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APPENDICES

Appendix A Hydrogen Capacities of Li–B–H Systems

Table A1 Hydrogen capacities of $LiBH_4$ in the 1st cycle of the hydrogen desorption/absorption

Sample	Hydrogen Capacity (wt%)
As-milled $LiBH_4$	2.9
1 mol% TiO_2–$LiBH_4$	2.1
1 mol% $TiCl_3$–$LiBH_4$	3.5
1 mol% VCl_3–$LiBH_4$	3.2
1 mol% $ZrCl_4$–$LiBH_4$	3.5

Table A2 Hydrogen capacities of $LiBH_4$ in the 2nd cycle of the hydrogen desorption/absorption

Sample	Hydrogen Capacity (wt%)
1 mol% TiO_2–$LiBH_4$	1.3
1 mol% $TiCl_3$–$LiBH_4$	1.2
1 mol% VCl_3–$LiBH_4$	2.3
1 mol% $ZrCl_4$–$LiBH_4$	1.5

Table A3 Hydrogen capacities of $LiBH_4$ in the 3rd cycle of the hydrogen desorption/absorption

Sample	Hydrogen Capacity (wt%)
1 mol% TiO_2–$LiBH_4$	1.1
1 mol% $TiCl_3$–$LiBH_4$	1.2
1 mol% VCl_3–$LiBH_4$	0.9
1 mol% $ZrCl_4$–$LiBH_4$	0.9

Appendix B Changed Pressure during the Desorption

Table B1 Changed pressure of as-milled $LiAlH_4$

Temperature (°C)	Pressure (psi)
27.7	0
55.2	0
84.1	0
111.4	0
145.6	2.20
165.5	93.77
178.8	120.90
192.1	138.46
205.2	163.37
221.0	178.75

Table B2 Changed pressure of 1 mol% TiO_2–$LiAlH_4$

Temperature (°C)	Pressure (psi)
27.5	0
54.3	0
81.7	2.20
96.8	7.33
121.9	30.04
134.7	100.37
146.0	124.54
165.9	152.38
181.8	179.49
195.5	186.08

Table B3 Changed pressure of 1 mol% $TiCl_3$–$LiAlH_4$

Temperature (°C)	Pressure (psi)
27.5	0
55.3	0
74.1	1.46
90.7	15.38
121.4	121.4
132.65	120.88
150.5	143.59
164.0	167.33
175.5	178.02
184.6	183.15

Table B4 Changed pressure of 1 mol% VCl_3–$LiAlH_4$

Temperature (°C)	Pressure (psi)
27.5	0
55.7	1.46
71.6	5.86
86.3	15.38
103.9	49.82
128.4	117.95
143.9	135.53
159.4	158.97
175.3	170.70
193.2	175.82

Table B5 Changed pressure of 1 mol% $ZrCl_4$–$LiAlH_4$

Temperature (°C)	Pressure (psi)
27.3	0
55.2	0
81.2	4.4
91.4	40.29
101.8	93.04
108.2	104.76
130.2	136.26
141.3	148.72
150.3	155.31
161.7	158.97

Table B6 Changed pressure of as-milled $LiBH_4$

Temperature (°C)	Pressure (psi)
28.4	0
54.7	0
83.0	1.46
121.1	2.93
159.3	3.66
201.6	5.86
241.8	8.06
281.8	10.25
323.7	41.76
371.6	84.25

Table B7 Changed pressure of 1 mol% TiO_2–$LiBH_4$ in the 1st desorption

Temperature (°C)	Pressure (psi)
27.3	0
55.2	0
81.0	1.46
143.3	5.13
174.7	6.59
210.4	8.06
246.1	10.26
281.5	15.38
321.4	41.03
358.8	71.06

Table B8 Changed pressure of 1 mol% TiO_2–$LiBH_4$ in the 2nd desorption

Temperature (°C)	Pressure (psi)
27.5	0
124.5	0
255.8	1.46
271.4	2.93
289.4	5.13
308.9	7.33
322.8	8.79
341.4	11.72
357.3	16.12
367.4	38.83

Table B9 Changed pressure of 1 mol% TiO_2–$LiBH_4$ in the 3rd desorption

Temperature (°C)	Pressure (psi)
31.0	0
125.8	0
273.0	1.46
286.8	2.93
301.6	4.40
314.1	5.86
328.8	8.06
340.7	9.52
351.6	12.45
360.2	24.18

Table B10 Changed pressure of 1 mol% $TiCl_3$–$LiBH_4$ in the 1st desorption

Temperature (°C)	Pressure (psi)
27.9	0
71.6	1.46
107.3	4.4.0
142.5	6.59
173.8	9.52
200.3	11.72
235.7	13.92
271.2	21.24
307.1	38.83
354.9	83.52

Table B11 Changed pressure of 1 mol% $TiCl_3$–$LiBH_4$ in the 2nd desorption

Temperature (°C)	Pressure (psi)
27.3	0
150.4	0
250.2	0
306.3	1.46
315.6	2.93
322.1	3.66
334.5	5.13
339.7	5.86
347.8	8.06
352.1	30.04

Table B12 Changed pressure of 1 mol% $TiCl_3$–$LiBH_4$ in the 3rd desorption

Temperature (°C)	Pressure (psi)
27.2	0
151.1	0
251.1	0
300.3	1.46
311.0	2.93
317.5	3.66
323.6	4.40
331.3	5.86
340.7	8.06
349.0	17.58

Table B13 Changed pressure of 1 mol% VCl_3–$LiBH_4$ in the 1st desorption

Temperature (°C)	Pressure (psi)
27.2	0
98.6	1.46
133.4	4.40
160.2	6.59
193.4	10.26
226.7	14.65
364.7	18.32
298.0	28.57
332.3	44.69
369.6	79.12

Table B14 Changed pressure of 1 mol% VCl_3–$LiBH_4$ in the 2nd desorption

Temperature (°C)	Pressure (psi)
27.3	0
174.5	1.46
216.1	2.20
234.0	2.93
256.2	3.66
273.8	4.40
294.6	5.86
316.6	8.06
339.1	11.72
356.9	53.48

Table B15 Changed pressure of 1 mol% VCl_3–$LiBH_4$ in the 3rd desorption

Temperature (°C)	Pressure (psi)
27.6	0
150.7	0
283.2	1.46
297.5	2.93
311.9	5.13
323.9	6.59
336.6	8.79
347.5	10.28
361.1	13.19
393.7	28.57

Table B16 Changed pressure of 1 mol% $ZrCl_4$–$LiBH_4$ in the 1st desorption

Temperature (°C)	Pressure (psi)
27.4	0
129.7	1.46
159.1	5.13
188.0	8.06
208.2	10.26
241.8	12.45
268.8	15.38
300.6	31.50
332.2	51.28
373.6	99.63

Table B17 Changed pressure of 1 mol% $ZrCl_4$–$LiBH_4$ in the 2nd desorption

Temperature (°C)	Pressure (psi)
28.0	0
150.8	0
272.9	1.46
283.8	2.93
296.3	4.40
318.2	6.60
333.4	8.79
343.5	11.00
354.0	13.92
366.7	46.15

Table B18 Changed pressure of 1 mol% $ZrCl_4$–$LiBH_4$ in the 3rd desorption

Temperature (°C)	Pressure (psi)
27.6	0
151.3	0
294.8	1.46
306.8	2.20
315.4	3.66
329.0	4.40
341.2	5.13
348.3	6.59
355.2	8.79
360.6	30.04

Table B19 Changed pressure of a 1:1 $LiAlH_4$:$LiBH_4$ molar ratio mixture

Temperature (°C)	Pressure (psi)
27.5	0
107.0	1.46
120.2	5.86
133.8	11.00
147.2	19.78
160.6	33.70
173.5	73.99
186.0	96.70
200.7	111.35
220.1	118.68

Table B20 Changed pressure of a 2:1 $LiAlH_4$:$LiBH_4$ molar ratio mixture

Temperature (°C)	Pressure (psi)
27.5	0
107.1	1.46
120.5	8.06
134.5	27.11
148.1	53.48
161.2	71.79
174.3	89.38
187.6	107.69
201.2	115.75
221.4	120.88

Table B21 Changed pressure of a 3:1 $LiAlH_4$:$LiBH_4$ molar ratio mixture

Temperature (°C)	Pressure (psi)
27.6	0
99.9	1.46
114.5	5.86
127.8	9.52
144.3	16.85
160.1	51.28
175.1	101.83
190.2	133.33
206.0	152.38
221.7	158.24

Table B22 Changed pressure of a 4:1 $LiAlH_4$:$LiBH_4$ molar ratio mixture

Temperature (°C)	Pressure (psi)
27.4	0
108.0	1.46
119.3	3.66
132.2	5.13
146.1	9.52
161.9	42.49
175.0	79.12
190.3	108.42
203.8	116.48
221.8	120.15

Table B23 Changed pressure of a 1:2 $LiAlH_4$:$LiBH_4$ molar ratio mixture

Temperature (°C)	Pressure (psi)
27.7	0
100.8	1.46
116.0	5.86
129.4	11.72
145.4	25.64
161.7	49.08
175.1	65.20
190.9	77.66
204.6	81.32
220.6	82.78

Table B24 Changed pressure of 1 mol% TiO_2–2$LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
29.0	0
104.9	2.20
116.2	20.51
125.5	46.89
135.9	65.20
146.4	79.12
155.1	98.17
166.6	106.23
179.9	109.16
195.4	111.35

Table B25 Changed pressure of 1 mol% VCl_3–2$LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
27.5	0
57.6	1.46
70.4	4.40
82.3	18.31
94.7	39.56
107.5	56.41
120.5	60.81
133.9	68.86
145.0	82.05
156.2	93.04

Table B26 Changed pressure of 1 mol% $ZrCl_4$–2$LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
27.6	0
74.1	1.46
84.1	19.05
94.5	69.60
105.3	76.92
114.1	82.78
125.0	98.17
136.1	116.48
143.1	119.41
152.2	120.88

Table B27 Changed pressure of 1 mol% $TiCl_3$–$2LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
28.7	0
48.4	1,46
64.3	4.40
80.1	15.38
94.8	46.89
110.2	73.99
125.7	87.91
141.2	113.55
159.4	120.15
175.1	123.08

Table B28 Changed pressure of 3 mol% $TiCl_3$–$2LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
27.9	0
62.4	1.46
76.1	17.58
90.7	43.22
114.1	64.47
130.1	82.05
144.0	86.45
155.5	91.58
164.6	94.51
173.7	95.97

Table B29 Changed pressure of 5 mol% $TiCl_3$–$2LiAlH_4$+ $LiBH_4$

Temperature (°C)	Pressure (psi)
27.3	0
47.9	1.46
60.6	5.86
72.7	11.00
96.0	21.98
109.3	36.63
122.8	43.22
134.2	46.15
143.3	47.62
154.6	48.35

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