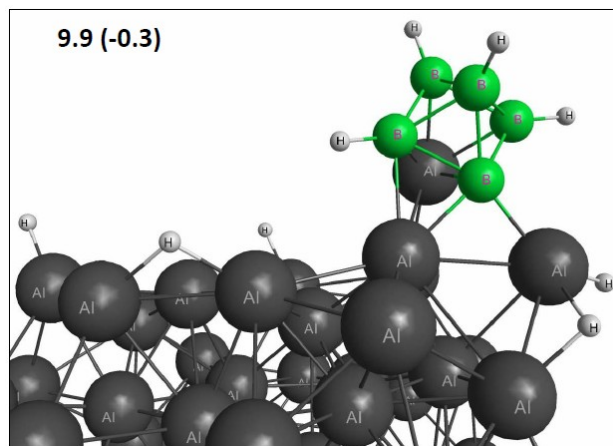
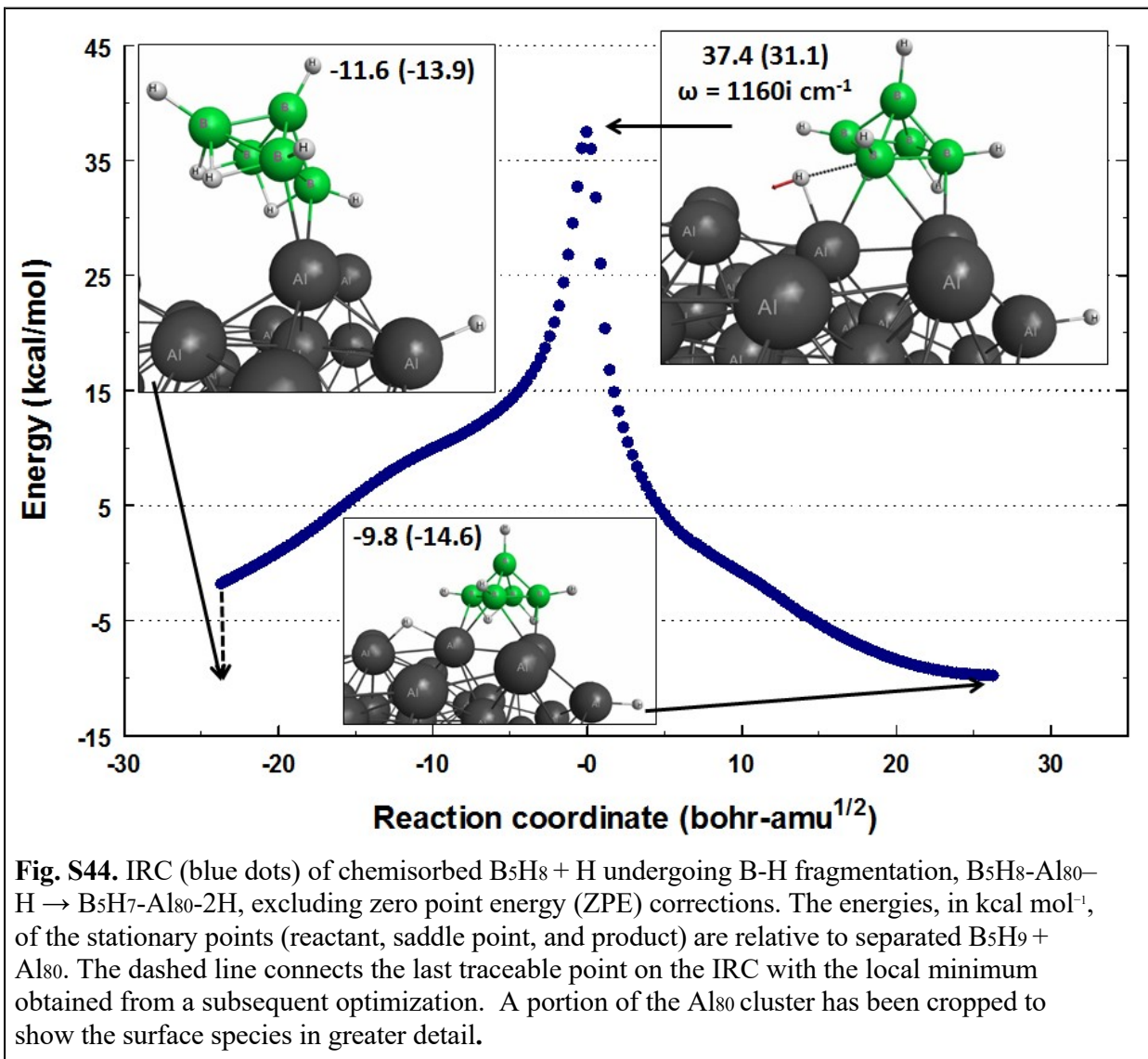


Fig. S43. M06/6-311++G(d,p) structure and binding energy of B₅H₄-Al₈₀-5H. Energies are in kcal mol⁻¹ and are relative to separated Al₈₀ + B₅H₉. The values in parentheses include scaled zero point vibrational energy corrections. A portion of the Al₈₀ cluster has been cropped to show the chemisorbed species in greater detail.



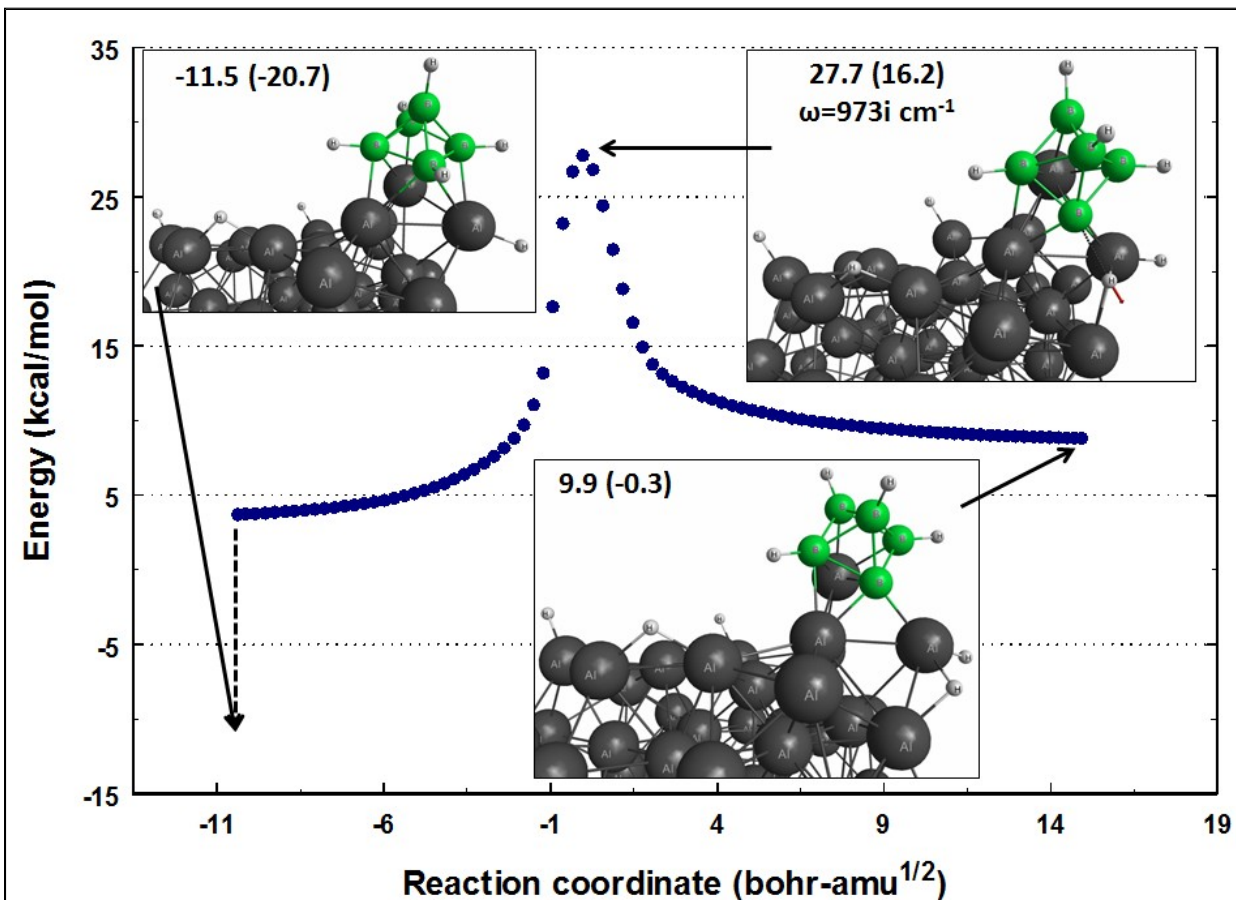
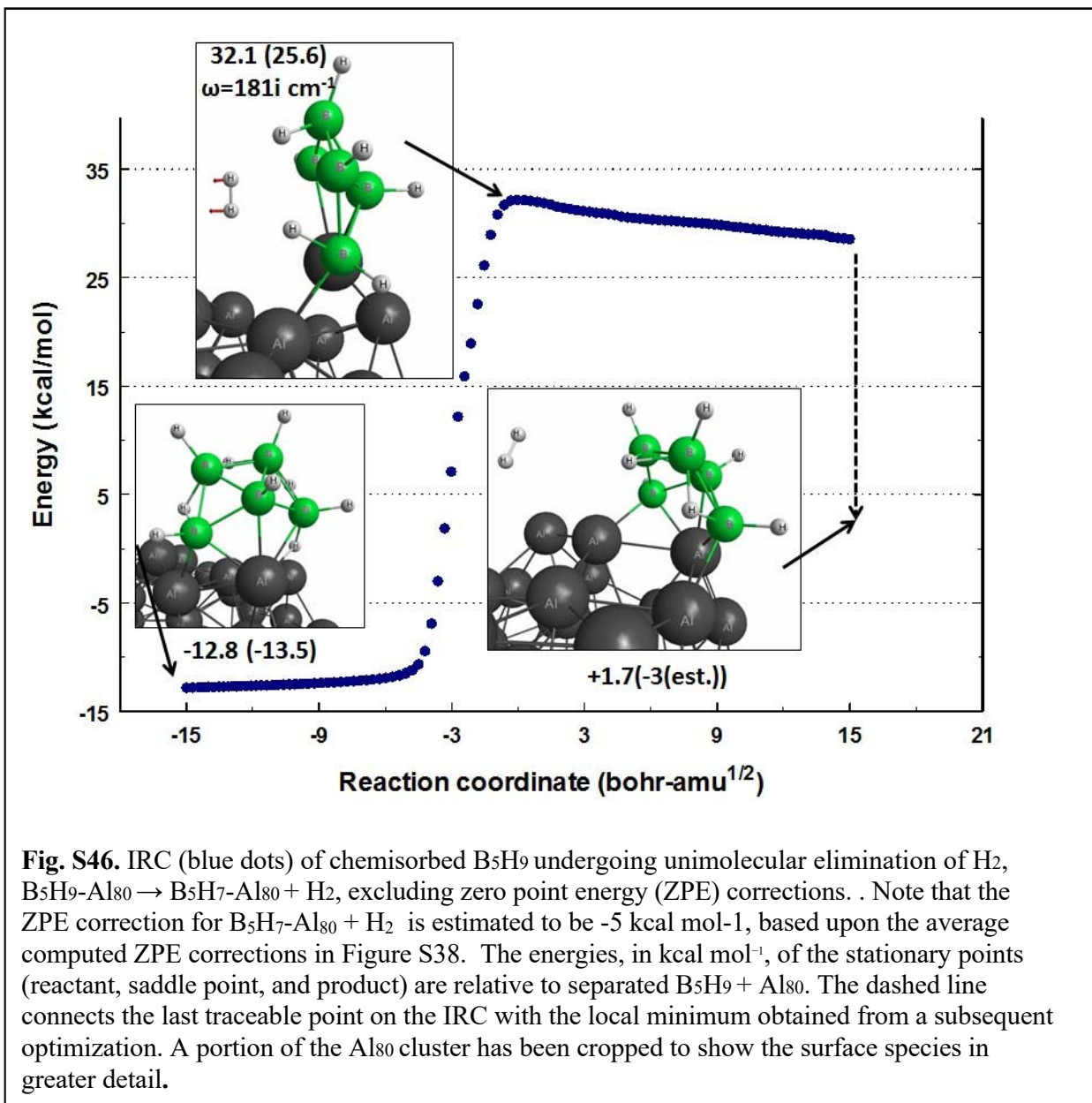


Fig. S45. IRC (blue dots) of chemisorbed $B_5H_5 + H$ undergoing B-H fragmentation, $B_5H_5-Al_{80}-4H \rightarrow B_5H_4-Al_{80}-5H$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $B_5H_9 + Al_{80}$. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.



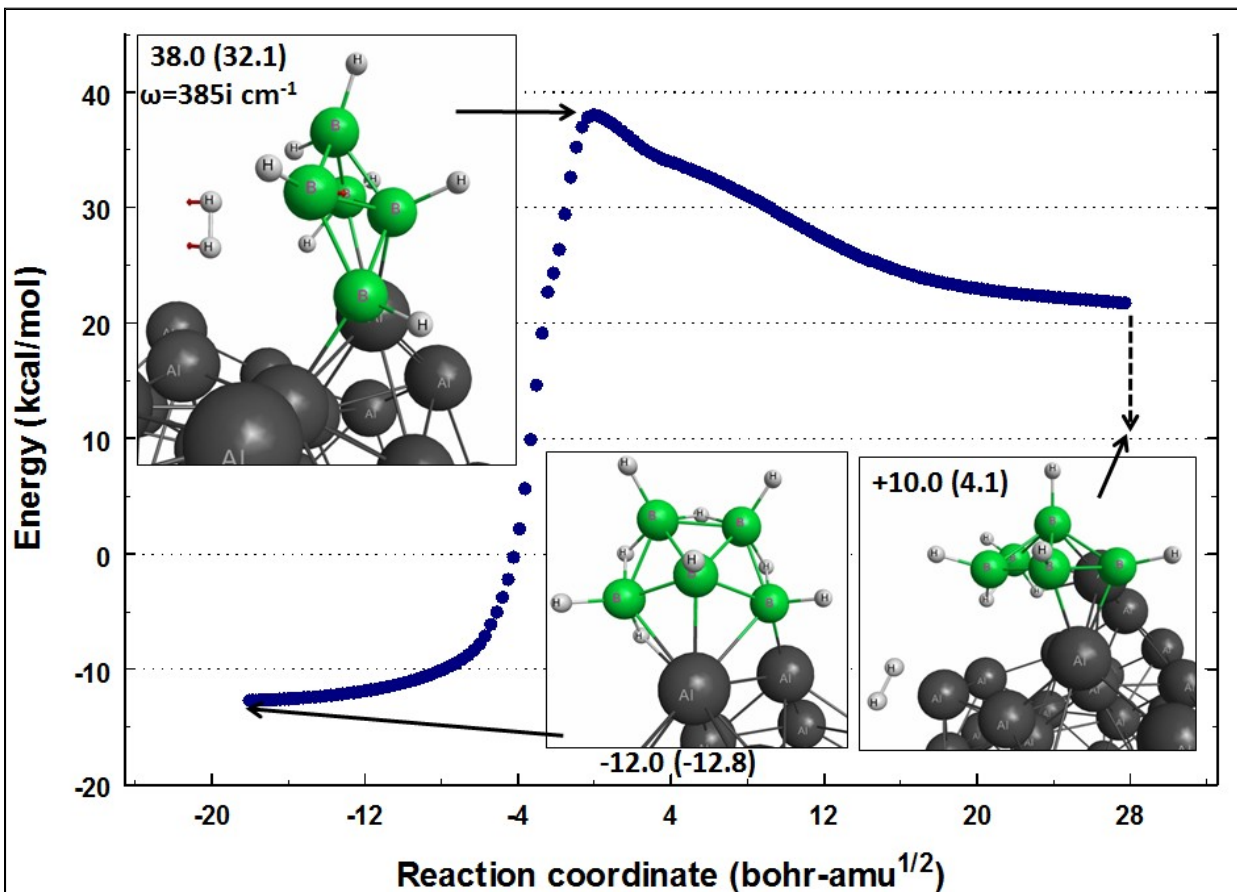


Fig. S47. IRC (blue dots) of chemisorbed B_5H_9 undergoing unimolecular elimination of H_2 , $B_5H_9-Al_{80} \rightarrow B_5H_7-Al_{80} + H_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol⁻¹, of the stationary points (reactant, saddle point, and product) are relative to separated $B_5H_9 + Al_{80}$. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

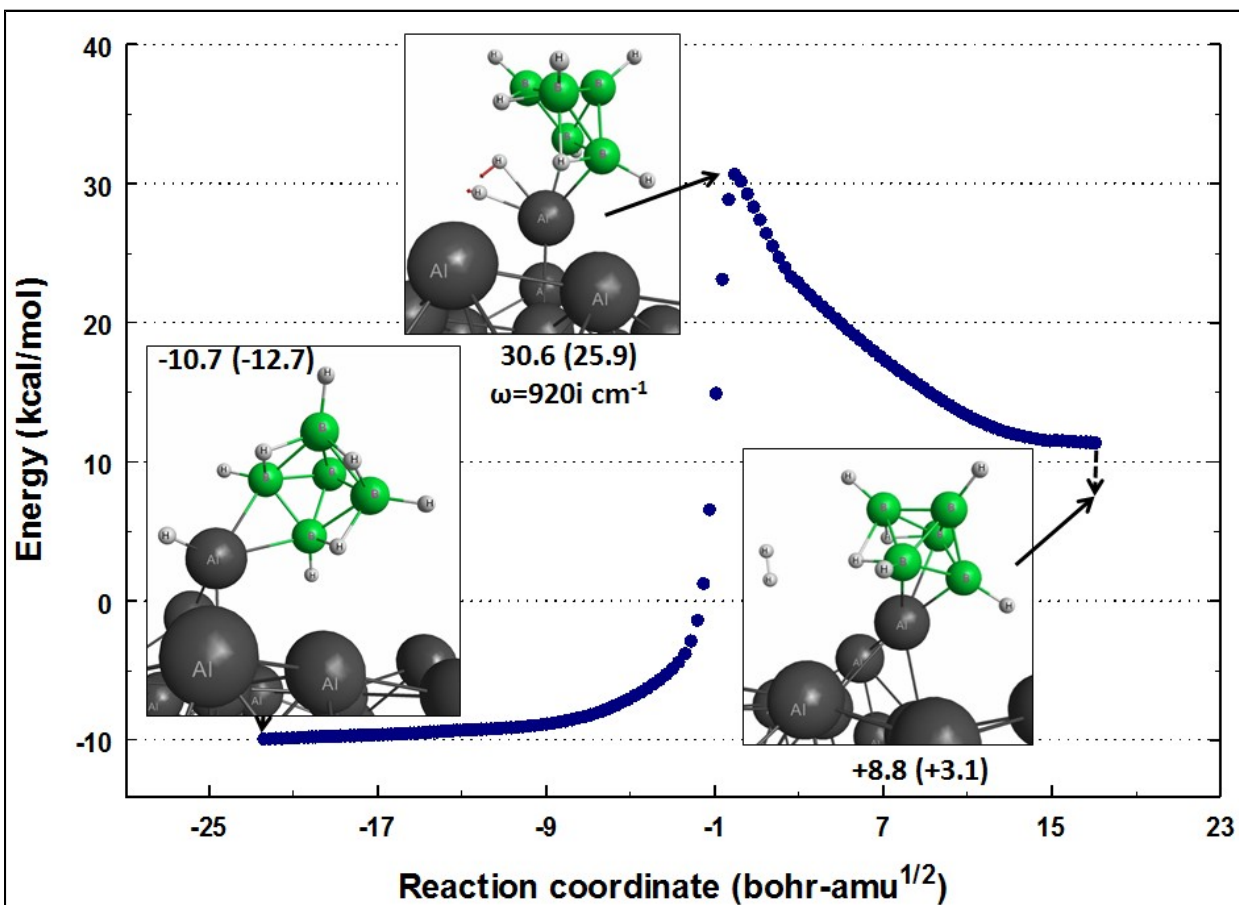


Fig. S48. IRC (blue dots) of chemisorbed B_5H_8 and H undergoing bimolecular elimination of H_2 , $B_5H_8-Al_{80}-H \rightarrow B_5H_7-Al_{80} + H_2$, excluding zero point energy (ZPE) corrections. The energies, in kcal mol^{-1} , of the stationary points (reactant, saddle point, and product) are relative to separated $B_5H_9 + Al_{80}$. The dashed line connects the last traceable point on the IRC with the local minimum obtained from a subsequent optimization. A portion of the Al_{80} cluster has been cropped to show the surface species in greater detail.

References

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Raw data

DLS (Figure. 2)

Diameter	Intensity	Diameter	Intensity	Diameter	Intensity	Diameter	Intensity
3	0	3	0	3	0	3	0
3.51	0	3.51	0	3.51	0	3.51	0
4.11	0	4.11	0	4.11	0	4.11	0
4.8	0	4.8	0	4.8	0	4.8	0
5.62	0	5.62	0	5.62	0	5.62	0
6.58	0	6.58	0	6.58	0	6.58	0
7.7	0	7.7	0	7.7	0	7.7	0
9	0	9	0	9	0	9	0
10.53	0	10.53	0	10.53	0	10.53	0
12.32	0	12.32	0	12.32	0	12.32	0
14.42	0	14.42	0	14.42	0	14.42	0
16.87	0	16.87	0	16.87	0	16.87	0
19.74	0	19.74	0	19.74	0	19.74	0
23.09	0	23.09	0	23.09	0	23.09	0
27.02	0	27.02	0	27.02	0	27.02	0
31.61	1	31.61	0	31.61	0	31.61	0
36.99	0.71	36.99	0	36.99	0.3	36.99	0
43.27	0.43	43.27	1	43.27	0.3	43.27	0
50.63	0.04	50.63	0.63	50.63	0.18	50.63	0
59.24	0	59.24	0.4	59.24	0.05	59.24	0
69.3	0	69.3	0	69.3	0	69.3	0
81.08	0	81.08	0	81.08	0	81.08	0
94.87	0	94.87	0	94.87	0	94.87	0
111	0	111	0	111	0	111	0
129.86	0	129.86	0	129.86	0	129.86	0
151.94	0	151.94	0	151.94	0	151.94	0
177.77	0	177.77	0	177.77	0	177.77	0
207.98	0	207.98	0	207.98	0	207.98	0
243.34	0	243.34	0	243.34	0	243.34	0
284.7	0	284.7	0	284.7	0	284.7	0
333.1	0	333.1	0	333.1	0	333.1	0
389.72	0	389.72	0	389.72	0	389.72	0
455.97	0	455.97	0	455.97	0	455.97	0
533.48	0	533.48	0	533.48	0	533.48	0
624.17	0.02	624.17	0	624.17	0	624.17	0
730.27	0.05	730.27	0.02	730.27	0	730.27	0
854.41	0.15	854.41	0.05	854.41	0	854.41	0
999.65	0.16	999.65	0.08	999.65	0	999.65	0

1169.58	0.15	1169.58	0.37	1169.58	0	1169.58	0
1368.4	0.01	1368.4	0.43	1368.4	0	1368.4	0.13
1601.01	0	1601.01	0.53	1601.01	0.14	1601.01	0.41
1873.16	0	1873.16	0	1873.16	0.48	1873.16	0.92
2191.58	0	2191.58	0	2191.58	1	2191.58	1
2564.13	0	2564.13	0	2564.13	1	2564.13	0.77
3000	0	3000	0	3000	0.64	3000	0.13

Diameter	Intensity	Diameter	Intensity	Diameter	Intensity	Diameter	Intensity
3	0	3	0	3	0	3	0
3.51	0	3.51	0	3.51	0	3.51	0
4.11	0	4.11	0	4.11	0	4.11	0
4.8	0	4.8	0	4.8	0	4.8	0
5.62	0	5.62	0	5.62	0	5.62	0
6.58	0	6.58	0	6.58	0	6.58	0
7.7	0	7.7	0	7.7	0	7.7	0
9	0	9	0	9	0	9	0
10.53	0	10.53	0	10.53	0	10.53	0
12.32	0	12.32	0	12.32	0	12.32	0
14.42	0	14.42	0	14.42	0	14.42	0
16.87	0	16.87	0	16.87	0	16.87	0
19.74	0	19.74	0	19.74	0	19.74	0
23.09	0	23.09	0	23.09	0	23.09	0
27.02	0	27.02	0	27.02	0	27.02	0
31.61	0.19	31.61	0	31.61	0	31.61	0
36.99	0.13	36.99	0	36.99	0	36.99	0
43.27	0.07	43.27	0	43.27	0	43.27	0
50.63	0	50.63	0	50.63	0	50.63	0
59.24	0	59.24	0	59.24	0	59.24	0
69.3	0	69.3	0	69.3	0	69.3	0
81.08	0	81.08	0.03	81.08	0	81.08	0
94.87	0	94.87	0.03	94.87	0	94.87	0
111	0	111	0.01	111	0.01	111	0
129.86	0	129.86	0	129.86	0.02	129.86	0
151.94	0	151.94	0	151.94	0.01	151.94	0
177.77	0	177.77	0	177.77	0.01	177.77	0
207.98	0	207.98	0	207.98	0	207.98	0
243.34	0	243.34	0	243.34	0	243.34	0
284.7	0	284.7	0	284.7	0	284.7	0
333.1	0	333.1	0	333.1	0	333.1	0
389.72	0	389.72	0	389.72	0	389.72	0
455.97	0	455.97	0	455.97	0	455.97	0

533.48	0	533.48	0	533.48	0	533.48	0
624.17	0	624.17	0	624.17	0	624.17	0
730.27	0	730.27	0	730.27	0	730.27	0
854.41	0	854.41	0	854.41	0	854.41	0
999.65	0	999.65	0	999.65	0	999.65	0
1169.58	0	1169.58	0.23	1169.58	0.03	1169.58	0
1368.4	0	1368.4	0.56	1368.4	0.29	1368.4	0
1601.01	0.09	1601.01	1	1601.01	0.62	1601.01	0.17
1873.16	0.36	1873.16	0.81	1873.16	1	1873.16	0.48
2191.58	0.91	2191.58	0.48	2191.58	0.77	2191.58	1
2564.13	1	2564.13	0	2564.13	0.44	2564.13	0.93
3000	0.76	3000	0	3000	0	3000	0.63

Headspace analysis (Fig 1, Figs S1-S5)

Diborane milling

2	1.79E-08	2.5	2.06E-08
3	0	3.5	0
4	0	4.5	0
5	0	5.5	0
6	0	6.5	0
7	0	7.5	0
8	0	8.5	0
9	0	9.5	0
10	2.57E-10	10.5	0
11	6.56E-10	11.5	0
12	2.99E-10	12.5	0
13	4.48E-10	13.5	0
14	0	14.5	0
15	0	15.5	0
16	0	16.5	0
17	0	17.5	0
18	0	18.5	0
19	0	19.5	0
20	9.50E-09	20.5	9.50E-09
21	0	21.5	0
22	4.23E-10	22.5	0
23	7.09E-10	23.5	0
24	1.03E-09	24.5	0
25	8.29E-10	25.5	0
26	1.26E-09	26.5	0
27	1.39E-09	27.5	0

28	0	28.5	0
29	0	29.5	0
30	0	30.5	0
31	0	31.5	0
32	0	32.5	0
33	0	33.5	0
34	0	34.5	0
35	0	35.5	0
36	4.85E-10	36.5	4.71E-10
37	0	37.5	0
38	0	38.5	0
39	0	39.5	0
40	1.38E-07	40.5	1.43E-07
41	0	41.5	0
42	0	42.5	0
43	0	43.5	0
44	0	44.5	0
45	0	45.5	0
46	0	46.5	0
47	0	47.5	0
48	0	48.5	0
49	0	49.5	0
50	0	50.5	0

2	2.06E-08
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0
12	0
13	0
14	0
15	0
16	0
17	0
18	0
19	0

20	9.50E-09
21	0
22	0
23	0
24	0
25	0
26	0
27	0
28	0
29	0
30	0
31	0
32	0
33	0
34	0
35	0
36	4.71E-10
37	0
38	0
39	0
40	1.43E-07
41	0
42	0
43	0
44	0
45	0
46	0
47	0
48	0
49	0
50	0

Pentaborane milling

1	0	2	4.85E-08	1	0
2	9.85E-08	3	0	2	1.84E-07
3	0	4	0	3	0
4	0	5	0	4	0
5	0	6	0	5	0
6	0	7	0	6	0
7	0	8	0	7	0
8	0	9	0	8	0
9	0	10	5.36E-10	9	0

10	8.53E-10	11	1.68E-09	10	3.62E-10
11	2.69E-09	12	2.83E-10	11	1.47E-09
12	6.81E-10	13	9.42E-10	12	3.80E-10
13	1.66E-09	14	1.67E-10	13	9.97E-10
14	5.69E-10	15	0	14	4.66E-11
15	0	16	0	15	0
16	0	17	0	16	0
17	0	18	0	17	0
18	0	19	0	18	0
19	0	20	0	19	0
20	0	21	0	20	0
21	0	22	0	21	0
22	0	23	0	22	0
23	4.11E-10	24	0	23	8.53E-11
24	3.98E-10	25	0	24	1.50E-10
25	1.13E-10	26	0	25	6.66E-11
26	4.61E-10	27	0	26	5.71E-11
27	4.37E-10	28	1.37E-09	27	1.40E-10
28	3.62E-09	29	0	28	4.45E-10
29	5.33E-10	30	0	29	8.16E-11
30	0	31	0	30	0
31	0	32	0	31	0
32	0	33	1.68E-10	32	0
33	4.00E-10	34	7.19E-10	33	1.10E-10
34	1.11E-09	35	7.73E-10	34	2.87E-10
35	1.23E-09	36	4.81E-10	35	4.05E-10
36	8.10E-10	37	4.53E-10	36	2.49E-10
37	6.00E-10	38	3.71E-10	37	9.66E-11
38	0	39	1.02E-10	38	0
39	0	40	2.80E-10	39	5.73E-11
40	4.65E-10	41	3.86E-10	40	5.65E-11
41	5.92E-10	42	2.58E-10	41	8.09E-11
42	4.17E-10	43	7.40E-10	42	8.84E-11
43	1.16E-09	44	0	43	2.90E-10
44	1.12E-09	45	1.75E-09	44	3.34E-10
45	2.78E-09	46	2.41E-09	45	8.62E-10
46	3.83E-09	47	3.10E-09	46	1.19E-09
47	4.70E-09	48	2.23E-09	47	1.37E-09
48	3.50E-09	49	7.41E-10	48	1.02E-09
49	1.03E-09	50	2.96E-10	49	2.29E-10
50	4.17E-10	51	0	50	5.94E-11
51	1.50E-10	52	3.30E-10	51	0
52	4.25E-10	53	7.29E-10	52	7.01E-11

53	1.15E-09	54	1.94E-09	53	3.44E-10
54	3.04E-09	55	2.76E-09	54	8.96E-10
55	4.36E-09	56	2.95E-09	55	1.27E-09
56	4.67E-09	57	3.37E-09	56	1.35E-09
57	5.32E-09	58	4.86E-09	57	1.60E-09
58	7.71E-09	59	7.31E-09	58	2.39E-09
59	1.16E-08	60	7.15E-09	59	3.65E-09
60	1.14E-08	61	4.96E-09	60	3.52E-09
61	7.86E-09	62	5.64E-09	61	2.46E-09
62	8.94E-09	63	4.14E-09	62	2.79E-09
63	6.54E-09	64	3.40E-09	63	2.13E-09
64	5.34E-09			64	1.68E-09
65	0			65	0
66	0			66	0
67	0			67	0
68	0			68	0
69	0			69	0
70	0			70	0

XPS

B 1s

B.E.	CPS	B.E.	CPS	B.E.	CPS
207.96	10710	200.50	6320.00	197.104	8820
207.86	10790	200.40	6415.00	197.004	8890
207.76	10830	200.30	6360.00	196.904	8826.667
207.66	10950	200.20	6490.00	196.804	8810
207.56	11230	200.10	6375.00	196.704	8733.333
207.46	11130	200.00	6690.00	196.604	8823.333
207.36	11280	199.90	6515.00	196.504	8940
207.26	11270	199.80	6610.00	196.404	8820
207.16	11060	199.70	6615.00	196.304	8963.333
207.06	11050	199.60	6645.00	196.204	8796.667
206.96	11250	199.50	6555.00	196.104	8796.667
206.86	11060	199.40	6455.00	196.004	8810
206.76	11060	199.30	6510.00	195.904	8810
206.66	10790	199.20	6575.00	195.804	8753.333
206.56	10860	199.10	6535.00	195.704	8843.333
206.46	11110	199.00	6415.00	195.604	8860
206.36	10790	198.90	6375.00	195.504	8970
206.26	10860	198.80	6685.00	195.404	8976.667
206.16	10910	198.70	6620.00	195.304	8876.667
206.06	11240	198.60	6630.00	195.204	8876.667
205.96	11130	198.50	6625.00	195.104	8836.667
205.86	10980	198.40	6510.00	195.004	8986.667
205.76	11120	198.30	6550.00	194.904	8930
205.66	10860	198.20	6550.00	194.804	8956.667
205.56	10990	198.10	6320.00	194.704	9080
205.46	10630	198.00	6460.00	194.604	9160
205.36	10750	197.90	6625.00	194.504	9083.333
205.26	11100	197.80	6525.00	194.404	9173.333
205.16	10990	197.70	6610.00	194.304	9150
205.06	10920	197.60	6520.00	194.204	9270
204.96	11020	197.50	6500.00	194.104	9336.667
204.86	10910	197.40	6490.00	194.004	9400
204.76	10940	197.30	6375.00	193.904	9506.667
204.66	11000	197.20	6570.00	193.804	9643.333
204.56	11280	197.10	6400.00	193.704	9710
204.46	11140	197.00	6390.00	193.604	10030
204.36	11150	196.90	6510.00	193.504	9973.333
204.26	11310	196.80	6455.00	193.404	10023.33

204.16	11310	196.70	6510.00	193.304	10046.67
204.06	11280	196.60	6605.00	193.204	10210
203.96	10980	196.50	6565.00	193.104	10293.33
203.86	10910	196.40	6400.00	193.004	10290
203.76	10870	196.30	6625.00	192.904	10250
203.66	11090	196.20	6585.00	192.804	10230
203.56	10960	196.10	6335.00	192.704	10143.33
203.46	11230	196.00	6460.00	192.604	10036.67
203.36	10720	195.90	6705.00	192.504	9903.333
203.26	11030	195.80	6385.00	192.404	9830
203.16	10900	195.70	6705.00	192.304	9723.333
203.06	10970	195.60	6505.00	192.204	9660
202.96	10930	195.50	6475.00	192.104	9626.667
202.86	11440	195.40	6410.00	192.004	9500
202.76	11100	195.30	6590.00	191.904	9480
202.66	10940	195.20	6715.00	191.804	9153.333
202.56	11190	195.10	6515.00	191.704	9040
202.46	10990	195.00	6480.00	191.604	9060
202.36	11000	194.90	6490.00	191.504	9010
202.26	10870	194.80	6625.00	191.404	9073.333
202.16	10990	194.70	6620.00	191.304	8953.333
202.06	10990	194.60	6720.00	191.204	8950
201.96	11130	194.50	6560.00	191.104	8856.667
201.86	10780	194.40	6770.00	191.004	8883.333
201.76	10870	194.30	6740.00	190.904	8986.667
201.66	10870	194.20	6945.00	190.804	8783.333
201.56	10940	194.10	6990.00	190.704	8936.667
201.46	11170	194.00	7030.00	190.604	8943.333
201.36	10640	193.90	7120.00	190.504	8860
201.26	11110	193.80	7220.00	190.404	8726.667
201.16	10840	193.70	7295.00	190.304	8860
201.06	11090	193.60	7375.00	190.204	8906.667
200.96	11300	193.50	7700.00	190.104	8890
200.86	10780	193.40	7815.00	190.004	8900
200.76	10920	193.30	7835.00	189.904	8946.667
200.66	11070	193.20	8025.00	189.804	8933.333
200.56	11210	193.10	8185.00	189.704	9006.667
200.46	11390	193.00	8230.00	189.604	8760
200.36	11040	192.90	8045.00	189.504	8860
200.26	10980	192.80	8085.00	189.404	8880
200.16	11020	192.70	8140.00	189.304	8820
200.06	10900	192.60	8060.00	189.204	8903.333
199.96	10580	192.50	8100.00	189.104	8943.333

199.86	10930	192.40	7940.00	189.004	8883.333
199.76	11200	192.30	7650.00	188.904	8896.667
199.66	11120	192.20	7545.00	188.804	8933.333
199.56	10870	192.10	7430.00	188.704	8986.667
199.46	10970	192.00	7295.00	188.604	8960
199.36	10940	191.90	7320.00	188.504	8926.667
199.26	10950	191.80	7000.00	188.404	8913.333
199.16	10890	191.70	7015.00	188.304	8976.667
199.06	10990	191.60	6890.00	188.204	8950
198.96	10860	191.50	7035.00	188.104	8960
198.86	11130	191.40	6945.00	188.004	8863.333
198.76	11170	191.30	6715.00	187.904	8836.667
198.66	10930	191.20	6830.00	187.804	8926.667
198.56	10790	191.10	6940.00	187.704	8903.333
198.46	10850	191.00	6670.00	187.604	8806.667
198.36	11080	190.90	6410.00	187.504	8956.667
198.26	10860	190.80	6465.00	187.404	8910
198.16	10950	190.70	6535.00	187.304	8923.333
198.06	11030	190.60	6455.00	187.204	8913.333
197.96	11040	190.50	6475.00	187.104	8880
197.86	10810	190.40	6575.00		
197.76	10810	190.30	6610.00		
197.66	11000	190.20	6525.00		
197.56	11020	190.10	6690.00		
197.46	11020	190.00	6690.00		
197.36	10920	189.90	6570.00		
197.26	11040	189.80	6590.00		
197.16	10970	189.70	6550.00		
197.06	10750	189.60	6590.00		
196.96	10810	189.50	6500.00		
196.86	10730	189.40	6720.00		
196.76	10800	189.30	6670.00		
196.66	11090	189.20	6595.00		
196.56	10880	189.10	6620.00		
196.46	11150	189.00	6645.00		
196.36	10820	188.90	6810.00		
196.26	10890	188.80	6785.00		
196.16	10940	188.70	6525.00		
196.06	10980	188.60	6745.00		
195.96	11140	188.50	6600.00		
195.86	11130	188.40	6550.00		
195.76	11130	188.30	6745.00		
195.66	11280	188.20	6770.00		

195.56	11090	188.10	6770.00
195.46	11000	188.00	6615.00
195.36	11270	187.90	6790.00
195.26	11360	187.80	6675.00
195.16	11510	187.70	6600.00
195.06	11180	187.60	6505.00
194.96	11410	187.50	6525.00
194.86	11490		
194.76	11470		
194.66	11470		
194.56	11390		
194.46	11400		
194.36	11490		
194.26	11210		
194.16	11520		
194.06	11860		
193.96	11890		
193.86	11780		
193.76	11830		
193.66	12000		
193.56	11980		
193.46	11940		
193.36	11950		
193.26	12030		
193.16	11860		
193.06	12140		
192.96	12150		
192.86	12100		
192.76	11960		
192.66	12130		
192.56	12010		
192.46	12040		
192.36	12030		
192.26	11990		
192.16	11660		
192.06	11580		
191.96	11740		
191.86	11460		
191.76	11500		
191.66	11240		
191.56	11250		
191.46	11100		
191.36	10990		

191.26	11110
191.16	10930
191.06	11030
190.96	10670
190.86	10870
190.76	11070
190.66	10930
190.56	11340
190.46	11070
190.36	11110
190.26	10960
190.16	10980
190.06	11080
189.96	11050
189.86	11070
189.76	10840
189.66	10930
189.56	11250
189.46	11390
189.36	11210
189.26	11600
189.16	11300
189.06	11250
188.96	11260
188.86	10810
188.76	11180
188.66	11130
188.56	10940
188.46	10900
188.36	11130
188.26	11140
188.16	11040
188.06	11150
187.96	11070
187.86	11230
187.76	11230
187.66	11320
187.56	11160
187.46	11120
187.36	10990
187.26	11130
187.16	11340
187.06	11050

186.96	11200
186.86	11280
186.76	11060
186.66	11110
186.56	11070
186.46	11100
186.36	11090
186.26	11040
186.16	11390
186.06	11160
185.96	11120
185.86	11090
185.76	11090
185.66	10900
185.56	10870
185.46	10950
185.36	10900
185.26	11060
185.16	11080
185.06	10870
184.96	10870
184.86	11070
184.76	11020
184.66	11010
184.56	10820
184.46	10990
184.36	10840
184.26	10980
184.16	11200
184.06	10880
183.96	10920
183.86	11160
183.76	10920
183.66	10980
183.56	11020
183.46	10760
183.36	11170
183.26	11090
183.16	10960
183.06	11010
182.96	10970

B.E.	CPS	B.E.	CPS	B.E.	CPS
207.659	4600	199.853	2912	199.331	1352
207.559	4580	199.753	2836	199.231	1298
207.459	4646.667	199.653	2896	199.131	1344
207.359	4600	199.553	2886	199.031	1324
207.259	4533.333	199.453	2868	198.931	1330
207.159	4586.667	199.353	2978	198.831	1384
207.059	4593.333	199.253	2924	198.731	1344
206.959	4573.333	199.153	2890	198.631	1296
206.859	4600	199.053	2902	198.531	1360
206.759	4583.333	198.953	2892	198.431	1352
206.659	4560	198.853	2912	198.331	1392
206.559	4566.667	198.753	2924	198.231	1316
206.459	4653.333	198.653	2878	198.131	1324
206.359	4586.667	198.553	2876	198.031	1366
206.259	4583.333	198.453	2946	197.931	1238
206.159	4590	198.353	2884	197.831	1342
206.059	4570	198.253	2868	197.731	1412
205.959	4630	198.153	2880	197.631	1406
205.859	4613.333	198.053	2870	197.531	1328
205.759	4636.667	197.953	2892	197.431	1328
205.659	4526.667	197.853	2878	197.331	1384
205.559	4606.667	197.753	2826	197.231	1342
205.459	4593.333	197.653	2828	197.131	1306
205.359	4553.333	197.553	2878	197.031	1372
205.259	4533.333	197.453	2900	196.931	1342
205.159	4560	197.353	2862	196.831	1346
205.059	4513.333	197.253	2926	196.731	1394
204.959	4523.333	197.153	2874	196.631	1330
204.859	4510	197.053	2936	196.531	1366
204.759	4570	196.953	2954	196.431	1332
204.659	4563.333	196.853	2968	196.331	1298
204.559	4523.333	196.753	2910	196.231	1316
204.459	4513.333	196.653	2920	196.131	1306
204.359	4570	196.553	2840	196.031	1374
204.259	4556.667	196.453	2934	195.931	1362
204.159	4636.667	196.353	2936	195.831	1356
204.059	4560	196.253	2888	195.731	1344
203.959	4546.667	196.153	3028	195.631	1326
203.859	4540	196.053	2988	195.531	1322
203.759	4560	195.953	2996	195.431	1380
203.659	4553.333	195.853	3008	195.331	1378
203.559	4606.667	195.753	2994	195.231	1294

203.459	4570	195.653	2956	195.131	1270
203.359	4516.667	195.553	3050	195.031	1354
203.259	4566.667	195.453	3104	194.931	1410
203.159	4553.333	195.353	3088	194.831	1414
203.059	4500	195.253	3050	194.731	1480
202.959	4466.667	195.153	3152	194.631	1398
202.859	4616.667	195.053	3174	194.531	1436
202.759	4533.333	194.953	3086	194.431	1496
202.659	4456.667	194.853	3174	194.331	1594
202.559	4483.333	194.753	3130	194.231	1604
202.459	4436.667	194.653	3168	194.131	1642
202.359	4433.333	194.553	3296	194.031	1772
202.259	4490	194.453	3296	193.931	1806
202.159	4446.667	194.353	3398	193.831	1814
202.059	4500	194.253	3468	193.731	1964
201.959	4436.667	194.153	3400	193.631	2064
201.859	4516.667	194.053	3502	193.531	2308
201.759	4423.333	193.953	3528	193.431	2296
201.659	4436.667	193.853	3556	193.331	2520
201.559	4443.333	193.753	3618	193.231	2594
201.459	4496.667	193.653	3760	193.131	2596
201.359	4500	193.553	3802	193.031	2598
201.259	4423.333	193.453	3852	192.931	2694
201.159	4493.333	193.353	3886	192.831	2668
201.059	4453.333	193.253	3998	192.731	2462
200.959	4416.667	193.153	4012	192.631	2468
200.859	4400	193.053	4064	192.531	2406
200.759	4483.333	192.953	3952	192.431	2392
200.659	4486.667	192.853	4002	192.331	2276
200.559	4490	192.753	3982	192.231	2120
200.459	4456.667	192.653	3964	192.131	2036
200.359	4453.333	192.553	3924	192.031	2032
200.259	4450	192.453	3918	191.931	1904
200.159	4503.333	192.353	3892	191.831	1818
200.059	4470	192.253	3748	191.731	1792
199.959	4496.667	192.153	3644	191.631	1692
199.859	4406.667	192.053	3534	191.531	1692
199.759	4566.667	191.953	3414	191.431	1626
199.659	4540	191.853	3362	191.331	1414
199.559	4450	191.753	3358	191.231	1506
199.459	4553.333	191.653	3212	191.131	1530
199.359	4526.667	191.553	3180	191.031	1490
199.259	4503.333	191.453	3150	190.931	1396

199.159	4450	191.353	3084	190.831	1358
199.059	4393.333	191.253	3068	190.731	1436
198.959	4426.667	191.153	3076	190.631	1416
198.859	4403.333	191.053	2954	190.531	1482
198.759	4473.333	190.953	3002	190.431	1458
198.659	4433.333	190.853	2920	190.331	1456
198.559	4413.333	190.753	2882	190.231	1406
198.459	4466.667	190.653	2900	190.131	1456
198.359	4446.667	190.553	3008	190.031	1526
198.259	4440	190.453	2966	189.931	1548
198.159	4536.667	190.353	2918	189.831	1528
198.059	4373.333	190.253	2912	189.731	1546
197.959	4366.667	190.153	2928	189.631	1576
197.859	4390	190.053	2946	189.531	1566
197.759	4470	189.953	3000	189.431	1700
197.659	4366.667	189.853	2928	189.331	1638
197.559	4403.333	189.753	2878	189.231	1650
197.459	4493.333	189.653	2946	189.131	1666
197.359	4486.667	189.553	2938	189.031	1732
197.259	4473.333	189.453	2976	188.931	1776
197.159	4420	189.353	2958	188.831	1820
197.059	4400	189.253	3012	188.731	1836
196.959	4493.333	189.153	2986	188.631	1884
196.859	4470	189.053	2956	188.531	1914
196.759	4503.333	188.953	2988	188.431	1910
196.659	4460	188.853	2952	188.331	2020
196.559	4463.333	188.753	3016	188.231	2000
196.459	4390	188.653	2992	188.131	2008
196.359	4486.667	188.553	3008	188.031	1988
196.259	4500	188.453	2996	187.931	2048
196.159	4493.333	188.353	2982	187.831	1932
196.059	4376.667	188.253	3020	187.731	1982
195.959	4473.333	188.153	3000	187.631	1864
195.859	4403.333	188.053	3046	187.531	1808
195.759	4470	187.953	3048	187.431	1864
195.659	4343.333	187.853	2990	187.331	1784
195.559	4486.667	187.753	2988	187.231	1720
195.459	4370	187.653	3012	187.131	1636
195.359	4366.667	187.553	3016	187.031	1588
195.259	4450	187.453	2976	186.931	1600
195.159	4436.667	187.353	2958	186.831	1562
195.059	4530	187.253	2948	186.731	1518
194.959	4583.333	187.153	3038	186.631	1508

194.859	4523.333	187.053	3070	186.531	1464
194.759	4603.333	186.953	2984	186.431	1418
194.659	4743.333	186.853	2898	186.331	1412
194.559	4643.333	186.753	2914	186.231	1374
194.459	4700	186.653	3008	186.131	1360
194.359	4820	186.553	2906	186.031	1312
194.259	4880	186.453	2812	185.931	1304
194.159	4963.333	186.353	2898	185.831	1272
194.059	5126.667	186.253	2952	185.731	1232
193.959	5133.333	186.153	2928	185.631	1308
193.859	5453.333	186.053	2882	185.531	1236
193.759	5513.333	185.953	2844	185.431	1238
193.659	5506.667	185.853	2898	185.331	1298
193.559	5596.667	185.753	2904	185.231	1362
193.459	5786.667	185.653	2868	185.131	1278
193.359	5976.667	185.553	2906	185.031	1240
193.259	6080	185.453	2878	184.931	1296
193.159	6026.667	185.353	2886	184.831	1238
193.059	6056.667	185.253	2838	184.731	1160
192.959	6060	185.153	2870	184.631	1252
192.859	6056.667	185.053	2892	184.531	1272
192.759	5906.667	184.953	2824	184.431	1238
192.659	5960	184.853	2868	184.331	1270
192.559	5903.333	184.753	2878	184.231	1296
192.459	5720	184.653	2952	184.131	1282
192.359	5590	184.553	2916	184.031	1218
192.259	5530	184.453	2894	183.931	1282
192.159	5420	184.353	2820	183.831	1246
192.059	5173.333	184.253	2812	183.731	1314
191.959	5146.667	184.153	2808	183.631	1244
191.859	4920	184.053	2824	183.531	1230
191.759	4736.667	183.953	2910	183.431	1232
191.659	4706.667	183.853	2912	183.331	1260
191.559	4646.667	183.753	2858	183.231	1328
191.459	4620	183.653	2840	183.131	1250
191.359	4500	183.553	2882	183.031	1242
191.259	4460	183.453	2872	182.931	1252
191.159	4526.667	183.353	2886	182.831	1274
191.059	4546.667	183.253	2900	182.731	1248
190.959	4493.333	183.153	2936	182.631	1208
190.859	4646.667	183.053	2910	182.531	1260
190.759	4736.667	182.953	2916	182.431	1326
190.659	4670	182.853	2934	182.331	1232

190.559	4586.667	182.753	2860	182.231	1266
190.459	4593.333	182.653	2884	182.131	1228
190.359	4616.667	182.553	2838	182.031	1324
190.259	4646.667	182.453	2878	181.931	1268
190.159	4713.333	182.353	2882	181.831	1298
190.059	4716.667	182.253	2886	181.731	1324
189.959	4793.333	182.153	2872	181.631	1266
189.859	4833.333	182.053	2840	181.531	1360
189.759	4803.333	181.953	2846	181.431	1316
189.659	4826.667	181.853	2836	181.331	1346
189.559	4730				
189.459	4816.667				
189.359	4876.667				
189.259	4863.333				
189.159	4896.667				
189.059	4963.333				
188.959	4863.333				
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188.659	5036.667				
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188.359	5166.667				
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188.159	5216.667				
188.059	5206.667				
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187.759	5043.333				
187.659	5093.333				
187.559	4970				
187.459	4913.333				
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187.159	4850				
187.059	4846.667				
186.959	4786.667				
186.859	4686.667				
186.759	4623.333				
186.659	4686.667				
186.559	4493.333				
186.459	4550				
186.359	4496.667				

186.259 4446.667
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 184.059 4330
 183.959 4330
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 183.359 4283.333
 183.259 4390
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 183.059 4386.667
 182.959 4300
 182.859 4350
 182.759 4320
 182.659 4386.667

Al 2p

B.E.	CPS	B.E.	CPS	B.E.	CPS
88.26	15940	82.802	8918	82.404	12334
88.16	15900	82.702	8932	82.304	12300

88.06	15825	82.602	8918	82.204	12290
87.96	15840	82.502	8899.333	82.104	12304
87.86	15855	82.402	8894.667	82.004	12320
87.76	15920	82.302	8899.333	81.904	12298
87.66	15895	82.202	8866.667	81.804	12318
87.56	15925	82.102	8859.667	81.704	12270
87.46	15900	82.002	8873.667	81.604	12258
87.36	16015	81.902	8831.667	81.504	12300
87.26	15920	81.802	8789.667	81.404	12300
87.16	15745	81.702	8817.667	81.304	12298
87.06	15880	81.602	8813	81.204	12286
86.96	15820	81.502	8836.333	81.104	12288
86.86	15770	81.402	8841	81.004	12302
86.76	15725	81.302	8841	80.904	12280
86.66	15685	81.202	8757	80.804	12302
86.56	15725	81.102	8785	80.704	12304
86.46	15710	81.002	8789.667	80.604	12314
86.36	15750	80.902	8827	80.504	12262
86.26	15765	80.802	8794.333	80.404	12282
86.16	15725	80.702	8827	80.304	12308
86.06	15635	80.602	8794.333	80.204	12276
85.96	15535	80.502	8808.333	80.104	12300
85.86	15565	80.402	8803.667	80.004	12308
85.76	15570	80.302	8799	79.904	12284
85.66	15625	80.202	8806	79.804	12294
85.56	15525	80.102	8808.333	79.704	12322
85.46	15545	80.002	8834	79.604	12274
85.36	15490	79.902	8859.667	79.504	12268
85.26	15480	79.802	8822.333	79.404	12314
85.16	15480	79.702	8810.667	79.304	12324
85.06	15505	79.602	8829.333	79.204	12298
84.96	15450	79.502	8813	79.104	12314
84.86	15480	79.402	8792	79.004	12300
84.76	15550	79.302	8794.333	78.904	12304
84.66	15475	79.202	8820	78.804	12298
84.56	15430	79.102	8838.667	78.704	12266
84.46	15470	79.002	8878.333	78.604	12308
84.36	15540	78.902	8848	78.504	12310
84.26	15460	78.802	8878.333	78.404	12304
84.16	15440	78.702	8906.333	78.304	12322
84.06	15445	78.602	8864.333	78.204	12304
83.96	15480	78.502	8906.333	78.104	12264
83.86	15510	78.402	8922.667	78.004	12342

83.76	15420	78.302	8878.333	77.904	12340
83.66	15445	78.202	8913.333	77.804	12312
83.56	15385	78.102	8845.667	77.704	12342
83.46	15395	78.002	8899.333	77.604	12318
83.36	15400	77.902	8857.333	77.504	12328
83.26	15355	77.802	8831.667	77.404	12322
83.16	15440	77.702	8869	77.304	12308
83.06	15345	77.602	8876	77.204	12344
82.96	15460	77.502	8876	77.104	12332
82.86	15470	77.402	8855	77.004	12344
82.76	15455	77.302	8878.333	76.904	12356
82.66	15480	77.202	8866.667	76.804	12402
82.56	15390	77.102	8871.333	76.704	12382
82.46	15445	77.002	8869	76.604	12412
82.36	15475	76.902	8831.667	76.504	12428
82.26	15440	76.802	8864.333	76.404	12482
82.16	15470	76.702	8876	76.304	12520
82.06	15465	76.602	8901.667	76.204	12570
81.96	15390	76.502	8955.333	76.104	12730
81.86	15435	76.402	8999.667	76.004	12742
81.76	15390	76.302	9016	75.904	12870
81.66	15420	76.202	9018.333	75.804	13002
81.56	15370	76.102	9130.333	75.704	13128
81.46	15425	76.002	9214.333	75.604	13288
81.36	15435	75.902	9335.667	75.504	13536
81.26	15410	75.802	9445.333	75.404	13636
81.16	15420	75.702	9601.667	75.304	13826
81.06	15385	75.602	9732.333	75.204	14082
80.96	15335	75.502	10021.67	75.104	14316
80.86	15435	75.402	10180.33	75.004	14412
80.76	15470	75.302	10406.67	74.904	14594
80.66	15500	75.202	10644.67	74.804	14850
80.56	15425	75.102	10854.67	74.704	14966
80.46	15445	75.002	11172	74.604	15046
80.36	15345	74.902	11426.33	74.504	14878
80.26	15405	74.802	11491.67	74.404	15102
80.16	15485	74.702	11662	74.304	14936
80.06	15410	74.602	11846.33	74.204	14946
79.96	15410	74.502	11727.33	74.104	14762
79.86	15415	74.402	11699.33	74.004	14480
79.76	15415	74.302	11697	73.904	14254
79.66	15490	74.202	11487	73.804	14004
79.56	15365	74.102	11400.67	73.704	13826

79.46	15395	74.002	11169.67	73.604	13674
79.36	15405	73.902	10784.67	73.504	13424
79.26	15370	73.802	10623.67	73.404	13220
79.16	15410	73.702	10367	73.304	13028
79.06	15420	73.602	10164	73.204	12920
78.96	15480	73.502	9797.667	73.104	12846
78.86	15405	73.402	9741.667	73.004	12656
78.76	15530	73.302	9473.333	72.904	12676
78.66	15505	73.202	9468.667	72.804	12698
78.56	15440	73.102	9277.333	72.704	12650
78.46	15420	73.002	9149	72.604	12630
78.36	15455	72.902	9095.333	72.504	12664
78.26	15550	72.802	9116.333	72.404	12712
78.16	15560	72.702	9086	72.304	12716
78.06	15525	72.602	9093	72.204	12794
77.96	15600	72.502	9081.333	72.104	12954
77.86	15630	72.402	9163	72.004	12914
77.76	15760	72.302	9200.333	71.904	12930
77.66	15575	72.202	9289	71.804	12984
77.56	15690	72.102	9382.333	71.704	13012
77.46	15805	72.002	9471	71.604	12952
77.36	15915	71.902	9515.333	71.504	12898
77.26	15755	71.802	9517.667	71.404	12842
77.16	15790	71.702	9636.667	71.304	12686
77.06	15785	71.602	9536.333	71.204	12550
76.96	15900	71.502	9438.333	71.104	12462
76.86	15985	71.402	9419.667	71.004	12426
76.76	15935	71.302	9230.667	70.904	12342
76.66	15985	71.202	9102.333	70.804	12266
76.56	15995	71.102	9067.333	70.704	12250
76.46	16005	71.002	8873.667	70.604	12238
76.36	16100	70.902	8850.333	70.504	12258
76.26	16165	70.802	8766.333	70.404	12230
76.16	16090	70.702	8808.333	70.304	12228
76.06	16205	70.602	8799	70.204	12258
75.96	16225	70.502	8761.667	70.104	12256
75.86	16255	70.402	8787.333	70.004	12250
75.76	16390	70.302	8773.333	69.904	12228
75.66	16480	70.202	8817.667	69.804	12230
75.56	16650	70.102	8845.667	69.704	12228
75.46	16715	70.002	8838.667	69.604	12252
75.36	16785	69.902	8789.667	69.504	12248
75.26	16900	69.802	8764	69.404	12236

75.16	17105	69.702	8764	69.304	12218
75.06	17280	69.602	8759.333	69.204	12218
74.96	17275	69.502	8808.333	69.104	12246
74.86	17290	69.402	8775.667	69.004	12256
74.76	17560	69.302	8759.333	68.904	12238
74.66	17630	69.202	8792	68.804	12252
74.56	17605	69.102	8864.333	68.704	12232
74.46	17635	69.002	8794.333	68.604	12258
74.36	17640	68.902	8799	68.504	12240
74.26	17405	68.802	8815.333	68.404	12258
74.16	17705			68.304	12256
74.06	17285			68.204	12276
73.96	17425			68.104	12254
73.86	17310			68.004	12256
73.76	17140			67.904	12234
73.66	16940			67.804	12260
73.56	16675			67.704	12196
73.46	16545			67.604	12248
73.36	16575			67.504	12274
73.26	16685			67.404	12214
73.16	16315			67.304	12244
73.06	16150			67.204	12262
72.96	16285			67.104	12234
72.86	16340			67.004	12246
72.76	16110			66.904	12246
72.66	16205			66.804	12284
72.56	16065			66.704	12266
72.46	16080			66.604	12276
72.36	16010			66.504	12236
72.26	16210			66.404	12250
72.16	16195			66.304	12242
72.06	16365			66.204	12264
71.96	16420			66.104	12226
71.86	16380			66.004	12210
71.76	16400			65.904	12242
71.66	16435			65.804	12232
71.56	16300			65.704	12210
71.46	16155			65.604	12220
71.36	16060			65.504	12226
71.26	15890			65.404	12214
71.16	15715				
71.06	15515				
70.96	15470				

70.86 15355
 70.76 15430
 70.66 15340
 70.56 15340
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 69.66 15260
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 69.06 15315
 68.96 15240
 68.86 15255
 68.76 15255
 68.66 15225
 68.56 15220
 68.46 15225
 68.36 15285
 68.26 15305
 68.16 15255
 68.06 15300
 67.96 15380
 67.86 15295
 67.76 15275
 67.66 15305
 67.56 15260
 67.46 15275
 67.36 15320
 67.26 15315

B.E.	CPS	B.E.	CPS	B.E.	CPS
87.959	6045	82.353	2970	84.231	296
87.859	5990	82.253	2934	84.131	264
87.759	5990	82.153	2928	84.031	290
87.659	6090	82.053	2910	83.931	284

87.559	5935	81.953	2904	83.831	286
87.459	5940	81.853	2886	83.731	284
87.359	6015	81.753	2886	83.631	300
87.259	6100	81.653	2982	83.531	274
87.159	5940	81.553	2904	83.431	270
87.059	6095	81.453	2892	83.331	244
86.959	6000	81.353	2958	83.231	240
86.859	5935	81.253	2916	83.131	246
86.759	5925	81.153	2964	83.031	260
86.659	5880	81.053	3024	82.931	242
86.559	5895	80.953	3000	82.831	214
86.459	5825	80.853	3006	82.731	214
86.359	5900	80.753	2940	82.631	242
86.259	5795	80.653	2970	82.531	258
86.159	5770	80.553	2952	82.431	256
86.059	5815	80.453	2940	82.331	234
85.959	5760	80.353	2952	82.231	248
85.859	5820	80.253	2814	82.131	226
85.759	5815	80.153	2874	82.031	224
85.659	5780	80.053	2958	81.931	238
85.559	5705	79.953	2964	81.831	236
85.459	5745	79.853	2880	81.731	228
85.359	5795	79.753	3060	81.631	174
85.259	5675	79.653	2910	81.531	232
85.159	5700	79.553	2940	81.431	180
85.059	5685	79.453	3030	81.331	216
84.959	5760	79.353	3006	81.231	238
84.859	5665	79.253	2904	81.131	214
84.759	5710	79.153	3000	81.031	246
84.659	5625	79.053	2982	80.931	176
84.559	5605	78.953	2964	80.831	238
84.459	5720	78.853	2982	80.731	212
84.359	5760	78.753	3048	80.631	242
84.259	5650	78.653	2964	80.531	206
84.159	5700	78.553	3048	80.431	222
84.059	5670	78.453	3054	80.331	224
83.959	5745	78.353	3066	80.231	224
83.859	5630	78.253	3090	80.131	222
83.759	5600	78.153	3162	80.031	230
83.659	5710	78.053	3198	79.931	240
83.559	5745	77.953	3120	79.831	188
83.459	5620	77.853	2970	79.731	244
83.359	5640	77.753	3102	79.631	200

83.259	5650	77.653	3138	79.531	184
83.159	5635	77.553	3048	79.431	210
83.059	5650	77.453	3288	79.331	184
82.959	5595	77.353	3234	79.231	222
82.859	5655	77.253	3318	79.131	236
82.759	5605	77.153	3240	79.031	200
82.659	5555	77.053	3282	78.931	202
82.559	5655	76.953	3264	78.831	204
82.459	5630	76.853	3396	78.731	234
82.359	5635	76.753	3318	78.631	192
82.259	5635	76.653	3336	78.531	192
82.159	5610	76.553	3174	78.431	214
82.059	5590	76.453	3408	78.331	190
81.959	5635	76.353	3642	78.231	210
81.859	5660	76.253	3612	78.131	224
81.759	5650	76.153	3510	78.031	210
81.659	5625	76.053	3636	77.931	246
81.559	5655	75.953	3756	77.831	226
81.459	5610	75.853	3714	77.731	218
81.359	5595	75.753	3720	77.631	170
81.259	5600	75.653	3732	77.531	208
81.159	5700	75.553	3798	77.431	216
81.059	5630	75.453	4128	77.331	214
80.959	5565	75.353	4200	77.231	214
80.859	5590	75.253	4206	77.131	222
80.759	5645	75.153	4224	77.031	198
80.659	5585	75.053	4356	76.931	202
80.559	5620	74.953	4434	76.831	170
80.459	5545	74.853	4602	76.731	190
80.359	5605	74.753	4872	76.631	222
80.259	5635	74.653	4746	76.531	224
80.159	5575	74.553	4896	76.431	280
80.059	5590	74.453	5088	76.331	228
79.959	5605	74.353	4848	76.231	262
79.859	5615	74.253	4968	76.131	278
79.759	5585	74.153	4680	76.031	296
79.659	5585	74.053	4860	75.931	304
79.559	5640	73.953	4860	75.831	338
79.459	5640	73.853	4698	75.731	432
79.359	5640	73.753	4704	75.631	522
79.259	5575	73.653	4584	75.531	532
79.159	5635	73.553	4410	75.431	628
79.059	5610	73.453	4218	75.331	772

78.959	5610	73.353	4284	75.231	804
78.859	5635	73.253	4062	75.131	932
78.759	5660	73.153	3918	75.031	1074
78.659	5580	73.053	3876	74.931	1216
78.559	5540	72.953	3888	74.831	1436
78.459	5595	72.853	3966	74.731	1654
78.359	5535	72.753	3798	74.631	1816
78.259	5580	72.653	3816	74.531	2012
78.159	5615	72.553	3684	74.431	2134
78.059	5670	72.453	3756	74.331	2314
77.959	5680	72.353	3786	74.231	2494
77.859	5630	72.253	3822	74.131	2540
77.759	5690	72.153	3780	74.031	2662
77.659	5595	72.053	3852	73.931	2636
77.559	5600	71.953	3990	73.831	2606
77.459	5620	71.853	3984	73.731	2582
77.359	5585	71.753	3942	73.631	2312
77.259	5585	71.653	3990	73.531	2246
77.159	5605	71.553	3972	73.431	2086
77.059	5665	71.453	4020	73.331	1890
76.959	5585	71.353	4002	73.231	1740
76.859	5665	71.253	3696	73.131	1480
76.759	5695	71.153	3708	73.031	1350
76.659	5705	71.053	3456	72.931	1244
76.559	5680	70.953	3306	72.831	1022
76.459	5770	70.853	3186	72.731	956
76.359	5810	70.753	3174	72.631	920
76.259	5855	70.653	3024	72.531	856
76.159	5805	70.553	2874	72.431	888
76.059	5835	70.453	2868	72.331	872
75.959	5865	70.353	2820	72.231	948
75.859	6005	70.253	2850	72.131	948
75.759	6045	70.153	2664	72.031	1068
75.659	6240	70.053	2736	71.931	1160
75.559	6330	69.953	2748	71.831	1312
75.459	6480	69.853	2778	71.731	1348
75.359	6510	69.753	2838	71.631	1504
75.259	6865.001	69.653	2790	71.531	1444
75.159	7085	69.553	2904	71.431	1338
75.059	7135.001	69.453	2688	71.331	1234
74.959	7250	69.353	2736	71.231	1140
74.859	7365	69.253	2874	71.131	902
74.759	7600.001	69.153	2880	71.031	684

74.659	7690.001	69.053	2832	70.931	536
74.559	7610	68.953	2772	70.831	360
74.459	7640	68.853	2808	70.731	270
74.359	7775	68.753	2832	70.631	210
74.259	7735.001	68.653	2820	70.531	196
74.159	7480.001	68.553	2796	70.431	174
74.059	7250	68.453	2784	70.331	158
73.959	7320	68.353	2766	70.231	154
73.859	7035	68.253	2772	70.131	138
73.759	7030.001	68.153	2658	70.031	160
73.659	6905	68.053	2742	69.931	130
73.559	6715	67.953	2784	69.831	104
73.459	6525	67.853	2730	69.731	90
73.359	6475	67.753	2736	69.631	118
73.259	6320	67.653	2790	69.531	134
73.159	6105	67.553	2706	69.431	130
73.059	6210	67.453	2748	69.331	106
72.959	6230	67.353	2688	69.231	124
72.859	6160	67.253	2688	69.131	158
72.759	6085	67.153	2718	69.031	112
72.659	6110	67.053	2766	68.931	118
72.559	6060	66.953	2856	68.831	112
72.459	6215	66.853	2712	68.731	118
72.359	6270	66.753	2742	68.631	128
72.259	6385	66.653	2706	68.531	124
72.159	6505	66.553	2790	68.431	102
72.059	6525	66.453	2730	68.331	110
71.959	6710	66.353	2772	68.231	134
71.859	6800			68.131	110
71.759	6735			68.031	92
71.659	6995			67.931	148
71.559	6745			67.831	136
71.459	6640			67.731	124
71.359	6455			67.631	134
71.259	6390			67.531	146
71.159	6180			67.431	160
71.059	5950			67.331	102
70.959	5885			67.231	90
70.859	5720			67.131	134
70.759	5605			67.031	130
70.659	5615			66.931	126
70.559	5575			66.831	92
70.459	5600			66.731	118

70.359	5505	66.631	142
70.259	5555	66.531	98
70.159	5540	66.431	132
70.059	5545	66.331	118
69.959	5550	66.231	140
69.859	5550	66.131	104
69.759	5500	66.031	132
69.659	5520	65.931	140
69.559	5475	65.831	104
69.459	5525	65.731	90
69.359	5585	65.631	110
69.259	5505	65.531	126
69.159	5510	65.431	118
69.059	5540	65.331	122
68.959	5480	65.231	148
68.859	5515		
68.759	5495		
68.659	5465		
68.559	5540		
68.459	5565		
68.359	5460		
68.259	5505		
68.159	5490		
68.059	5545		
67.959	5515		
67.859	5500		
67.759	5520		
67.659	5505		
67.559	5465		
67.459	5450		
67.359	5480		
67.259	5570		
67.159	5520		
67.059	5545		
66.959	5460		