Electronic Supplementary Material (ESI) for Chemical Science

Supporting Information

Structure Determination of an Amorphous Compound AlB_4H_{11}

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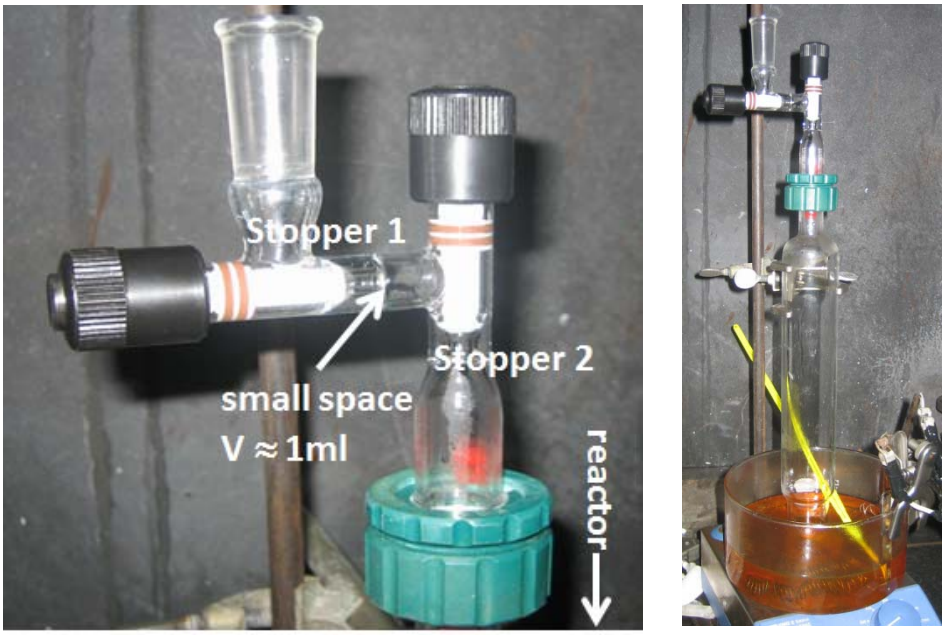

Figure S1. Special apparatus for sample collections during reaction from a reactor containing diborane (at 1.5 atm).

Table S1: PEGS+DFT predicted AlB_4H_{11} structures: Str-0, Str-86, Str-108, Str-260, Str-400, and Str-640.

System	Atom	Wyckoff site	x	y	z
Str-0	Al	1a	-0.44327	0.07529	0.44095
(P1)	Al	1a	0.25901	-0.40984	0.04455
a=7.117Å	B	1a	0.33880	0.20507	-0.38801
b=7.955Å	B	1a	0.47405	0.17428	-0.21548
c=6.907Å	B	1a	0.35658	0.36078	-0.15702
α=106.46	B	1a	0.43389	-0.18080	0.22807
β=80.58	B	1a	0.30656	-0.33644	0.36654
γ=104.90	B	1a	-0.43998	-0.22000	0.39979
	B	1a	-0.17581	0.21875	0.30673
	B	1a	0.01013	-0.35839	-0.04867
	H	1a	0.43761	-0.48804	-0.17949
	H	1a	0.46223	0.33136	-0.04371
	H	1a	0.41879	0.28021	0.47733
	H	1a	0.18214	0.10784	-0.42222
	H	1a	-0.34855	0.20866	-0.22975
	H	1a	0.39646	0.05862	-0.13024
	H	1a	0.18977	0.34394	-0.06864
	H	1a	-0.30447	-0.28630	0.32443
	H	1a	0.43613	-0.34775	0.47748
	H	1a	-0.48174	-0.21488	0.05748
	H	1a	0.35053	-0.05857	0.25459
	H	1a	0.26511	-0.49904	0.28316
	H	1a	0.17547	-0.28901	0.48311
	H	1a	-0.40907	-0.11057	-0.43620
	H	1a	-0.18196	0.13505	0.43871
	H	1a	-0.33302	0.17114	0.22644
	H	1a	-0.15023	0.37636	0.39042
	H	1a	-0.05711	0.16436	0.17516
	H	1a	0.00234	-0.43241	0.09403
	H	1a	-0.02592	-0.21375	0.02836
	H	1a	0.18216	-0.32977	-0.13697
	H	1a	-0.08746	-0.46746	-0.17290
System	Atom	Wyckoff site	x	y	z
Str-86	Al	1a	0.16965	-0.25467	0.39606
(P1)	Al	1a	0.13917	-0.48621	-0.08570
a=6.193Å	B	1a	0.09545	-0.23402	-0.25260
b=6.220Å	B	1a	0.04321	-0.32365	-0.41054
c=10.044Å	B	1a	-0.11438	-0.45940	-0.28307
α=79.98	B	1a	0.07102	0.49067	0.27420
β=103.98	B	1a	-0.08744	-0.29191	0.20253
γ=99.84	B	1a	0.03835	-0.42480	0.09994
	B	1a	0.44313	-0.02140	0.40044
	B	1a	0.35602	0.28745	-0.04608
	H	1a	-0.09534	0.34684	-0.23609
	H	1a	-0.11194	-0.49141	-0.42004
	H	1a	0.29418	-0.25486	-0.19701
	H	1a	0.04181	-0.06557	-0.23762
	H	1a	0.20442	-0.40415	-0.42399
	H	1a	-0.03418	-0.18647	0.49312
	H	1a	-0.30085	-0.41891	-0.29626
	H	1a	0.21853	-0.33911	0.07003
	H	1a	-0.07825	-0.26228	0.06011
	H	1a	0.27522	-0.47871	0.32523
	H	1a	-0.02240	0.32008	0.32118
	H	1a	-0.02183	-0.09643	0.21388

	H	1a	-0.28432	-0.33921	0.19757
	H	1a	-0.07319	0.43305	0.03017
	H	1a	-0.40564	0.12232	0.42544
	H	1a	0.40096	-0.06681	0.28230
	H	1a	0.48083	-0.19180	0.48282
	H	1a	0.27068	0.03748	0.41987
	H	1a	0.47520	0.14875	0.00046
	H	1a	0.32169	0.33768	-0.17193
	H	1a	0.17001	0.21970	-0.01435
	H	1a	0.43565	0.45646	0.00909
System	Atom	Wyckoff site	x	y	z
Str-108	Al	1a	0.43120	0.44856	-0.46516
(P1)	Al	1a	0.13889	0.03663	0.04353
a=7.779Å	B	1a	0.31947	-0.27472	-0.33388
b=7.344Å	B	1a	0.21151	-0.21815	-0.16773
c=7.893Å	B	1a	0.19105	-0.44388	-0.34374
α=108.47	B	1a	0.30516	0.23432	0.27406
β=112.83	B	1a	0.28865	0.45622	0.22369
γ=74.30	B	1a	0.31796	0.22940	0.05536
	B	1a	-0.12045	0.02117	0.07192
	B	1a	-0.27438	0.32836	-0.32779
	H	1a	0.03746	-0.45064	-0.46141
	H	1a	0.13554	-0.35666	-0.17634
	H	1a	0.25799	-0.17753	-0.44808
	H	1a	0.49222	-0.29783	-0.25788
	H	1a	0.07318	-0.08823	-0.20628
	H	1a	0.32110	-0.18595	-0.00165
	H	1a	0.26981	0.40188	-0.29870
	H	1a	0.46063	0.14413	0.02463
	H	1a	0.31146	0.41083	0.05558
	H	1a	0.44585	0.14862	0.37245
	H	1a	0.15992	0.23060	0.29709
	H	1a	0.42356	-0.45678	0.31188
	H	1a	0.13772	-0.44083	0.20208
	H	1a	0.17485	0.20020	-0.08590
	H	1a	-0.16118	0.11775	0.20915
	H	1a	-0.10180	0.14151	-0.00403
	H	1a	0.03823	-0.08488	0.13399
	H	1a	-0.22179	-0.08443	-0.05239
	H	1a	-0.18200	0.43071	-0.18871
	H	1a	-0.41340	0.31253	-0.29193
	H	1a	-0.32814	0.41520	-0.45907
	H	1a	-0.20432	0.16525	-0.38809
System	Atom	Wyckoff site	x	y	z
Str-260	Al	1a	0.31640	-0.46829	-0.11083
(P1)	Al	1a	0.46445	-0.01467	0.44132
a=6.700Å	B	1a	0.23310	0.15864	0.35678
b=7.746Å	B	1a	0.31265	0.35257	0.16516
c=8.150Å	B	1a	0.46040	0.29217	0.35525
α=67.80	B	1a	0.42474	-0.17344	-0.25340
β=87.70	B	1a	-0.32611	-0.07982	-0.33827
γ=96.16	B	1a	-0.37915	-0.31584	-0.17815
	B	1a	0.08607	0.42385	-0.23905
	B	1a	-0.45100	-0.15428	0.26389
	H	1a	0.45620	0.38136	0.44658
	H	1a	0.48248	0.43721	0.18167
	H	1a	0.09534	0.15656	0.45540
	H	1a	0.22111	0.01827	0.31796

	H	1a	0.19633	0.47167	0.13130
	H	1a	0.35010	0.29345	0.04708
	H	1a	-0.37034	0.25255	0.33360
	H	1a	-0.32897	-0.33832	-0.03302
	H	1a	-0.21817	-0.22271	-0.28935
	H	1a	0.34143	-0.10033	-0.16901
	H	1a	0.30980	-0.22012	-0.34962
	H	1a	-0.25118	0.03592	-0.28831
	H	1a	-0.27017	-0.04354	-0.49520
	H	1a	-0.38666	-0.45870	-0.21160
	H	1a	0.04054	-0.47753	-0.38187
	H	1a	0.27342	0.41492	-0.25921
	H	1a	0.05376	-0.49157	-0.13583
	H	1a	0.00517	0.26541	-0.16527
	H	1a	-0.29490	-0.21929	0.27456
	H	1a	-0.40636	0.01842	0.22912
	H	1a	0.43664	-0.16740	0.15683
	H	1a	0.45016	-0.23637	0.41350

System	Atom	Wyckoff site	x	y	z
Str-400	Al	1a	0.44213	0.34031	-0.01863
(P1)	B	1a	0.24063	0.16418	0.23529
a=5.967Å	B	1a	-0.41067	-0.27126	0.04782
b=5.073Å	B	1a	-0.44926	0.07029	-0.15947
c=6.904Å	B	1a	0.33448	-0.20446	-0.13774
α=69.76	H	1a	0.15761	0.25469	0.04216
β=100.43	H	1a	0.17984	0.31991	0.31319
γ=93.39	H	1a	0.19104	-0.08106	0.29766
	H	1a	0.45615	0.17486	0.26079
	H	1a	-0.28869	-0.46210	0.04566
	H	1a	-0.41682	-0.28536	0.22310
	H	1a	-0.34039	0.16778	-0.30003
	H	1a	0.37601	0.00478	-0.29864
	H	1a	0.16163	-0.17488	-0.08330
	H	1a	0.30340	-0.35518	-0.25116
	H	1a	-0.26244	-0.09001	-0.03597

System	Atom	Wyckoff site	x	y	z
Str-640	Al	1a	-0.03369	0.38552	-0.44839
(P1)	B	1a	-0.41784	0.29967	-0.21890
a=5.112Å	B	1a	0.29355	0.29463	-0.31465
b=6.070Å	B	1a	0.12034	-0.37324	0.26592
c=6.563Å	B	1a	-0.40022	0.16507	-0.44080
α=84.23	H	1a	-0.27808	0.24215	0.37433
β=74.23	H	1a	0.33597	0.19933	-0.48615
γ=94.50	H	1a	0.16284	0.42367	0.27443
	H	1a	-0.04702	-0.33765	0.43910
	H	1a	-0.31625	0.49655	-0.23385
	H	1a	-0.43303	0.19526	-0.05087
	H	1a	0.27924	0.49398	-0.36775
	H	1a	0.10054	0.19066	-0.18248
	H	1a	0.33415	-0.26617	0.25193
	H	1a	0.00412	-0.34171	0.13101
	H	1a	-0.42380	-0.03454	-0.41228

Table S2. Simulated chemical shifts (ppm) of boron atoms in ^{11}B NMR spectra of predicted Str-0, Str-86, Str-108, and Str-260.

Atoms	Str-0	Str-86	Str-108	Str-260
B1	-60.96	-59.41	-54.14	-59.18
B2	-33.45	-43.64	-55.22	-45.64
B3	-58.48	-30.50	-40.23	-39.01
B4	-61.82	-70.40	-59.57	-58.94
B5	-46.61	-39.31	-44.40	-39.77
B6	-46.50	-41.55	-42.76	-45.65
B7	-47.61	-35.66	-38.88	-56.25
B8	-41.29	-44.13	-51.24	-55.80

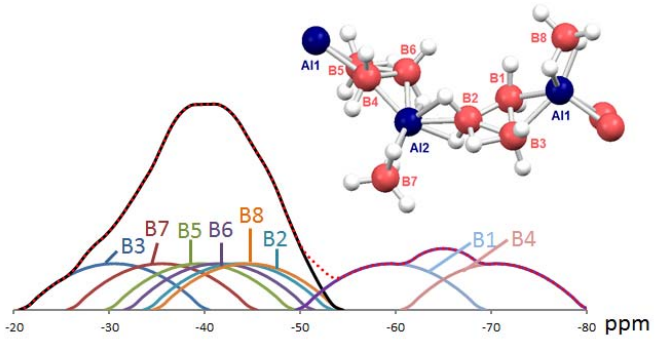

Figure S2. Simulated ^{11}B NMR spectra of AlB_4H_{11} based on the predicted Str-86.

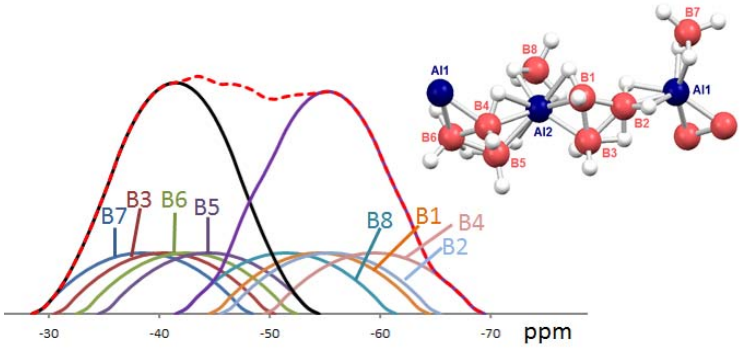

Figure S3. Simulated ^{11}B NMR spectra of AlB_4H_{11} based on the predicted Str-108.

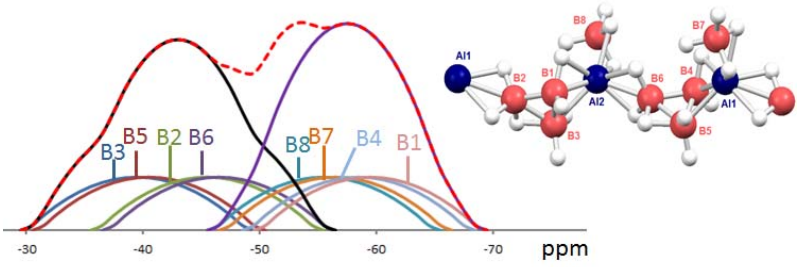

Figure S4. Simulated ^{11}B NMR spectra of AlB_4H_{11} based on the predicted Str-260.