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Crystal Structures, Phase Stabilities, and Hydrogen Storage Properties of Metal Amidoboranes — Supporting Information

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Table A: PEGS+DFT predicted LiAB, NaAB and KAB crystal structures.

System	Atom	Wyckoff site	x	y	z
LiAB (P-1)	Li	2i	0.11775	0.32825	0.86631
a=7.209Å	B	2i	0.18967	0.81212	0.93418
b=5.154Å	N	2i	0.72976	0.92376	0.22091
c=4.813Å	H	2i	0.96477	0.32178	0.19580
α=90.229	H	2i	0.69943	0.33491	0.03714
β=94.890	H	2i	0.84533	0.13798	0.82635
γ=106.056	H	2i	0.72763	0.96409	0.42884
	H	2i	0.58804	0.83353	0.15129
NaAB (P1)	Na	1a	0.33878	-0.12097	-0.23706
a=5.312Å	Na	1a	-0.16615	0.19508	0.40596
b=7.715Å	B	1a	-0.29467	-0.16213	0.38272
c=4.305Å	B	1a	0.19752	0.23679	0.06300
α=105.041	N	1a	-0.06340	-0.28071	-0.47060
β=107.012	N	1a	0.42545	0.35325	0.32141
γ=85.000	H	1a	0.48425	-0.23585	0.26508
	H	1a	-0.31715	-0.02613	-0.39793
	H	1a	-0.25013	-0.11201	0.15264
	H	1a	-0.04591	-0.39824	0.35934
	H	1a	-0.09203	-0.31809	-0.27222
	H	1a	-0.02524	0.31181	0.01373
	H	1a	0.24433	0.18728	-0.21293
	H	1a	0.17771	0.10019	0.15463
	H	1a	0.39684	0.38652	-0.44516
	H	1a	0.43891	0.47300	0.26686
KAB (P1)	K	1a	0.88092	0.86648	0.27800
a=5.337Å	K	1a	0.64687	0.28848	0.06996
b=7.524Å	B	1a	0.00080	0.32323	0.39578
c=5.364Å	B	1a	0.54548	0.84450	0.95043
α=103.983	N	1a	0.19244	0.36889	0.54864
β=64.247	N	1a	0.57649	0.65016	0.97340
γ=104.200	H	1a	0.76687	0.23852	0.51877
	H	1a	0.97179	0.46871	0.34945
	H	1a	0.09654	0.22407	0.16162
	H	1a	0.19174	0.27210	0.65332
	H	1a	0.19503	0.49475	0.67243
	H	1a	0.41142	0.84630	0.81461
	H	1a	0.43589	0.93065	0.18961
	H	1a	0.77466	0.93653	0.83867
	H	1a	0.65177	0.57230	0.77913
	H	1a	0.39040	0.57749	0.07995

Table B: PEGS+DFT predicted BeAB, MgAB, CaAB and SrAB crystal structures. For SrAB, we also show the structure using experimental CaAB prototype structure (C2).

System	Atom	Wyckoff site	x	y	z
BeAB (P-1)	Be	2i	0.12785	0.15099	0.16624
a=4.740Å	B	2i	-0.45079	0.25512	0.41703
b=7.942Å	B	2i	0.09157	0.19812	-0.09371
c=7.526Å	N	2i	0.27418	0.31550	0.30119
α=87.02	N	2i	-0.02038	0.05437	-0.23802
β=99.53	H	2i	-0.25013	0.37722	0.46808
γ=103.05	H	2i	0.46625	0.16733	-0.45405
	H	2i	-0.36607	0.16159	0.31995
	H	2i	0.34352	0.42757	0.23212
	H	2i	0.13638	0.34532	0.38045
	H	2i	0.31123	0.16438	0.00873
	H	2i	0.16141	0.34388	-0.15070
	H	2i	-0.10322	0.19435	0.00235
	H	2i	0.14182	0.06198	-0.31598
	H	2i	-0.19212	0.08659	-0.32647
MgAB (C2)	Mg	2a	0.00000	0.06261	0.00000
a=8.383Å	B	2a	0.77157	0.28899	0.16870
b=6.006Å	N	2a	0.97502	0.28346	0.20721
c=7.272Å	H	2a	0.75980	0.45165	0.26857
α=90.0	H	2a	0.13592	0.79975	0.96134
β=126.094	H	2a	0.24618	0.62190	0.24361
γ=90.0	H	2a	0.08272	0.25088	0.37576
	H	2a	0.01041	0.43827	0.18143
CaAB (P1)	Ca	1a	0.91313	0.53622	0.77497
a=5.156Å	B	1a	0.44184	0.76531	0.83815
b=6.006Å	B	1a	0.91242	0.35021	0.32657
c=5.066Å	N	1a	0.24549	0.81378	0.62740
α=85.051	N	1a	0.92732	0.20993	0.08555
β=85.058	H	1a	0.66409	0.84497	0.77089
γ=90.453	H	1a	0.36603	0.84109	0.04798
	H	1a	0.45965	0.55755	0.88571
	H	1a	0.31876	0.78470	0.43920
	H	1a	0.18871	0.97673	0.61365
	H	1a	0.72993	0.29699	0.49576
	H	1a	0.11877	0.34347	0.43520
	H	1a	0.88053	0.55529	0.25919
	H	1a	0.76777	0.10921	0.07901
	H	1a	0.08389	0.10692	0.07879

Table C: Continue Table Table B.

System	Atom	Wyckoff site	x	y	z
SrAB (P-1)	Sr	2i	0.21883	0.17214	0.17914
a=4.669Å	B	2i	0.67263	0.28077	0.38037
b=8.222Å	B	2i	0.82833	0.19977	0.91619
c=8.454Å	N	2i	0.55920	0.40920	0.28735
α=91.415	N	2i	0.90918	0.13639	0.74285
β=78.928	H	2i	0.92862	0.31983	0.40371
γ=99.481	H	2i	0.50749	0.24653	0.51075
	H	2i	0.66449	0.14686	0.30383
	H	2i	0.71847	0.47479	0.20213
	H	2i	0.46691	0.49457	0.36109
	H	2i	0.02702	0.30085	0.95879
	H	2i	0.60613	0.26580	0.93360
	H	2i	0.77137	0.08161	0.01725
	H	2i	0.12817	0.16837	0.69265
	H	2i	0.79831	0.18133	0.66494
SrAB (C2)	Sr	2c	0.00000	-0.40514	0.00000
a=9.437Å	B	2c	-0.17047	0.08626	-0.21282
b=4.521Å	N	2c	0.17546	0.49811	-0.27731
c=6.948Å	H	2c	0.42327	0.43435	-0.28315
α=90.000	H	2c	0.14955	0.34436	0.26021
β=93.636	H	2c	-0.14993	0.07121	-0.03226
γ=90.000	H	2c	-0.35612	0.09863	-0.40467
	H	2c	-0.16587	0.27675	0.30561

Table D: PEGS+DFT predicted ScAB crystal structure.

System	Atom	Wyckoff site	x	y	z
ScAB (P1)	Sc	1a	0.53537	0.89265	0.72297
a=7.330Å	B	1a	0.53145	0.42151	0.55598
b=4.906Å	B	1a	0.21321	0.04859	0.14009
c=6.799Å	B	1a	0.80920	0.04000	0.84397
α=104.350	N	1a	0.52938	0.10550	0.46422
β=65.218	N	1a	0.22360	0.22112	0.97484
γ=80.661	N	1a	0.87268	0.83344	0.59716
	H	1a	0.35297	0.60564	0.66779
	H	1a	0.60282	0.45163	0.69673
	H	1a	0.64169	0.51725	0.40954
	H	1a	0.65915	0.99168	0.30472
	H	1a	0.40350	0.10325	0.43408
	H	1a	0.19911	0.19603	0.32274
	H	1a	0.07886	0.92213	0.16747
	H	1a	0.38651	0.84273	0.04288
	H	1a	0.22035	0.43566	0.03313
	H	1a	0.10722	0.21997	0.92875
	H	1a	0.84932	0.90471	0.95623
	H	1a	0.87060	0.25693	0.84640
	H	1a	0.60867	0.14966	0.95042
	H	1a	0.96067	0.62098	0.54860
	H	1a	0.94800	0.90960	0.46691