Supplementary Information for

Using First Principles Calculations To Identify New Destabilized Metal Hydride Reactions for Reversible Hydrogen Storage

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Table S1: Enthalpy of reaction per mole of H_2 released for the reactions studied using the PW91 functional. ** indicates results for final materials with varying Si loading. For reactions involving $LiBH_4$, the enthalpy for the reaction with the hexagonal and orthorhombic polymorphs of $LiBH_4$ is denoted by (h) and (o), respectively.

No	Reaction	wt.% H_2	ΔU_0 (PAW)
	Calibration reactions and reactions for comparison with previous work		
1	$MgH_2 \rightarrow Mg + H_2$	7.67	65.1
2	$2\ LiH \rightarrow 2\ Li + H_2$	12.70	171.4
3	$2\ MgH_2 + Si \rightarrow Mg_2Si + 2\ H_2$	5.00	37.9
4	$MgH_2 + 2\ LiBH_4 \rightarrow 2\ LiH + MgB_2 + 4\ H_2$	11.56	66.8 (o) 58.6 (h)
5	$CaH_2 \rightarrow Ca + H_2$	4.80	175.2
6	$2\ AlH_3 \rightarrow 2\ Al + 3\ H_2$	10.07	11.1
7	$Ca(AlH_4)_2 \rightarrow 2\ Al + Ca + 4\ H_2$	7.91	54.3
8	$Ca(AlH_4)_2 \rightarrow 2\ Al + CaH_2 + 3\ H_2$	5.93	14.0
9	$LiBH_4 \rightarrow LiH + B + 1.5\ H_2$	13.91	82.4 (o) 71.5 (h)
10	$LiNH_2 + 2\ LiH \rightarrow Li_3N + 2\ H_2$	10.39	109.4
11	$LiBH_4 + 2\ LiNH_2 \rightarrow Li_3BN_2 + 4\ H_2$	11.93	24.3 (o) 20.2 (h)
	Reaction with $LiNH_2$		
12	**$3\ LiNH_2 + 2\ LiH + Si \rightarrow Li_5N_3Si + 4\ H_2$ (10/11 Si atoms)	7.16	34.2/23.3
13	$LiNH_2 + MgH_2 \rightarrow LiMgN + 2\ H_2$	8.19	32.0
14	$2\ LiNH_2 + 3\ MgH_2 \rightarrow Mg_3N_2 + 2\ LiH + 4\ H_2$	6.47	6.9

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15	$2 LiNH_2 + MgH_2 + Si \rightarrow MgN_2Si + 2 LiH + 2 H_2$	4.02	-86.0
16	$LiBH_4 + 3 MgH_2 + 3 LiNH_2 \rightarrow Mg_3BN_3 + 4 LiH + 6 H_2$	7.14	5.8 (o) 3.1 (h)
17	$N(SiH_3)_3 + 3 LiNH_2 \rightarrow N_4Si_3 + 3 LiH + 6 H_2$	6.86	-38.0
	Reaction with LiBH$_4$		
18	$6 LiBH_4 + Si \rightarrow 6 LiH + B_6Si + 9 H_2$	11.45	117.9 (o) 106.9 (h)
19	$4 LiBH_4 + MgH_2 \rightarrow 4 LiH + MgB_4 + 7 H_2$	12.46	69.2 (o) 59.9 (h)
20	$7 LiBH_4 + MgH_2 \rightarrow 7 LiH + MgB_7 + 11.5 H_2$	12.99	71.5-75.5 (o) 61.5-65.5 (h)
21	$6 LiBH_4 + 7 Si \rightarrow 6 LiSi + SiB_6 + 12 H_2$	7.39	109.9(o) 101.8(h)
22	$MgH_2 + 9 LiBH_4 + LiNH_2 \rightarrow MgB_9N + 10 LiH + 14 H_2$	11.5	108.4(o) 98.0(h)
	Reaction of MgH$_2$, LiH and Si		
23	$12 LiH + 3 MgH_2 + 4 Si \rightarrow Li_{12}Mg_3Si_4 + 9 H_2$	6.34	85.0
24	$2 NaMgH_3 + 3 Si \rightarrow Mg_2Si + 2 NaSi + 3 H_2$	3.27	57.5
25	$4 MgH_2 + Al + 6 Si \rightarrow AlMg_4Si_6 + 4 H_2$	2.68	92.4
26	$4 MgH_2 + AlH_3 + 6 Si \rightarrow AlMg_4Si_6 + 5.5 H_2$	3.65	70.2
27	$2 LiH + 2 Si \rightarrow 2 LiSi + H_2$	2.80	91.3
28	$2 LiH + Si \rightarrow Li_2Si + H_2$	4.58	103.6
29	$7 LiH + 2 Si \rightarrow Li_7Si_2 + 1.5 H_2$	2.70	1139.9
	Reactions with CaH$_2$		
30	$CaH_2 + 2 Al \rightarrow Al_2Ca + H_2$	2.10	73.8
31	$3 CaH_2 + 2 Al + 2 Si \rightarrow Al_2Ca_3Si_2 + 3 H_2$	2.56	71.8
32	$CaH_2 + 2 Al + 2 Si \rightarrow Al_2CaSi_2 + H_2$	1.33	16.3
33	$CaH_2 + Si \rightarrow CaSi + H_2$	2.88	80.9
34	$CaH_2 + 2 Si \rightarrow CaSi_2 + H_2$	2.06	61.7
35	$5 CaH_2 + 3 Si \rightarrow Ca_5Si_3 + 5 H_2$	3.43	100.9
36	$CaH_2 + LiH + 2 Si \rightarrow CaLiSi_2 + 1.5 H_2$	2.85	65.0
37	$2 CaH_2 + LiH + 3 Si \rightarrow Ca_2LiSi_3 + 2.5 H_2$	2.86	64.6
38	$CaH_2 + 2 LiH \rightarrow CaLi_2 + 2 H_2$	6.96	78.3
39	$CaH_2 + 6 LiBH_4 \rightarrow CaB_6 + 6 LiH + 10 H_2$	11.69	62.7 (o) 52.9 (h)
40	$CaH_2 + MgH_2 + Si \rightarrow CaMgSi + 2 H_2$	4.19	51.8
41	$3 CaH_2 + LiBH_4 + 3 LiNH_2 \rightarrow Ca_3BN_3 + 4 LiH + 6 H_2$	5.58	38.8 (o) 36.1 (h)
42	$CaH_2 + 2 MgH_2 \rightarrow CaMg_2 + 3 H_2$	6.38	88.3
43	$CaH_2 + LiNH_2 \rightarrow CaLiN + 2 H_2$	6.20	88.1
44	$2 CaH_2 + LiNH_2 \rightarrow Ca_2HN + LiH + 2 H_2$	3.76	74.7
45	$3 CaH_2 + 3 LiNH_2 + Al \rightarrow Ca_3AlN_3 + 3 LiH + 4.5 H_2$	4.08	34.8
46	$3 CaH_2 + 3 LiNH_2 + AlH_3 \rightarrow Ca_3AlN_3 + 3 LiH + 6 H_2$	5.37	28.9

47	$CaH_2 + 2\ MgH_2 + 2\ LiNH_2 \rightarrow CaMg_2N_2 + 2\ LiH + 4\ H_2$	5.73	29.2
	Reaction of Ca(AlH$_4$)$_2$ and Si		
48	$Ca(AlH_4)_2 + Si \rightarrow 2\ Al + CaSi + 4\ H_2$	6.30	30.7
49	$Ca(AlH_4)_2 + 2\ Si \rightarrow Al_2CaSi_2 + 4\ H_2$	5.10	14.5
50	$3\ Ca(AlH_4)_2 + 2\ Si \rightarrow 2\ Al_2Ca + Al_2CaSi_2 + 12\ H_2$	6.69	24.1
51	$3\ Ca(AlH_4)_2 + 2\ Si \rightarrow 4\ Al + Al_2Ca_3Si_2 + 12\ H_2$	6.69	28.4
52	$3\ Ca(AlH_4)_2 + 2\ Si \rightarrow 4\ AlH_3 + Al_2Ca_3Si_2 + 6\ H_2$	3.34	45.4
	Reaction of Ca(AlH$_4$)$_2$ and MgH$_2$		
53	$6\ Ca(AlH_4)_2 + 17\ MgH_2 \rightarrow Al_{12}Mg_{17} + 6\ CaH_2 + 35\ H_2$	6.67	35.5
54	$Ca(AlH_4)_2 + 2\ MgH_2 \rightarrow CaMg_2 + 2\ Al + 6\ H_2$	7.83	51.6
55	$Ca(AlH_4)_2 + 2\ MgH_2 \rightarrow CaMg_2 + 2\ AlH_3 + 3\ H_2$	3.92	91.7
	Reaction of Ca(AlH$_4$)$_2$ and LiH		
56	$Ca(AlH_4)_2 + 2\ LiH \rightarrow 2\ AlLi + CaH_2 + 4\ H_2$	6.85	33.3
57	$2\ Ca(AlH_4)_2 + 6\ LiH \rightarrow 2\ Al_2Li_3 + 2\ CaH_2 + 9\ H_2$	7.22	43.9
58	$2\ Ca(AlH_4)_2 + 9\ LiH \rightarrow Al_4Li_9 + 2\ CaH_2 + 10.5\ H_2$	7.69	60.5
59	$3\ Ca(AlH_4)_2 + 2\ LiH \rightarrow 2\ Al_3Li + 3\ CaH_2 + 10\ H_2$	6.27	20.5
60	$3\ Ca(AlH_4)_2 + 4\ LiH \rightarrow 4\ AlLi + Al_2Ca + 2\ CaH_2 + 12\ H_2$	7.17	31.8
61	$3\ Ca(AlH_4)_2 + 8\ LiH \rightarrow 2\ Al_3Li + 3\ CaLi_2 + 16\ H_2$	8.74	76.9
62	$4\ Ca(AlH_4)_2 + 26\ LiH \rightarrow 2\ Al_4Li_9 + 4\ CaLi_2 + 29\ H_2$	9.65	91.0
	Reaction of Ca(AlH$_4$)$_2$, LiH and Si		
63	$Ca(AlH_4)_2 + 2\ LiH + 2\ Si \rightarrow 2\ AlLiSi + CaH_2 + 4\ H_2$	4.64	17.6
64	$Ca(AlH_4)_2 + LiH + 2\ Si \rightarrow 2\ Al + CaLiSi_2 + 4.5\ H_2$	5.47	31.0
65	$Ca(AlH_4)_2 + LiH + 2\ Si \rightarrow 2\ AlH_3 + CaLiSi_2 + 1.5\ H_2$	1.82	70.2
66	$2\ Ca(AlH_4)_2 + LiH + 3\ Si \rightarrow 4\ Al + Ca_2LiSi_3 + 8.5\ H_2$	5.79	28.8
67	$2\ Ca(AlH_4)_2 + LiH + 3\ Si \rightarrow 4\ AlH_3 + Ca_2LiSi_3 + 2.5\ H_2$	1.70	70.7
	Reaction of Ca(AlH$_4$)$_2$ and LiBH$_4$		
68	$2\ Ca(AlH_4)_2 + 4\ LiBH_4 \rightarrow 2\ AlB_2 + 2\ AlH_3 + 2\ CaLi_2 + 13\ H_2$	9.14	92.0 (o) 86.9 (h)
69	$4\ Ca(AlH_4)_2 + 4\ LiBH_4 \rightarrow 2\ Al_3Li + 2\ AlB_2 + 2\ LiH + 2\ CaH_2 + 21\ H_2$	8.56	67.9 (o) 64.7 (h)
70	$2\ Ca(AlH_4)_2 + 6\ LiBH_4 \rightarrow CaB_6 + 2\ Al_2Li_3 + CaH_2 + 19\ H_2$	10.85	53.4 (o) 48.3 (h)
	Reaction of Ca(AlH$_4$)$_2$ and LiNH$_2$		
71	$Ca(AlH_4)_2 + LiNH_2 \rightarrow CaH_2 + AlLi + AlN + 4\ H_2$	6.46	-20.5
72	$Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow CaH_2 + 2\ LiH + 2\ AlN + 4\ H_2$	5.46	-73.3
73	$Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow CaLi_2 + 2\ AlN + 6\ H_2$	8.19	7.4
74	$Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow CaH_2 + AlLi_3N_2 + AlN + 6\ H_2$	7.09	-26.4

3

75	$Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow CaH_2 + 2\ AlN + Li_3N + 6\ H_2$	7.09	-12.4
76	$Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow CaH_2 + 2\ AlLi + LiN_3 + 6\ H_2$	7.09	86.0
77	$Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow CaLi_2 + LiN_3 + 2\ Al + 7\ H_2$	8.27	109.1
78	$Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow CaLi_2 + LiN_3 + 2\ AlH_3 + 4\ H_2$	4.72	182.7
79	$Ca(AlH_4)_2 + 4\ LiNH_2 \rightarrow CaH_2 + AlN + AlLi + LiN_3 + 2\ LiH + 6\ H_2$	6.25	40.9
80	$Ca(AlH_4)_2 + 4\ LiNH_2 \rightarrow CaLi_2 + AlN + AlLi + LiN_3 + 8\ H_2$	8.33	80.3
81	$Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow CaH_2 + 4\ LiH + 2\ AlN + LiN_3 + 6\ H_2$	5.33	15.6
82	$Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow CaH_2 + AlLi_3N_2 + LiN_3 + AlLi + 8\ H_2$	7.45	55.0
83	$Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow CaLi_2 + 2\ LiH + 2\ AlN + LiN_3 + 8\ H_2$	7.45	54.0
84	$Ca(AlH_4)_2 + 6\ LiNH_2 \rightarrow CaH_2 + 2\ LiN_3 + 2\ AlLi + 2\ LiH + 8\ H_2$	8.38	27.6
85	$Ca(AlH_4)_2 + 6\ LiNH_2 \rightarrow CaLi_2 + 2\ LiN_3 + 2\ AlLi + 10\ H_2$	9.31	124.1
86	$2\ Ca(AlH_4)_2 + LiNH_2 \rightarrow 2\ CaH_2 + AlN + Al_3Li + 7\ H_2$	6.22	-7.0
87	$2\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + AlLi + 3\ Al + 9\ H_2$	8.00	41.7
88	$2\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + Al_3Li + AlH_3 + 7.5\ H_2$	6.67	47.0
89	$2\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + AlLi + 3\ AlH_3 + 4.5\ H_2$	4.00	72.2
90	$2\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + Al_3Li + Al + 9\ H_2$	8.00	112.9
91	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow 2\ CaH_2 + 2\ AlN + 2\ LiH + 2\ AlH_3 + 4\ H_2$	3.23	-71.9
92	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow 2\ CaH_2 + 2\ AlN + 2\ LiH + 2\ Al + 7\ H_2$	5.65	-36.3
93	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow CaLi_2 + CaH_2 + 2\ AlN + 2\ Al + 9\ H_2$	7.27	9.3
94	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow CaLi_2 + CaH_2 + 2\ AlN + 2\ AlH_3 + 6\ H_2$	4.84	8.4
95	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow Ca_2N + AlN + 3\ Al + 2\ LiH + 9\ H_2$	7.27	18.2
96	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow Ca_2N + Al_3Li + AlN + LiH + 9.5\ H_2$	7.67	21.4
97	$2\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow Ca_2N + AlN + 3\ AlH_3 + 2\ LiH + 4.5\ H_2$	3.63	25.3
98	$2\ Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow 2\ CaH_2 + 3\ AlN + 3\ LiH + AlH_3 + 6\ H_2$	4.44	-72.8
99	$2\ Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow 2\ CaH_2 + 3\ AlN + 3\ LiH +$	5.54	-56.1

	Al + 7.5 H_2		
100	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → 2 CaH_2 + Li_3N + 2 AlN + 2 AlH_3 + 6 H_2	4.44	-11.4
101	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → 2 CaH_2 + Li_3N + 2 AlN + 2 Al + 9 H_2	6.65	-3.9
102	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → CaH_2 + $CaLi_2$ + AlLi + 3 AlN + 10 H_2	7.39	-3.8
103	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → Ca_2N + 2 AlN + 2 AlLi + LiH + 10.5 H_2	7.76	8.4
104	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → Ca_2N + Al_2Li_3 + 2 AlN + 11 H_2	8.13	13.7
105	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → Ca_2N + Li_3N + AlN + 3 Al + 11 H_2	8.13	34.8
106	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → Ca_2N + Li_3N + AlN + 3 AlH_3 + 6.5 H_2	4.81	51.2
107	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → 2 CaH_2 + LiN_3 + 2 AlLi + 2 Al + 9 H_2	6.65	61.7
108	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → $CaLi_2$ + Al_2Ca + LiN_3 + 2 Al + 11 H_2	8.13	79.6
109	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → CaH_2 + $CaLi_2$ + LiN_3 + 4 Al + 10 H_2	7.39	80.3
110	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → 2 CaH_2 + LiN_3 + 2 AlLi + 2 AlH_3 + 6 H_2	4.44	87.0
111	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → $CaLi_2$ + Al_2Ca + LiN_3 + 2 AlH_3 + 8 H_2	5.92	105.2
112	2 $Ca(AlH_4)_2$ + 3 $LiNH_2$ → CaH_2 + $CaLi_2$ + LiN_3 + 4 AlH_3 + 4 H_2	2.96	184.1
113	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → 2 CaH_2 + Li_3N + 3 AlN + AlLi + 10 H_2	6.82	-15.6
114	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + $AlLi_3N_2$ + AlLi + AlN + Al + 12 H_2	8.19	14.8
115	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + $AlLi_3N_2$ + AlLi + AlN + AlH_3 + 10.5 H_2	7.16	15.3
116	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + Li_3N + 2 AlN + AlLi + Al + 12 H_2	8.19	21.8
117	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + Li_3N + 2 AlN + AlLi + AlH_3 + 10.5 H_2	7.16	23.3
118	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → 2 CaH_2 + LiN_3 + 3 AlLi + AlN + 10 H_2	6.82	43.4
119	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → 2 CaH_2 + Al_2Li_3 + LiN_3 + AlN + Al + 10 H_2	6.82	45.2
120	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → 2 CaH_2 + Al_2Li_3 + LiN_3 + AlN + AlH_3 + 8.5 H_2	5.80	51.3
121	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + LiN_3 + 3 AlLi + Al + 12 H_2	8.19	71.0
122	2 $Ca(AlH_4)_2$ + 4 $LiNH_2$ → Ca_2N + LiN_3 + 3 AlLi +	7.16	79.6

	$AlH_3 + 10.5\ H_2$		
123	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow 2\ CaH_2 + Li_3N + 2\ LiH + 4\ AlN + 10\ H_2$	6.33	-36.8
124	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow Ca_2N + 4\ AlN + 5\ LiH + 10.5\ H_2$	6.65	-31.9
125	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow 2\ CaH_2 + LiN_3 + 2\ AlN + 2\ AlLi + 2\ LiH + 10\ H_2$	6.33	22.3
126	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow Ca_2N + LiN_3 + Al_3Li + AlN + 3\ LiH + 11.5\ H_2$	7.28	51.3
127	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow Ca_2N + LiN_3 + 3\ AlLi + AlN + LiH + 12.5\ H_2$	7.91	54.9
128	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow 2\ CaLi_2 + LiN_3 + 2\ AlN + 2\ Al + 13\ H_2$	8.23	62.2
129	$2\ Ca(AlH_4)_2 + 5\ LiNH_2 \rightarrow 2\ CaLi_2 + LiN_3 + 2\ AlN + 2\ AlH_3 + 10\ H_2$	6.33	77.5
130	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow 3\ CaH_2 + Al_3Li + AlN + 2\ AlH_3 + 7\ H_2$	4.29	-6.1
131	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow 3\ CaH_2 + Al_3Li + AlN + 2\ Al + 10\ H_2$	6.13	-1.0
132	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + CaH_2 + Al_3Li + 3\ Al + 12\ H_2$	7.36	34.0
133	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + CaH_2 + AlLi + 5\ Al + 12\ H_2$	7.36	34.5
134	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + Al_2Ca + Al_3Li + Al + 13\ H_2$	7.97	38.0
135	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + Al_2Ca + Al_3Li + AlH_3 + 11.5\ H_2$	7.05	40.3
136	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + CaH_2 + Al_3Li + 3\ AlH_3 + 7.5\ H_2$	4.60	47.8
137	$3\ Ca(AlH_4)_2 + LiNH_2 \rightarrow Ca_2N + CaH_2 + AlLi + 5\ AlH_3 + 4.5\ H_2$	2.76	73.5
138	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow 3\ CaH_2 + 2\ AlLi + 2\ AlN + 2AlH_3 + 8\ H_2$	4.59	-19.8
139	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow 3\ CaH_2 + 2\ AlLi + 2\ AlN + 2\ Al + 11\ H_2$	6.31	-11.4
140	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow CaH_2 + 2\ Al_2Ca + 2\ AlN + 2\ LiH + 12\ H_2$	6.88	-5.9
141	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow 2\ CaH_2 + Al_2Ca + 2\ AlN + 2\ AlLi + 12\ H_2$	6.88	-4.4
142	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow Ca_2N + CaLi_2 + AlN + 5\ Al + 14\ H_2$	8.03	38.6
143	$3\ Ca(AlH_4)_2 + 2\ LiNH_2 \rightarrow Ca_2N + CaLi_2 + AlN + 5\ AlH_3 + 6.5\ H_2$	3.73	70.4
144	$3\ Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow 3\ CaH_2 + 3\ AlN + Al_3Li + 2\ LiH + 11\ H_2$	5.92	-31.1
145	$3\ Ca(AlH_4)_2 + 3\ LiNH_2 \rightarrow 3\ CaH_2 + Al_2Li_3 + 3\ AlN$	5.65	-23.3

	$+ AlH_3 + 10.5 \, H_2$		
146	$3 \, Ca(AlH_4)_2 + 3 \, LiNH_2 \rightarrow 3 \, CaH_2 + Al_2Li_3 + 3 \, AlN + Al + 12 \, H_2$	6.46	-19.0
147	$3 \, Ca(AlH_4)_2 + 3 \, LiNH_2 \rightarrow 3 \, CaH_2 + Li_3N + 2 \, AlN + 4 \, AlH_3 + 6 \, H_2$	3.23	-10.5
148	$3 \, Ca(AlH_4)_2 + 3 \, LiNH_2 \rightarrow 3 \, CaH_2 + Li_3N + 2 \, AlN + 4 \, Al + 12 \, H_2$	6.46	0.3
149	$3 \, Ca(AlH_4)_2 + 3 \, LiNH_2 \rightarrow 3 \, CaH_2 + LiN_3 + 2 \, AlLi + 4 \, Al + 12 \, H_2$	6.46	49.5
150	$3 \, Ca(AlH_4)_2 + 3 \, LiNH_2 \rightarrow 3 \, CaH_2 + LiN_3 + 2 \, AlLi + 4 \, AlH_3 + 6 \, H_2$	3.23	87.9
151	$3 \, Ca(AlH_4)_2 + 5 \, LiNH_2 \rightarrow 3 \, CaH_2 + Li_3N + 2 \, AlLi + 4 \, AlN + 14 \, H_2$	6.71	-17.0
152	$3 \, Ca(AlH_4)_2 + 5 \, LiNH_2 \rightarrow 3 \, CaH_2 + LiN_3 + 4 \, AlLi + 2 \, AlN + 14 \, H_2$	6.71	25.1
153	$3 \, Ca(AlH_4)_2 + 6 \, LiNH_2 \rightarrow 3 \, CaH_2 + 3 \, AlLi + 3 \, AlN + LiN_3 + 2 \, LiH + 14 \, H_2$	6.37	10.1
154	$4 \, Ca(AlH_4)_2 + 2 \, LiNH_2 \rightarrow 3 \, CaH_2 + CaLi_2 + 2 \, AlN + 6 \, Al + 15 \, H_2$	6.67	10.8
155	$4 \, Ca(AlH_4)_2 + 2 \, LiNH_2 \rightarrow 3 \, CaH_2 + CaLi_2 + 2 \, AlN + 6 \, AlH_3 + 6 \, H_2$	2.67	10.3
	Reactions including Sc		
156	$ScH_2 + 3 \, Al \rightarrow Al_3Sc + H_2$	1.58	19.6
157	$ScH_2 + 2 \, Si \rightarrow ScSi_2 + H_2$	1.95	95.5
158	$ScH_2 + 2 \, Al \rightarrow Al_2Sc + H_2$	2.00	57.9
159	$ScH_2 + Si \rightarrow ScSi + H_2$	2.68	39.8
160	$ScH_2 + Al \rightarrow AlSc + H_2$	2.73	111.1
161	$5 \, ScH_2 + 3 \, Si \rightarrow Sc_5Si_3 + 5 \, H_2$	3.16	81.9
162	$2 \, ScH_2 + Al \rightarrow AlSc_2 + 2 \, H_2$	3.33	148.0
163	$ScH_2 \rightarrow Sc + H_2$	4.29	200.0
164	$ScH_2 + LiNH_2 \rightarrow ScN + LiH + 1.5 \, H_2$	4.32	-43.8
165	$2 \, ScH_2 + 3 \, LiNH_2 \rightarrow Li_3ScN_2 + ScN + 5 \, H_2$	6.19	11.3
166	$ScH_2 + 2 \, LiBH_4 \rightarrow ScB_2 + 2 \, LiH + 4 \, H_2$	8.91	49.7
167	$ScH_2 + 12 \, LiBH_4 \rightarrow ScB_{12} + 12 \, LiH + 19 \, H_2$	12.42	74.1
168	$2 \, ScH_2 + Al + 2 \, Si \rightarrow AlSc_2Si_2 + 2 \, H_2$	2.28	28.9
169	$2 \, ScH_2 + AlH_3 + 2 \, Si \rightarrow AlSc_2Si_2 + 3.5 \, H_2$	3.92	21.3
	Reactions including Ti		
170	$TiH_2 \rightarrow Ti + H_2$	4.04	142.7
171	$TiH_2 + LiBH_4 \rightarrow LiH + TiB + 2.5 \, H_2$ (TiB – SG: $F\bar{4}3m$)	7.03	162.0 (o) 155.6 (h)
172	$TiH_2 + LiBH_4 \rightarrow LiH + TiB + 2.5 \, H_2$ (TiB – SG: Pnma)	7.03	43.7 (o) 37.2 (h)
173	$TiH_2 + 2 \, LiBH_4 \rightarrow 2 \, LiH + TiB_2 + 4 \, H_2$	8.63	22.2 (o) 14.1 (h)
174	$TiH_2 + Si \rightarrow TiSi + H_2$	2.59	-0.1

175	$TiH_2 + 2\,Si \rightarrow TiSi_2 + H_2$	1.90	-6.2
176	$5\,TiH_2 + 3\,Si \rightarrow Ti_5Si_3 + 5\,H_2$	3.02	28.4
177	$5\,TiH_2 + 4\,Si \rightarrow Ti_5Si_4 + 5\,H_2$	2.79	10.6
178	$TiH_2 + Al \rightarrow AlTi + H_2$	2.62	63.3
179	$TiH_2 + 2\,Al \rightarrow Al_2Ti + H_2$ (Al$_2$Ti – SG: Cmmm)	1.94	18.5
180	$TiH_2 + 2\,Al \rightarrow Al_2Ti + H_2$ (Al$_2$Ti – SG: I4$_1$/amd)	1.94	17.2
181	$TiH_2 + 3\,Al \rightarrow Al_3Ti + H_2$	1.54	-11.9
182	$3\,TiH_2 + Al \rightarrow AlTi_3 + H_2$	1.14	106.5
183	$TiH_2 + LiNH_2 \rightarrow LiH + TiN + 2\,H_2$	5.53	-46.4
184	$2\,TiH_2 + LiNH_2 \rightarrow LiH + Ti_2N + 2.5\,H_2$ (Ti$_2$N – SG: I4$_1$/amd)	4.11	11.7
185	$2\,TiH_2 + LiNH_2 \rightarrow LiH + Ti_2N + 2.5\,H_2$ (Ti$_2$N – SG: P4$_2$/mnm)	4.11	9.2
186	$3\,TiH_2 + Al + C \rightarrow Ti_3AlC + 3\,H_2$	3.21	50.1
187	$3\,TiH_2 + Al + LiNH_2 \rightarrow LiH + Ti_3AlN + 3.5\,H_2$	3.53	26.1
188	$3\,TiH_2 + 2\,Al + LiNH_2 \rightarrow AlLi + Ti_3AlN + 4\,H_2$	3.56	34.1
189	$3\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_3Li + Ti_3AlN + 4\,H_2$	3.18	-56.5
190	$3\,TiH_2 + 2\,Al + 3\,LiNH_2 \rightarrow AlLi_3N_2 + Ti_3AlN + 6\,H_2$	4.44	10.0
191	$4\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_3AlN + LiH + 5\,H_2$ (Al$_2$Ti – SG: Cmmm)	3.32	-43.6
192	$4\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_3AlN + LiH + 5\,H_2$ (Al$_2$Ti – SG: I4$_1$/amd)	3.32	-43.8
193	$9\,TiH_2 + 5\,Al + 3\,LiNH_2 \rightarrow Al_2Li_3 + 3\,Ti_3AlN + 12\,H_2$	3.71	35.6
194	$27\,TiH_2 + 13\,Al + 9\,LiNH_2 \rightarrow Al_4Li_9 + 9\,Ti_3AlN + 36\,H_2$	3.81	38.0
195	$2\,TiH_2 + Al + LiNH_2 \rightarrow LiH + Ti_2AlN + 2.5\,H_2$	3.37	-19.3
196	$2\,TiH_2 + 2\,Al + LiNH_2 \rightarrow AlLi + Ti_2AlN + 3\,H_2$	3.42	-1.1
197	$2\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_3Li + Ti_2AlN + 3\,H_2$	2.97	-121.7
198	$2\,TiH_2 + 2\,Al + 3\,LiNH_2 \rightarrow AlLi_3N_2 + Ti_2AlN + 5\,H_2$	4.53	-15.9
199	$3\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_2AlN + LiH + 4\,H_2$ (Al$_2$Ti – SG: Cmmm)	3.18	-89.3
200	$3\,TiH_2 + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_2AlN + LiH + 4\,H_2$ (Al$_2$Ti – SG: I4$_1$/amd)	3.18	-89.6
201	$6\,TiH_2 + 5\,Al + 3\,LiNH_2 \rightarrow Al_2Li_3 + 3\,Ti_2AlN + 9\,H_2$	3.61	1.0
202	$18\,TiH_2 + 13\,Al + 9\,LiNH_2 \rightarrow Al_4Li_9 + 9\,Ti_2AlN + 27\,H_2$	3.74	4.1
203	$4\,TiH_2 + Al + 3\,LiNH_2 \rightarrow 3\,LiH + Ti_4AlN_3 + 5.5\,H_2$	3.75	-37.7
204	$4\,TiH_2 + 4\,Al + 3\,LiNH_2 \rightarrow 3\,AlLi + Ti_4AlN_3 + 7\,H_2$	3.75	-10.3
205	$4\,TiH_2 + 10\,Al + 3\,LiNH_2 \rightarrow 3\,Al_3Li + Ti_4AlN_3 + 7\,H_2$	2.62	-12.7
206	$4\,TiH_2 + 4\,Al + 5\,LiNH_2 \rightarrow 2\,AlLi + AlLi_3N_2 + Ti_4AlN_3 + 9\,H_2$	4.30	-16.5

207	5 TiH$_2$ + 3 Al + 3 LiNH$_2$ → Al$_2$Ti + Ti$_4$AlN$_3$ + 3 LiH + 6.5 H$_2$ (Al$_2$Ti – SG: Cmmm)	3.28	-29.0
208	5 TiH$_2$ + 3 Al + 3 LiNH$_2$ → Al$_2$Ti + Ti$_4$AlN$_3$ + 3 LiH + 6.5 H$_2$ (Al$_2$Ti – SG: I4$_1$/amd)	3.28	-29.2
209	4 TiH$_2$ + 3 Al + 3 LiNH$_2$ → Al$_2$Li$_3$ + Ti$_4$AlN$_3$ + 7 H$_2$	4.04	-7.7
210	12 TiH$_2$ + 7 Al + 9 LiNH$_2$ → Al$_4$Li$_9$ + 3 Ti$_4$AlN$_3$ + 21 H$_2$	4.26	-3.6
211	TiH → Ti + 0.5 H$_2$	2.06	139.7
212	TiH + LiBH$_4$ → LiH + TiB + 2 H$_2$ (TiB – SG: F$\bar{4}$3m)	5.71	166.1 (o) 158.0 (h)
213	TiH + LiBH$_4$ → LiH + TiB + 2 H$_2$ (TiB – SG: Pnma)	5.71	18.2 (o) 10.1 (h)
214	TiH + 2 LiBH$_4$ → 2 LiH + TiB$_2$ + 3.5 H$_2$	7.63	4.5 (o) -4.7 (h)
215	TiH + Si → TiSi + 0.5 H$_2$	1.31	-145.8
216	TiH + 2 Si → TiSi$_2$ + 0.5 H$_2$	0.96	-158.0
217	5 TiH + 3 Si → Ti$_5$Si$_3$ + 2.5 H$_2$	1.53	-88.9
218	5 TiH + 4 Si → Ti$_5$Si$_4$ + 2.5 H$_2$	1.41	-124.5
219	TiH + Al → AlTi + 0.5 H$_2$	1.33	-19.2
220	TiH + 2 Al → Al$_2$Ti + 0.5 H$_2$ (Al$_2$Ti – SG: Cmmm)	0.98	-108.6
221	TiH + 2 Al → Al$_2$Ti + 0.5 H$_2$ (Al$_2$Ti – SG: I4$_1$/amd)	0.98	-111.3
222	TiH + 3 Al → Al$_3$Ti + 0.5 H$_2$	0.78	-169.4
223	3 TiH + Al → AlTi$_3$ + 1.5 H$_2$	1.74	67.2
224	TiH + LiNH$_2$ → LiH + TiN + H$_2$	2.81	-142.4
225	2 TiH + LiNH$_2$ → LiH + Ti$_2$N + 1.5 H$_2$ (Ti$_2$N – SG: I4$_1$/amd)	2.50	-77.6
226	2 TiH + LiNH$_2$ → LiH + Ti$_2$N + 1.5 H$_2$ (Ti$_2$N – SG: P4$_2$/mnm)	2.50	-81.9
227	3 TiH + Al + LiNH$_2$ → LiH + Ti$_3$AlN + 2 H$_2$	2.05	-63.7
228	3 TiH + 2 Al + LiNH$_2$ → AlLi + Ti$_3$AlN + 2.5 H$_2$	2.25	-32.9
229	3 TiH + 3 Al + LiNH$_2$ → Al$_3$Li + Ti$_3$AlN + 2.5 H$_2$	2.01	-177.7
230	3 TiH + 2 Al + 3 LiNH$_2$ → AlLi$_3$N$_2$ + Ti$_3$AlN + 4.5 H$_2$	3.37	-35.3
231	4 TiH + 3 Al + LiNH$_2$ → Al$_2$Ti + Ti$_3$AlN + LiH + 3 H$_2$ (Al$_2$Ti – SG: Cmmm)	2.02	-169.7
232	4 TiH + 3 Al + LiNH$_2$ → Al$_2$Ti + Ti$_3$AlN + LiH + 3 H$_2$ (Al$_2$Ti – SG: I4$_1$/amd)	2.02	-170.1
233	9 TiH + 5 Al + 3 LiNH$_2$ → Al$_2$Li$_3$ + 3 Ti$_3$AlN + 7.5 H$_2$	2.35	-30.5
234	27 TiH + 13 Al + 9 LiNH$_2$ → Al$_4$Li$_9$ + 9 Ti$_3$AlN + 22.5 H$_2$	2.42	-26.7
235	2 TiH + Al + LiNH$_2$ → LiH + Ti$_2$AlN + 1.5 H$_2$	2.05	-129.3
236	2 TiH + 2 Al + LiNH$_2$ → AlLi + Ti$_2$AlN + 2 H$_2$	2.31	-74.4

237	$2\,TiH + 3\,Al + LiNH_2 \rightarrow Al_3Li + Ti_2AlN + 2\,H_2$	2.00	-255.4
238	$2\,TiH + 2\,Al + 3\,LiNH_2 \rightarrow AlLi_3N_2 + Ti_2AlN + 4\,H_2$	3.65	-56.3
239	$3\,TiH + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_2AlN + LiH + 2.5\,H_2\ (Al_2Ti - SG:\ Cmmm)$	2.01	-230.2
240	$3\,TiH + 3\,Al + LiNH_2 \rightarrow Al_2Ti + Ti_2AlN + LiH + 2.5\,H_2\ (Al_2Ti - SG:\ I4_1/amd)$	2.01	-230.8
241	$6\,TiH + 5\,Al + 3\,LiNH_2 \rightarrow Al_2Li_3 + 3\,Ti_2AlN + 6\,H_2$	2.43	-71.4
242	$18\,TiH + 13\,Al + 9\,LiNH_2 \rightarrow Al_4Li_9 + 9\,Ti_2AlN + 18\,H_2$	2.52	-66.6
243	$4\,TiH + Al + 3\,LiNH_2 \rightarrow 3\,LiH + Ti_4AlN_3 + 3.5\,H_2$	2.42	-142.4
244	$4\,TiH + 4\,Al + 3\,LiNH_2 \rightarrow 3\,AlLi + Ti_4AlN_3 + 5\,H_2$	2.71	-72.7
245	$4\,TiH + 10\,Al + 3\,LiNH_2 \rightarrow 3\,Al_3Li + Ti_4AlN_3 + 5\,H_2$	1.89	-76.0
246	$4\,TiH + 4\,Al + 5\,LiNH_2 \rightarrow 2\,AlLi + AlLi_3N_2 + Ti_4AlN_3 + 7\,H_2$	3.37	-62.8
247	$5\,TiH + 3\,Al + 3\,LiNH_2 \rightarrow Al_2Ti + Ti_4AlN_3 + 3\,LiH + 4\,H_2\ (Al_2Ti - SG:\ Cmmm)$	2.05	-138.2
248	$5\,TiH + 3\,Al + 3\,LiNH_2 \rightarrow Al_2Ti + Ti_4AlN_3 + 3\,LiH + 4\,H_2\ (Al_2Ti - SG:\ I4_1/amd)$	2.05	-138.5
249	$4\,TiH + 3\,Al + 3\,LiNH_2 \rightarrow Al_2Li_3 + Ti_4AlN_3 + 5\,H_2$	2.92	-69.0
250	$12\,TiH + 7\,Al + 9\,LiNH_2 \rightarrow Al_4Li_9 + 3\,Ti_4AlN_3 + 15\,H_2$	3.08	-63.3
	Reactions including V		
251	$VH_2 \rightarrow V + H_2$	3.81	63.3
252	$2\,VH_2 \rightarrow V_2H + 1.5\,H_2$ $(V_2H - SG:\ I4_1/amd)$	2.86	57.4
253	$2\,VH_2 \rightarrow V_2H + 1.5\,H_2$ $(V_2H - SG:\ Cm)$	2.86	57.2
254	$VH_2 + 3\,Al \rightarrow Al_3V + H_2$	1.51	-47.0
255	$VH_2 + 10\,Al \rightarrow Al_{10}V + H_2$	0.62	-48.6
256	$3\,VH_2 + Al \rightarrow AlV_3 + 3\,H_2$	3.25	46.6
257	$VH_2 + 2\,Si \rightarrow VSi_2 + H_2$	1.85	-60.9
258	$3\,VH_2 + Si \rightarrow V_3Si + 3\,H_2$	3.23	5.2
259	$6\,VH_2 + 5\,Si \rightarrow V_6Si_5 + 6\,H_2$	2.64	-25.3
260	$VH_2 + LiNH_2 \rightarrow VN + LiH + 1.5\,H_2$	3.98	-5.4
261	$2\,VH_2 + 3\,LiNH_2 \rightarrow 2\,VN + Li_3N + 5\,H_2$	5.77	40.5
262	$4\,VH_2 + 7\,LiNH_2 \rightarrow Li_7N_4V + 3\,VN + 11\,H_2$ $(Li_7N_4V - SG:\ P\overline{4}3n)$	5.95	14.3
263	$4\,VH_2 + 7\,LiNH_2 \rightarrow Li_7N_4V + 3\,VN + 11\,H_2$ $(Li_7N_4V - SG:\ Pa\overline{3})$	5.95	14.1
264	$4\,VH_2 + 7\,LiNH_2 \rightarrow Li_7N_4V + 3\,VN + 11\,H_2$ $(Li_7N_4V - SG:\ P4_2/nmc)$	5.95	14.8
265	$VH_2 + LiBH_4 \rightarrow VB + LiH + 2.5\,H_2$	6.74	11.6 (o) 5.1 (h)
266	$VH_2 + 2\,LiBH_4 \rightarrow VB_2 + 2\,LiH + 4\,H_2$	8.35	25.5 (o)

			17.4 (h)
267	$2\ VH_2 + 3\ LiBH_4 \rightarrow V_2B_3 + 3\ LiH + 6.5\ H_2$	7.65	19.0 (o) 11.5 (h)
268	$3\ VH_2 + 2\ LiBH_4 \rightarrow V_3B_2 + 2\ LiH + 6\ H_2$	5.98	16.3 (o) 10.9 (h)
269	$VH_2 + 4\ LiNH_2 + 3\ LiH \rightarrow Li_7N_4V + 6.5\ H_2$ (Li_7N_4V – SG: $P\bar{4}3n$)	7.77	28.0
270	$VH_2 + 4\ LiNH_2 + 3\ LiH \rightarrow Li_7N_4V + 6.5\ H_2$ (Li_7N_4V – SG: $Pa\bar{3}$)	7.77	27.5
271	$VH_2 + 4\ LiNH_2 + 3\ LiH \rightarrow Li_7N_4V + 6.5\ H_2$ (Li_7N_4V – SG: $P4_2/nmc$)	7.77	28.7
272	$3\ VH_2 + 2\ ScH_2 + 4\ Si \rightarrow Sc_2V_3Si_4 + 5\ H_2$	3.17	-7.7
273	$VH_2 + 3\ CaH_2 + 3\ LiNH_2 \rightarrow Ca_3N_3V + 3\ LiH + 5.5\ H_2$	4.47	35.0
274	$VH_2 + 2\ CaH_2 + 3\ LiNH_2 \rightarrow Ca_2N_3V + 3\ LiH + 4.5\ H_2$	4.40	12.3
	Using V_2H with SG: $I4_1/amd$		
275	$V_2H \rightarrow 2\ V + 0.5\ H_2$	1.94	80.9
276	$V_2H + 6\ Al \rightarrow 2\ Al_3V + 0.5\ H_2$	0.47	-360.1
277	$V_2H + 20\ Al \rightarrow 2\ Al_{10}V + 0.5\ H_2$	0.17	-366.7
278	$3\ V_2H + 2\ Al \rightarrow 2\ AlV_3 + 1.5\ H_2$	1.44	14.0
279	$V_2H + 4\ Si \rightarrow 2\ VSi_2 + 0.5\ H_2$	0.61	-416.0
280	$3\ V_2H + 2\ Si \rightarrow 2\ V_3Si + 1.5\ H_2$	1.43	-151.3
281	$3\ V_2H + 5\ Si \rightarrow V_6Si_5 + 1.5\ H_2$	1.02	-273.5
282	$V_2H + 2\ LiNH_2 \rightarrow 2\ VN + 2\ LiH + 1.5\ H_2$	3.09	-68.2
283	$V_2H + 3\ LiNH_2 \rightarrow 2\ VN + Li_3N + 3.5\ H_2$	5.84	33.3
284	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: $P\bar{4}3n$)	6.09	-1.8
285	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: $Pa\bar{3}$)	6.09	-2.2
286	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: $P4_2/nmc$)	6.09	-1.2
287	$V_2H + 2\ LiBH_4 \rightarrow 2\ VB + 2\ LiH + 3.5\ H_2$	7.39	-8.1 (o) -17.4 (h)
288	$V_2H + 3\ LiBH_4 \rightarrow V_2B_3 + 3\ LiH + 5\ H_2$	8.59	341.7 (o) 331.9 (h)
289	$V_2H + 4\ LiBH_4 \rightarrow 2\ VB_2 + 4\ LiH + 6.5\ H_2$	9.42	-496.1 (o) -506.1 (h)
290	$3\ V_2H + 4\ LiBH_4 \rightarrow 2\ V_3B_2 + 4\ LiH + 7.5\ H_2$	6.22	-8.4 (o) -17.0 (h)
291	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: $P\bar{4}3n$)	8.18	24.2
292	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: $Pa\bar{3}$)	8.18	23.6

293	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: P4$_2$/nmc)	8.18	25.0
294	$3\ V_2H + 4\ ScH_2 + 8\ Si \rightarrow 2\ Sc_2V_3Si_4 + 5.5\ H_2$	2.91	-61.1
	Using V$_2$H with SG: Cm		
295	$V_2H \rightarrow 2\ V + 0.5\ H_2$	1.94	81.6
296	$V_2H + 6\ Al \rightarrow 2\ Al_3V + 0.5\ H_2$	0.47	-359.5
297	$V_2H + 20\ Al \rightarrow 2\ Al_{10}V + 0.5\ H_2$	1.70	-366.1
298	$3\ V_2H + 2\ Al \rightarrow 2\ AlV_3 + 1.5\ H_2$	1.44	14.6
299	$V_2H + 4\ Si \rightarrow 2\ VSi_2 + 0.5\ H_2$	0.61	-415.4
300	$3\ V_2H + 2\ Si \rightarrow 2\ V_3Si + 1.5\ H_2$	1.43	-150.7
301	$3\ V_2H + 5\ Si \rightarrow V_6Si_5 + 1.5\ H_2$	1.02	-272.8
302	$V_2H + 2\ LiNH_2 \rightarrow 2\ VN + 2\ LiH + 1.5\ H_2$	3.09	-68.0
303	$V_2H + 3\ LiNH_2 \rightarrow 2\ VN + Li_3N + 3.5\ H_2$	5.84	33.4
304	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: P$\bar{4}$3n)	6.09	-1.7
305	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: Pa$\bar{3}$)	6.09	-2.1
306	$4\ V_2H + 14\ LiNH_2 \rightarrow 2\ Li_7N_4V + 6\ VN + 16\ H_2$ (Li_7N_4V – SG: P4$_2$/nmc)	6.09	-1.2
307	$V_2H + 2\ LiBH_4 \rightarrow 2\ VB + 2\ LiH + 3.5\ H_2$	7.39	-8.0 (o) -17.7 (h)
308	$V_2H + 3\ LiBH_4 \rightarrow V_2B_3 + 3\ LiH + 5\ H_2$	8.59	341.7 (o) 332.0 (h)
309	$V_2H + 4\ LiBH_4 \rightarrow 2\ VB_2 + 4\ LiH + 6.5\ H_2$	9.42	-496.1 (o) -506.0 (h)
310	$3\ V_2H + 4\ LiBH_4 \rightarrow 2\ V_3B_2 + 4\ LiH + 7.5\ H_2$	6.22	-8.3 (o) -16.9 (h)
311	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: P$\bar{4}$3n)	8.18	24.2
312	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: Pa$\bar{3}$)	8.18	23.6
313	$V_2H + 8\ LiNH_2 + 6\ LiH \rightarrow 2\ Li_7N_4V + 11.5\ H_2$ (Li_7N_4V – SG: P4$_2$/nmc)	8.18	25.0
314	$3\ V_2H + 4\ ScH_2 + 8\ Si \rightarrow 2\ Sc_2V_3Si_4 + 5.5\ H_2$	2.91	-60.9
	Reactions including C		
315	$ScH_2 + C \rightarrow ScC + H_2$	3.42	163.6
316	$2\ ScH_2 + C \rightarrow Sc_2C + 2\ H_2$	3.81	134.4
317	$2\ ScH_2 + 3\ C \rightarrow Sc_2C_3 + 2\ H_2$	3.10	123.6
318	$3\ ScH_2 + 4\ C \rightarrow Sc_3C_4 + 3\ H_2$	3.20	99.0
319	$4\ ScH_2 + 3\ C \rightarrow Sc_4C_3 + 4\ H_2$	3.60	109.8
320	$MgH_2 + 2\ C \rightarrow MgC_2 + H_2$	4.00	173.3
321	$2\ MgH_2 + 3\ C \rightarrow Mg_2C_3 + 2\ H_2$	4.55	93.2
322	$LiNH_2 + C \rightarrow LiCN + H_2$	5.76	119.6
323	$LiBH_4 + C \rightarrow LiBC + 2\ H_2$	11.95	43.6(o)

			35.3(h)
324	$2 LiNH_2 + C \rightarrow Li_2CN_2 + 2 H_2$	6.97	31.4
325	$3 ScH_2 + Al + C \rightarrow Sc_3AlC + 3 H_2$	3.36	101.1
326	$ScH_2 + 3 Al + 3 C \rightarrow ScAl_3C_3 + H_2$	1.23	-68.5
327	$CaH_2 + 2 LiNH_2 + C \rightarrow CaCN_2 + 2 LiH + 2 H_2$	4.03	24.6
328	$MgH_2 + 2 LiNH_2 + C \rightarrow MgCN_2 + 2 LiH + 2 H_2$	4.79	126.5
329	$MgH_2 + 2 LiNH_2 + C \rightarrow Mg(NCN) + 2 LiH + 2 H_2$	4.79	23.8
330	$CaH_2 + 2 LiBH_4 + 2 C \rightarrow CaB_2C_2 + 2 LiH + 4 H_2$	7.35	59.7(o) 51.6(h)
331	$ScH_2 + 2 LiBH_4 + C \rightarrow ScB_2C + 2 LiH + 4 H_2$	7.86	52.9(o) 44.8(h)
332	$ScH_2 + 2 LiBH_4 + 2 C \rightarrow ScB_2C_2 + 2 LiH + 4 H_2$	7.04	52.4(o) 44.3(h)
333	$MgH_2 + 2 LiBH_4 + 2 C \rightarrow MgB_2C_2 + 2 LiH + 4 H_2$	8.59	55.3(o) 47.2(h)
334	$TiH_2 + C \rightarrow TiC + H_2$	3.26	-9.5
335	$2 TiH_2 + C \rightarrow Ti_2C + 2 H_2$	3.61	53.3
336	$8 TiH_2 + 5 C \rightarrow Ti_8C_5 + 8 H_2$	3.51	33.1
337	$3 TiH_2 + Si + 2 C \rightarrow Ti_3SiC_2 + 3 H_2$	3.00	-12.0
338	$3 TiH_2 + Al + 2 C \rightarrow Ti_3AlC_2 + 3 H_2$	3.48	-1.6
339	$TiH + C \rightarrow TiC + 0.5 H_2$	1.66	-164.6
340	$2 TiH + C \rightarrow Ti_2C + H_2$	1.84	-39.1
341	$8 TiH + 5 C \rightarrow Ti_8C_5 + 4 H_2$	1.79	-79.5
342	$3 TiH + Al + C \rightarrow Ti_3AlC + 1.5 H_2$	1.63	-45.4
343	$3 TiH + Si + 2 C \rightarrow Ti_3SiC_2 + 1.5 H_2$	1.52	-169.7
344	$3 TiH + Al + 2 C \rightarrow Ti_3AlC_2 + 1.5 H_2$	1.53	-148.9
345	$VH_2 + C \rightarrow VC + H_2$	3.10	-13.6
346	$2 VH_2 + C \rightarrow V_2C + 2 H_2$	3.42	-1.9
347	$6 VH_2 + 5 C \rightarrow V_6C_5 + 6 H_2$	3.20	-30.8
348	$V_2H + C \rightarrow V_2C + 0.5 H_2$ ($V_2H - SG$: $I4_1/amd$)	1.58	-179.9
349	$V_2H + 2 C \rightarrow 2 VC + 0.5 H_2$ ($V_2H - SG$: $I4_1/amd$)	1.33	-226.8
350	$3 V_2H + 5 C \rightarrow V_6C_5 + 1.5 H_2$ ($V_2H - SG$: $I4_1/amd$)	1.40	-295.5
351	$V_2H + C \rightarrow V_2C + 0.5 H_2$ ($V_2H - SG$: Cm)	4.73	-179.3
352	$V_2H + 2 C \rightarrow 2 VC + 0.5 H_2$ ($V_2H - SG$: Cm)	1.33	-226.2
353	$3 V_2H + 5 C \rightarrow V_6C_5 + 1.5 H_2$ ($V_2H - SG$: Cm)	1.40	-294.9

Table S2: Enthalpy of formation at 0 K for the compounds studied at the energy cutoff of 425 eV. For any compound A_xB_y, the enthalpy of formation is defined as $\Delta H_f = E_{A_xB_y} - xE_A - yE_B$, where $E_{A_xB_y}$, E_A and E_B are the DFT calculated total energies of A_xB_y, **A** and **B** respectively.[1]

Compound	Space Group	ΔH_f (kJ/mol)
$Al_{10}V$	$Fd\overline{3}m$	-111.91
$Al_{12}Mg_{17}$	$I\overline{4}3m$	-114.68
Al_2Ca	$Fd\overline{3}m$	-100.88
$Al_2Ca_3Si_2$	Immm	-302.58
Al_2CaSi_2	$P\overline{3}m1$	-157.98
Al_2Li_3	$R\overline{3}m$	-102.49
Al_2Sc	$Fd\overline{3}mS$	-142.07
Al_2Ti	Cmmm	-124.14
Al_2Ti	$I4_1$/amd	-125.46
Al_3Li	$Pm\overline{3}m$	-45.84
Al_3Sc	$Pm\overline{3}m$	-180.34
Al_3Ti	I4/mmm	-154.53
Al_3V	I4/mmm	-110.26
Al_4Li_9	C2/m	-223.06
AlB_2	P6/mmm	-13.34
AlH_3	$R\overline{3}c$	-16.62
AlLi	$Fd\overline{3}m$	-40.27
$AlLi_3N_2$	$Ia\overline{3}$	-530.27
AlLiSi	$F\overline{4}3m$	-71.29
$AlMg_4Si_6$	C12/m1	110.69
AlN	$P6_3mc$	-287.56
AlSc	$Pm\overline{3}m$	-88.87
$AlSc_2$	$P6_3$/mmc	-103.91
$AlSc_2Si_2$	P4/mbm	-342.00
AlTi	P4/mmm	-79.41
$AlTi_3$	$P6_3$/mmc	-108.66
AlV_3	$Pm\overline{3}n$	-50.23

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[1] Corrections to a number of typographical errors in this table were made to this table in July 2007. We greatly appreciate Prof. C. Ahn and Prof. D. Jenkins, who pointed out these errors. All calculations reported in our paper were performed with the data listed in this corrected table; the incorrect information for some entries of this table that appeared previously was not used in any of the calculated results reported in our paper.

$Ca(AlH_4)_2$	Pbca	-212.11
Ca_2HN	$Fd\overline{3}m$	-318.41
Ca_2LiSi_3	Pnnm	-274.45
Ca_2N	$R\overline{3}m$	-215.91
Ca_2N_3V	C2/c	-718.74
Ca_3AlN_3	$P2_1/c$	-727.36
Ca_3BN_3	P4/mmm	-774.64
Ca_3N_2	$Ia\overline{3}$	-405.47
Ca_3N_3V	Cmcm	-754.56
Ca_5Si_3	I4/mcm	-352.76
CaB_2C_2	$P\overline{4}2c$	-107.42
CaB_2C_2	I4/mcm	-180.77
CaB_6	$Pm\overline{3}m$	-291.60
$CaCN_2$	$R\overline{3}mR$	-366.90
CaH_2	Pnma	-173.15
$CaLi_2$	$P6_3/mmc$	-5.97
$CaLiN$	Pnma	-203.65
$CaLiSi_2$	Pnma	-163.46
$CaMgSi$	Pnma	-134.22
$CaMg_2$	$P6_3/mmc$	-38.00
$CaMg_2N_2$	$P\overline{3}m1$	-428.51
$CaSi$	Cmcm	-99.05
$CaSi_2$	$R\overline{3}mH$	-113.42
$Li_{12}Mg_3Si_4$	$I\overline{4}3d$	-455.05
Li_2CN_2	I4/mmm	-350.73
Li_2Si	C2/m	-250.11
Li_3AlH_6	$R\overline{3}H$	-298.94
Li_3BN_2	$P4_2/mnm$	-520.85
Li_3N	$P6_3/mmc$	-158.51
Li_3ScN_2	$Ia\overline{3}$	-576.78
Li_4BNH_{10}	$I2_13$	-833.26
Li_4NH	$I4_1/a$	-250.67
Li_5N_3Si (10 Si atoms)	$Ia\overline{3}$	-677.74
Li_5N_3Si (11 Si atoms)	$Ia\overline{3}$	-688.11
Li_7N_4V	$P\overline{4}3a$	-964.21
Li_7N_4V	$Pa\overline{3}$	-967.44

Li$_7$N$_4$V	P4$_2$/nmc	-959.56
Li$_7$Si$_2$	Pbam	-198.63
LiAlH$_4$	P2/c	-104.73
LiBC	P6$_3$/mmc	-118.40
LiBH$_4$	Pnma	-208.87
LiBH$_4$	P6$_3$mc	-192.36
LiCN	Pnma	-87.15
LiH	Fm$\overline{3}$m	-85.29
LiMgN	Pnma	-207.46
LiN$_3$	C2/m	-62.70
LiNH$_2$	I$\overline{4}$	-206.77
LiSi	I4$_1$/a	-40.26
Mg(NCN)	R$\overline{3}$mH	-260.02
Mg$_2$C$_3$	Pnnm	56.95
Mg$_2$Si	Fm$\overline{3}$m	-54.25
Mg$_3$BN$_3$	P6$_3$/mmc	-647.14
Mg$_3$N$_2$	Ia$\overline{3}$	-409.28
MgB$_2$	P6/mmm	-46.49
MgB$_2$C$_2$	Cmca	-981.26
MgB$_4$	Pnma	-75.79
MgB$_7$ (Mg$_8$B$_{56}$)	Imma	-109.28
MgB$_7$ (Mg$_7$B$_{56}$)	Imma	-93.59
MgB$_9$N	R$\overline{3}$mH	-433.08
MgC$_2$	P4$_2$/mnm	108.56
MgCN$_2$	I$\overline{4}$2d	-54.58
MgH$_2$	P4$_2$/mnm	-64.68
MgSiN$_2$	Pna2$_1$	-479.67
N(SiH$_3$)$_3$	P$\overline{1}$	-176.35
N$_4$Si$_3$-α	P31c	-768.20
N$_4$Si$_3$-β	P6$_3$/m	-768.89
Na$_3$AlH$_6$	P2$_1$/n	-208.16
NaAlH$_4$	I4$_1$/a	-101.25
NaH	Fm$\overline{3}$m	-43.99
NaMgH$_3$	Pnma	-119.33
NaSi	C2/c	-5.88
Sc$_2$BC$_2$	I4/mmm	-295.61

Sc_2C	$P\bar{3}m1$	-131.04
Sc_2C_3	$I\bar{4}3d$	-152.64
$Sc_2V_3Si_4$	$P4_12_12$	-628.51
Sc_3AlC	$Pm\bar{3}m$	-296.68
Sc_3C_4	$P4/mnc$	-302.81
Sc_4C_3	$I\bar{4}3d$	-360.84
Sc_5Si_3	$P6_3/mcm$	-590.07
$ScAl_3C_3$	$P6_3mc$	-268.46
ScB_{12}	$Fm\bar{3}m$	-272.43
ScB_2	$P6/mmm$	-247.86
ScB_2C	$P4_2/mbc$	-234.95
ScB_2C_2	$Pbam$	-237.08
ScC	$Fm\bar{3}m$	-36.37
ScH_2	$Fm\bar{3}m$	-199.94
ScN	$Fm\bar{3}m$	-387.02
$ScSi$	$Cmcm$	-160.17
$ScSi_2$	$P6/mmm$	-32.01
SiB_6	$Pm3m$	301.99
Ti_2AlN	$P6_3/mmc$	-455.00
Ti_2C	$Fd\bar{3}m$	-178.77
Ti_2N	$I4_1/amd$	-377.59
Ti_2N	$P4_2/mnm$	-383.91
Ti_3AlC	$Pm\bar{3}m$	-277.57
Ti_3AlC_2	$P6_3/mmc$	-432.87
Ti_3AlN	$Pm\bar{3}m$	-458.30
Ti_3SiC_2	$P6_3/mmc$	-463.99
Ti_4AlN_3	$P6_3/mmc$	-1142.13
Ti_5Si_3	$P6_3/mcm$	-571.51
Ti_5Si_4	$P4_12_12$	-660.34
Ti_8C_5	$R\bar{3}mH$	-876.74
TiB	$F\bar{4}3m$	139.10
TiB	$Pnma$	-156.74
TiB_2	$P6/mmm$	-300.58
TiC	$Fm\bar{3}m$	-152.14
TiH	$P4_2/n$	-69.84
TiH_2	$Fm\bar{3}m$	-142.66
TiN	$Fm\bar{3}m$	-333.64

TiSi	Pnma	-142.71
TiSi$_2$	Fddd	-148.82
V$_2$B$_3$	Cmcm	-373.13
V$_2$C	Pbcn	-274.62
V$_2$H	I4$_1$/amd	-40.47
V$_2$H	Cm	-40.77
V$_3$B$_2$	P4/mbm	-338.66
V$_3$Si	Pm$\bar{3}$n	-174.20
V$_6$C$_5$	P3$_1$12	-1285.57
V$_6$Si$_5$	Ibam	-531.53
VB	Cmcm	-157.69
VB$_2$	P6/mmm	-207.95
VC	Fm$\bar{3}$m	-221.13
VH$_2$	Fm$\bar{3}$m	-63.31
VN	Fm$\bar{3}$m	-192.88
VSi$_2$	P6$_4$22	-124.23