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(<http://www.ovonic-hydrogen.com/solutions/technology1.htm>)

APPENDICES

Appendix A Calculated Volume of the Manifold and Sample Holder

Table A1 Manifold volume estimated by gas expansion

| Experiment 1 | P initial (psia) | P final (psia) | Volume (cm ³) |
|--------------|---------------------|-------------------|------------------------------|
| 1 | 1458.75 | 1001.25 | 35.07 |
| 2 | 1001.25 | 693.75 | 35.60 |
| 3 | 693.75 | 481.88 | 35.82 |
| 4 | 481.88 | 335.63 | 36.01 |
| 5 | 335.63 | 234.38 | 36.17 |
| 6 | 234.38 | 165.00 | 36.51 |
| 7 | 165.00 | 114.38 | 35.97 |
| Average | | | 35.88 |

| Experiment 2 | P initial (psia) | P final (psia) | Volume (cm ³) |
|--------------|---------------------|-------------------|------------------------------|
| 1 | 1475.63 | 1012.50 | 35.06 |
| 2 | 1012.50 | 699.38 | 35.49 |
| 3 | 699.38 | 485.63 | 35.81 |
| 4 | 485.63 | 339.38 | 36.13 |
| 5 | 339.38 | 236.25 | 36.05 |
| 6 | 236.25 | 165.00 | 36.21 |
| 7 | 165.00 | 116.25 | 36.57 |
| Average | | | 35.90 |

Table A1 Manifold volume estimated by gas expansion

| Experiment 3 | P initial (psia) | P final (psia) | Volume (cm ³) |
|--------------|---------------------|-------------------|------------------------------|
| 1 | 1468.13 | 1006.88 | 35.04 |
| 2 | 1006.88 | 697.5 | 35.59 |
| 3 | 697.50 | 483.75 | 35.76 |
| 4 | 483.75 | 337.50 | 36.07 |
| 5 | 337.50 | 236.25 | 36.25 |
| 6 | 236.25 | 165.00 | 36.21 |
| 7 | 165.00 | 116.25 | 36.57 |
| Average | | | 35.93 |

| Experiment | Volume (cm ³) |
|------------|------------------------------|
| 1 | 35.88 |
| 2 | 35.90 |
| 3 | 35.93 |
| Average | 35.90 |

Table A2 Dead volume of the sample holder

| Experiment | P initial (psia) | P final (psia) | Volume (cm ³) |
|------------|---------------------|-------------------|------------------------------|
| 1 | 504.38 | 241.88 | 43.70 |
| 2 | 500.63 | 241.88 | 43.07 |
| 3 | 502.50 | 243.75 | 42.74 |
| 4 | 504.38 | 247.50 | 41.79 |
| 5 | 504.38 | 243.75 | 43.06 |

Appendix B Hydrogen Capacities of Li-N-H Systems

Table B1 Hydrogen Capacities of LiNH₂ and LiH Mixtures

| 1:1 mol ratio of LiNH ₂ and LiH mixtures | Hydrogen Capacity (wt%) |
|--|-------------------------|
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% TiO ₂ mixed by mortar | 0.50 |
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% Fe mixed by mortar | 0.36 |
| 1:1 mol ratio of LiNH ₂ and LiH mixed by mortar | 0.40 |
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% TiO ₂ mixed by ball milling | 1.50 |
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% ZrCl ₄ mixed by ball milling | 0.78 |
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% Ni mixed by ball milling | 0.76 |
| 1:1 mol ratio of LiNH ₂ and LiH doped with 1 mol% Fe mixed by ball milling | 0.68 |
| 1:1 mol ratio of LiNH ₂ and LiH mixed by ball milling | 0.44 |

Table B2 Hydrogen Capacities of LiNH₂ and LiAlH₄ mixtures

| LiNH ₂ and LiAlH ₄ mixtures | Hydrogen Capacity (wt%) |
|--|-------------------------|
| 1:1 mol ratio of LiNH ₂ and LiAlH ₄ | 2.62 |
| 1:3 mol ratio of LiNH ₂ and LiAlH ₄ | 2.47 |
| 1:5 mol ratio of LiNH ₂ and LiAlH ₄ | 5.19 |
| 1:5 mol ratio of LiNH ₂ and LiAlH ₄ doped with 1 mol% ZrCl ₄ | 6.42 |
| 1:5 mol ratio of LiNH ₂ and LiAlH ₄ doped with 4 mol% ZrCl ₄ | 7.84 |
| 1:5 mol ratio of LiNH ₂ and LiAlH ₄ doped with 4 mol% TiO ₂ | 4.92 |
| Two-layered 1:5 mol ratio of LiNH ₂ and LiAlH ₄ each of which doped with 1 mol% ZrCl ₄ | 8.61 |
| Two-layered 1:5 mol ratio of LiNH ₂ and LiAlH ₄ only LiAlH ₄ doped with 1 mol% ZrCl ₄ | 8.09 |
| Two-layered 1:1 mol ratio of LiNH ₂ and LiAlH ₄ each of which doped with 1 mol% VCl ₃ | 6.16 |
| Two-layered 1:1 mol ratio of LiNH ₂ and LiAlH ₄ each of which doped with 1 mol% ZrCl ₄ | 5.53 |

Appendix C Changes of Pressure during the Dehydrogenation

Table C1 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiH

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 27.7 |
| 3.75 | 67.6 |
| 5.63 | 84.8 |
| 9.38 | 109.8 |
| 15.00 | 132.0 |
| 18.75 | 149.9 |
| 24.38 | 168.7 |
| 31.88 | 199.8 |

Table C2 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiH
doped with 1 mol% Fe

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 42.5 |
| 3.75 | 84.8 |
| 5.63 | 91.5 |
| 9.38 | 112.4 |
| 11.25 | 119.2 |
| 18.75 | 142.5 |
| 24.38 | 153.1 |
| 30.00 | 171.7 |
| 37.50 | 187.6 |
| 41.25 | 191.1 |
| 45.00 | 200.7 |

Table C3 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiH
doped with 1 mol% Ni

| Pressure (psi) | Temperature (°C) |
|----------------|-------------------|
| 0.00 | 31.9 |
| 3.75 | 63.4 |
| 5.63 | 77.6 |
| 9.38 | 91.8 |
| 15.00 | 111.9 |
| 18.75 | 123.7 |
| 22.50 | 140.3 |
| 28.13 | 150.7 |
| 33.75 | 165.1 |
| 39.38 | 178.0 |
| 45.00 | 192.5 |
| 48.75 | 200.3 |

Table C4 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiH
doped with 1 mol% ZrCl₄

| Pressure (psi) | Temperature (°C) |
|----------------|-------------------|
| 0.00 | 58.1 |
| 3.75 | 79.4 |
| 5.63 | 93.9 |
| 9.38 | 108.0 |
| 11.25 | 114.8 |
| 18.75 | 144.9 |
| 24.38 | 175.1 |
| 26.25 | 183.6 |
| 28.13 | 191.4 |
| 30.00 | 200.2 |

Table C5 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiH
doped with 1 mol% TiO₂

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 31.0 |
| 3.75 | 67.7 |
| 5.63 | 74.4 |
| 11.25 | 106.1 |
| 16.88 | 133.8 |
| 22.50 | 163.2 |
| 24.38 | 171.5 |
| 26.25 | 182.8 |
| 30.00 | 200.9 |

Table C6 Pressure Changing of 1:1 Mol Ratio of LiNH₂ and LiAlH₄

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 42.5 |
| 3.75 | 79.6 |
| 5.63 | 91.5 |
| 9.38 | 108.5 |
| 15.00 | 124.0 |
| 18.75 | 134.0 |
| 24.38 | 143.6 |
| 35.63 | 161.3 |
| 50.63 | 182.7 |
| 65.63 | 193.3 |
| 75.00 | 197.4 |
| 78.75 | 199.3 |
| 81.00 | 200.3 |

Table C7 Pressure Changing of 1:3 Mol Ratio of LiNH₂ and LiAlH₄

| Pressure (psi) | Temperature (°C) |
|----------------|-------------------|
| 0.00 | 51.2 |
| 3.75 | 79.8 |
| 5.63 | 85.5 |
| 9.38 | 96.5 |
| 11.25 | 112.7 |
| 18.75 | 133.3 |
| 24.38 | 148.0 |
| 33.75 | 165.9 |
| 50.63 | 187.7 |
| 67.50 | 200.8 |

Table C8 Pressure Changing of 1:5 Mol Ratio of LiNH₂ and LiAlH₄

| Pressure (psi) | Temperature (°C) |
|----------------|-------------------|
| 0.00 | 57.5 |
| 5.63 | 108.3 |
| 11.25 | 127.2 |
| 16.88 | 133.1 |
| 22.50 | 138.9 |
| 31.88 | 144.5 |
| 39.88 | 149.6 |
| 48.75 | 154.5 |
| 60.00 | 159.4 |
| 69.38 | 163.6 |
| 78.75 | 167.8 |
| 86.25 | 171.6 |
| 95.63 | 181.3 |
| 106.88 | 191.1 |
| 114.38 | 196.4 |
| 127.50 | 200.9 |

Table C9 Pressure Changing of 1:5 Mol Ratio of LiNH_2 and LiAlH_4
doped with 1 mol% ZrCl_4

| Pressure (psi) | Temperature ($^{\circ}\text{C}$) |
|----------------|------------------------------------|
| 0.00 | 41.6 |
| 5.63 | 72.6 |
| 9.38 | 81.7 |
| 16.88 | 90.7 |
| 30.00 | 100.1 |
| 46.88 | 109.3 |
| 73.13 | 118.3 |
| 97.50 | 127.3 |
| 108.75 | 136.4 |
| 116.25 | 145.0 |
| 121.88 | 153.2 |
| 129.38 | 161.2 |
| 135.00 | 168.8 |
| 142.50 | 175.8 |
| 153.75 | 182.5 |
| 165.00 | 188.8 |
| 178.13 | 194.2 |
| 193.13 | 199.6 |

Table C10 Pressure Changing of 1:5 Mol Ratio of LiNH_2 and LiAlH_4
doped with 4 mol% ZrCl_4

| Pressure (psi) | Temperature ($^{\circ}\text{C}$) |
|----------------|------------------------------------|
| 0.00 | 44.1 |
| 5.63 | 76.5 |
| 11.25 | 83.1 |
| 16.88 | 89.7 |
| 26.25 | 96.2 |
| 39.38 | 102.5 |
| 52.50 | 108.6 |
| 63.75 | 114.5 |
| 71.25 | 120.3 |
| 80.63 | 131.3 |
| 88.13 | 141.8 |
| 95.63 | 151.8 |
| 103.13 | 161.4 |
| 106.88 | 166.0 |
| 118.13 | 174.6 |
| 127.50 | 182.6 |
| 136.88 | 189.8 |
| 146.25 | 199.4 |

Table C11 Pressure Changing of 1:5 Mol Ratio of LiNH_2 and LiAlH_4
doped with 4 mol% TiO_2

| Pressure (psi) | Temperature ($^{\circ}\text{C}$) |
|----------------|------------------------------------|
| 0.00 | 39.9 |
| 5.63 | 91.6 |
| 15.00 | 108.6 |
| 24.38 | 116.8 |
| 39.38 | 125.1 |
| 52.50 | 133.2 |
| 65.63 | 148.4 |
| 73.13 | 162.3 |
| 88.13 | 185.8 |
| 110.63 | 199.3 |

Table C12 Pressure Changing of two-layered on 1:5 Mol Ratio of
 LiNH_2 and LiAlH_4 each of which doped with 4 mol% ZrCl_4

| Pressure (psi) | Temperature ($^{\circ}\text{C}$) |
|----------------|------------------------------------|
| 0.00 | 44.1 |
| 7.50 | 66.4 |
| 16.88 | 75.7 |
| 28.13 | 85.7 |
| 50.63 | 96.2 |
| 99.38 | 107.4 |
| 180.00 | 118.7 |
| 211.88 | 130.0 |
| 226.88 | 141.0 |
| 260.63 | 162.7 |
| 281.25 | 173.2 |
| 301.88 | 183.0 |
| 318.75 | 192.7 |
| 330.00 | 200.5 |

Table C14 Pressure Changing of two-layered on 1:1 Mol Ratio of
LiNH₂ and LiAlH₄ each of which doped with 4 mol% VCl₃

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 36.3 |
| 5.63 | 60.9 |
| 13.13 | 77.1 |
| 26.25 | 94.4 |
| 54.38 | 112.1 |
| 93.75 | 129.6 |
| 114.38 | 138.0 |
| 131.25 | 146.2 |
| 142.50 | 153.9 |
| 155.63 | 169.0 |
| 168.75 | 182.3 |
| 193.13 | 199.2 |

Table C13 Pressure Changing of two-layered on 1:1 Mol Ratio of
LiNH₂ and LiAlH₄ each of which doped with 4 mol% ZrCl₄

| Pressure (psi) | Temperature (°C) |
|----------------|------------------|
| 0.00 | 36.3 |
| 5.63 | 68.0 |
| 13.13 | 87.0 |
| 28.13 | 109.2 |
| 37.50 | 117.6 |
| 52.50 | 129.0 |
| 69.38 | 145.7 |
| 80.63 | 163.0 |
| 91.88 | 175.5 |
| 101.25 | 181.5 |
| 146.25 | 199.7 |

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