Supporting information for: First-principles study of structural prototypes for NaAlH$_4$: Elevated pressure polymorph in symmetry Fmm2 leads to a single-step decomposition pathway

E.H. Majzoub,* † E. Hazrati,‡ and G.A. de Wijs‡

Center for Nanoscience, and Department of Physics and Astronomy,
University of Missouri – St. Louis, St. Louis, MO 63121, and Radboud University Nijmegen,
Institute for Molecules and Materials Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

E-mail: majzoube@umsl.edu

*To whom correspondence should be addressed  †Center for Nanoscience, and Department of Physics and Astronomy, University of Missouri – St. Louis, St. Louis, MO 63121  ‡Radboud University Nijmegen, Institute for Molecules and Materials Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands
Table S1: Experimentally reported shifts of the line positions for $^{27}\text{Al}$ and $^{23}\text{Na}$ in NaAlH$_4$ (I4$_1$/a), Na$_3$AlH$_6$, NaH, $\alpha$-AlH$_3$, Al and S105. Reported were resonance peak positions referenced to aqueous Al(NO$_3$)$_3$. The field strength in Refs. 1, 2 and 3 were 8.32 T, 11.74 T and 11.7 T respectively.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$^{23}\text{Na}$</th>
<th>$\delta_{\text{Na}}$</th>
<th>$^{27}\text{Al}$</th>
<th>$\delta_{\text{Al}}$</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaAlH$_4$</td>
<td>−9.4 ± 0.2</td>
<td>0.0</td>
<td>95.2 ± 0.5</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>93</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>S105</td>
<td>22.8 ± 0.2</td>
<td>32.2</td>
<td>−42.7 ± 0.3</td>
<td>−137.9</td>
<td>2</td>
</tr>
<tr>
<td>Na$_3$AlH$_6$</td>
<td>−10.2 ± 0.2</td>
<td>−0.8</td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>NaH</td>
<td>18.3 ± 0.2</td>
<td>27.7</td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Al</td>
<td>1639.5 ± 0.5</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>$\alpha$-AlH$_3$</td>
<td>5.5</td>
<td>−89.7</td>
<td></td>
<td></td>
<td>3</td>
</tr>
</tbody>
</table>

Table S2: Calculated isotropic chemical shifts in ppm for $^{27}\text{Al}$ and $^{23}\text{Na}$ for various compounds. Absolute shifts are reported, but the relative shifts $\delta_{\text{Na}}(B_0)$ and $\delta_{\text{Al}}(B_0)$ are referenced to NaAlH$_4$ (I4$_1$/a). The relative shifts also account for the contribution of the second order quadrupole-induced shifts (QIS), as calculated from the electric field gradients (Eq. 2 of Ref. 4). The QIS are dependent on the $B_0$ field, and vanish for $B_0 \rightarrow \infty$. The relative shifts for $B_0 = 11.74$ T can be compared directly with the relative shifts $\delta_{\text{Na}}$ and $\delta_{\text{Al}}$ in Table S1.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$^{23}\text{Na}$</th>
<th>$\delta_{\text{Na}}(B_0)_{B_0 \rightarrow \infty}$</th>
<th>$\delta_{\text{Na}}(B_0)_{B_0 = 11.74}$</th>
<th>$^{27}\text{Al}$</th>
<th>$\delta_{\text{Al}}(B_0)_{B_0 \rightarrow \infty}$</th>
<th>$\delta_{\text{Al}}(B_0)_{B_0 = 11.74}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaAlH$_4$ (I4$_1$/a)</td>
<td>−566.67</td>
<td>0.0</td>
<td>0.0</td>
<td>−467.45</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Na$_3$AlH$_6$ (P2$_1$)</td>
<td>−528.74</td>
<td>37.92</td>
<td>38.21</td>
<td>−609.53</td>
<td>−142.09</td>
<td>−139.52</td>
</tr>
<tr>
<td></td>
<td>−567.10</td>
<td>−0.44</td>
<td>−1.38</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NaH (Fm$\bar{3}$m)</td>
<td>−537.54</td>
<td>29.12</td>
<td>30.35</td>
<td>−565.07</td>
<td>−97.62</td>
<td>−94.46</td>
</tr>
<tr>
<td>$\alpha$-AlH$_3$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table S3: PBE absolute isotropic all-electron chemical shifts in ppm of some small molecules calculated with VASP and the quantum-chemical code DALTON$^5$ (GIAO/aug-cc-pCVQZ).

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Symmetry</th>
<th>VASP</th>
<th>Q-CHEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlH$_3$</td>
<td>D$_{3h}$</td>
<td>−258.98</td>
<td>−251.77</td>
</tr>
<tr>
<td>Al$_2$H$_6$</td>
<td>O$_h$</td>
<td>−408.22</td>
<td>−406.38</td>
</tr>
<tr>
<td>(AlH$_4$)$^-$</td>
<td>T$_d$</td>
<td>−484.12</td>
<td>−480.72</td>
</tr>
</tbody>
</table>

Table S4: Structure prototypes for NaAlH$_4$ at $T = 0$ K containing tetrahedral AlH$_4$ units and their relative total energies $\Delta E$ and zero-point vibrational energies (ZPE).

<table>
<thead>
<tr>
<th>Prototype</th>
<th>Space Group</th>
<th>$\Delta E$ kJ/mol</th>
<th>ZPE meV/f.u.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaAlH$_4$</td>
<td>I$_4$/a</td>
<td>0.00</td>
<td>796</td>
</tr>
<tr>
<td>R2-n199</td>
<td>P21/m</td>
<td>3.42</td>
<td>766</td>
</tr>
<tr>
<td>R2-n160</td>
<td>P21</td>
<td>4.93</td>
<td>772</td>
</tr>
<tr>
<td>R3-n172</td>
<td>P-4</td>
<td>5.04</td>
<td>790</td>
</tr>
<tr>
<td>R3-n139</td>
<td>I222</td>
<td>6.05</td>
<td>795</td>
</tr>
<tr>
<td>R2-n159</td>
<td>*Cmcm</td>
<td>7.61</td>
<td>770</td>
</tr>
<tr>
<td>R2-n111</td>
<td>Pmn21</td>
<td>8.14</td>
<td>772</td>
</tr>
<tr>
<td>R3-n142</td>
<td>Fmm2</td>
<td>8.17</td>
<td>774</td>
</tr>
<tr>
<td>R2-n48</td>
<td>Pm</td>
<td>8.32</td>
<td>776</td>
</tr>
<tr>
<td>R3-n170</td>
<td>C2</td>
<td>8.53</td>
<td>775</td>
</tr>
<tr>
<td>R2-n146</td>
<td>P4nbm</td>
<td>8.94</td>
<td>792</td>
</tr>
<tr>
<td>R2-n121</td>
<td>Cc</td>
<td>9.02</td>
<td>779</td>
</tr>
<tr>
<td>R2-n140</td>
<td>Ama2</td>
<td>9.08</td>
<td>775</td>
</tr>
<tr>
<td>R2-n127</td>
<td>C2m</td>
<td>9.12</td>
<td>778</td>
</tr>
<tr>
<td>R3-n187</td>
<td>Cm</td>
<td>9.13</td>
<td>783</td>
</tr>
<tr>
<td>R3-n144</td>
<td>C2</td>
<td>9.34</td>
<td>785</td>
</tr>
<tr>
<td>R3-n103</td>
<td>Cm</td>
<td>9.67</td>
<td>777</td>
</tr>
<tr>
<td>R2-n23</td>
<td>Cc</td>
<td>9.73</td>
<td>786</td>
</tr>
<tr>
<td>R2-n107</td>
<td>I-42m</td>
<td>10.03</td>
<td>771</td>
</tr>
<tr>
<td>R1-n104</td>
<td>I-42m</td>
<td>10.04</td>
<td>771</td>
</tr>
<tr>
<td>R1-n197</td>
<td>Fmm2</td>
<td>10.13</td>
<td>774</td>
</tr>
<tr>
<td>R2-n172</td>
<td>Fdd2</td>
<td>10.18</td>
<td>774</td>
</tr>
<tr>
<td>R2-n165</td>
<td>C2221</td>
<td>10.36</td>
<td>783</td>
</tr>
<tr>
<td>R3-n181</td>
<td>Cm</td>
<td>12.02</td>
<td>774</td>
</tr>
<tr>
<td>R2-n138</td>
<td>C2</td>
<td>15.20</td>
<td>772</td>
</tr>
<tr>
<td>R2-n129</td>
<td>P21</td>
<td>18.46</td>
<td>755</td>
</tr>
</tbody>
</table>

*Identical to the Wood-Marzari Cmcm structure (Ref. 6)
Table S5: NMR parameters of structure prototypes for NaAlH₄ containing tetrahedral AlH₄ units. \( \delta_{Na} \) and \( \delta_{Al} \): relative chemical shifts. \( \delta_{QIS}^{Al}(B_0) \): relative shifts including the second order quadrupole-induced shifts calculated from the electric field gradients (Eq. 2 of Ref. 4). \( V_{zz}, \eta \): electric field gradients, converted to \( C_q \) using the Al quadrupole moment of Ref. 7.

<table>
<thead>
<tr>
<th>Prototype</th>
<th>Space Group</th>
<th>( \delta_{Na} ) ppm</th>
<th>( \delta_{Al} ) ppm</th>
<th>( \delta_{QIS}^{Al}(20.0 \text{T}) ) ppm</th>
<th>( \delta_{QIS}^{Al}(8.32 \text{T}) ) ppm</th>
<th>( V_{zz}[\text{Al}] ) V/Å²</th>
<th>( C_q[\text{Al}] ) MHz</th>
<th>( \eta[\text{Al}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaAlH4</td>
<td>I4/m</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>8.4</td>
<td>3.0</td>
<td>0.00</td>
</tr>
<tr>
<td>R2-n199</td>
<td>P21/m</td>
<td>0.99</td>
<td>11.97</td>
<td>12.26</td>
<td>13.67</td>
<td>−7.2</td>
<td>−2.6</td>
<td>0.05</td>
</tr>
<tr>
<td>R2-n160</td>
<td>P21</td>
<td>4.27</td>
<td>13.13</td>
<td>13.85</td>
<td>17.33</td>
<td>4.7</td>
<td>1.7</td>
<td>0.46</td>
</tr>
<tr>
<td>R3-n172</td>
<td>P-4</td>
<td>1.46</td>
<td>−5.32</td>
<td>−5.53</td>
<td>−6.54</td>
<td>9.2</td>
<td>3.3</td>
<td>0.00</td>
</tr>
<tr>
<td>R3-n139</td>
<td>I222</td>
<td>−1.36</td>
<td>8.48</td>
<td>7.53</td>
<td>2.98</td>
<td>−11.4</td>
<td>−4.0</td>
<td>0.30</td>
</tr>
<tr>
<td>R2-n159</td>
<td>*Cmcm</td>
<td>0.42</td>
<td>12.47</td>
<td>12.81</td>
<td>14.45</td>
<td>−6.4</td>
<td>−2.3</td>
<td>0.74</td>
</tr>
<tr>
<td>R2-n111</td>
<td>Pmn21</td>
<td>5.51</td>
<td>12.80</td>
<td>12.88</td>
<td>13.30</td>
<td>7.9</td>
<td>2.8</td>
<td>0.40</td>
</tr>
<tr>
<td>R3-n142</td>
<td>Fmm2</td>
<td>1.26</td>
<td>12.67</td>
<td>12.93</td>
<td>14.16</td>
<td>−7.1</td>
<td>−2.5</td>
<td>0.44</td>
</tr>
<tr>
<td>R2-n48</td>
<td>Pm</td>
<td>1.41</td>
<td>19.14</td>
<td>19.19</td>
<td>19.45</td>
<td>7.9</td>
<td>2.6</td>
<td>0.48</td>
</tr>
<tr>
<td>R3-n170</td>
<td>C2</td>
<td>7.40</td>
<td>12.06</td>
<td>12.40</td>
<td>14.03</td>
<td>6.9</td>
<td>2.4</td>
<td>0.32</td>
</tr>
<tr>
<td>R2-n146</td>
<td>P4nbm</td>
<td>7.08</td>
<td>5.60</td>
<td>3.15</td>
<td>−8.56</td>
<td>−15.2</td>
<td>−5.4</td>
<td>0.02</td>
</tr>
<tr>
<td>R2-n121</td>
<td>Cc</td>
<td>1.57</td>
<td>11.44</td>
<td>10.97</td>
<td>8.72</td>
<td>−8.9</td>
<td>−3.1</td>
<td>0.94</td>
</tr>
<tr>
<td>R2-n140</td>
<td>Ama2</td>
<td>0.99</td>
<td>10.44</td>
<td>10.77</td>
<td>12.35</td>
<td>7.0</td>
<td>2.5</td>
<td>0.25</td>
</tr>
<tr>
<td>R2-n127</td>
<td>C2m</td>
<td>0.98</td>
<td>12.33</td>
<td>12.23</td>
<td>11.75</td>
<td>8.6</td>
<td>3.1</td>
<td>0.34</td>
</tr>
<tr>
<td>R3-n187</td>
<td>Cm</td>
<td>3.78</td>
<td>14.15</td>
<td>13.81</td>
<td>12.17</td>
<td>−9.6</td>
<td>−3.4</td>
<td>0.25</td>
</tr>
<tr>
<td>R3-n144</td>
<td>C2</td>
<td>6.75</td>
<td>7.90</td>
<td>8.28</td>
<td>10.07</td>
<td>6.1</td>
<td>2.2</td>
<td>0.84</td>
</tr>
<tr>
<td>R3-n103</td>
<td>Cm</td>
<td>5.22</td>
<td>12.79</td>
<td>13.30</td>
<td>15.70</td>
<td>5.7</td>
<td>2.0</td>
<td>0.70</td>
</tr>
<tr>
<td>R2-n23</td>
<td>Cc</td>
<td>8.66</td>
<td>8.57</td>
<td>8.03</td>
<td>5.44</td>
<td>−9.5</td>
<td>−3.4</td>
<td>0.75</td>
</tr>
<tr>
<td>R2-n107</td>
<td>I-42m</td>
<td>0.43</td>
<td>8.56</td>
<td>9.50</td>
<td>13.97</td>
<td>−3.1</td>
<td>−1.1</td>
<td>0.00</td>
</tr>
<tr>
<td>R1-n104</td>
<td>I-42m</td>
<td>0.31</td>
<td>8.48</td>
<td>9.40</td>
<td>13.76</td>
<td>−3.4</td>
<td>−1.2</td>
<td>0.00</td>
</tr>
<tr>
<td>R1-n197</td>
<td>Fmm2</td>
<td>0.48</td>
<td>8.64</td>
<td>9.61</td>
<td>14.23</td>
<td>−2.8</td>
<td>−1.0</td>
<td>0.02</td>
</tr>
<tr>
<td>R2-n172</td>
<td>Fdd2</td>
<td>12.57</td>
<td>5.00</td>
<td>3.46</td>
<td>−3.93</td>
<td>12.7</td>
<td>4.5</td>
<td>0.46</td>
</tr>
<tr>
<td>R2-n165</td>
<td>C2221</td>
<td>3.98</td>
<td>7.12</td>
<td>7.44</td>
<td>8.97</td>
<td>−6.2</td>
<td>−2.2</td>
<td>0.95</td>
</tr>
<tr>
<td>R3-n181</td>
<td>Cm</td>
<td>9.00</td>
<td>7.42</td>
<td>5.96</td>
<td>−1.05</td>
<td>12.5</td>
<td>4.4</td>
<td>0.47</td>
</tr>
<tr>
<td>R2-n138</td>
<td>C2</td>
<td>5.79</td>
<td>11.80</td>
<td>10.96</td>
<td>6.94</td>
<td>10.0</td>
<td>3.5</td>
<td>0.90</td>
</tr>
<tr>
<td>R2-n129</td>
<td>P21</td>
<td>22.66</td>
<td>4.26</td>
<td>5.28</td>
<td>10.19</td>
<td>−1.8</td>
<td>−6.6</td>
<td>0.90</td>
</tr>
</tbody>
</table>

*Identical to the Wood-Marzari Cmcm structure (Ref. 6)
Table S6: Energy ordering of structures ($F = E - TS$) at $T = 10$ K and $T = 360$ K. Assuming there is no Fmm2 phase, 360 K is the predicted critical temperature of the first decomposition step to Na$_3$AlH$_6$ at an overpressure of about 5 bar H$_2$.

<table>
<thead>
<tr>
<th>Prototype</th>
<th>Space Group</th>
<th>$\Delta F$ (kJ/mol)</th>
<th>$\rho$ (g/cc)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T = 10$ K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NaAlH$_4$</td>
<td>I4-1/a</td>
<td>0.0000</td>
<td>1.2995</td>
</tr>
<tr>
<td>R2-n199</td>
<td>P21/m</td>
<td>0.5555</td>
<td>1.1326</td>
</tr>
<tr>
<td>R2-n160</td>
<td>Pmn21</td>
<td>2.6526</td>
<td>1.1367</td>
</tr>
<tr>
<td>R3-n78</td>
<td>Cm</td>
<td>2.8716</td>
<td>1.1598</td>
</tr>
<tr>
<td>R3-n172</td>
<td>P-4</td>
<td>4.4855</td>
<td>1.2465</td>
</tr>
<tr>
<td>R2-n41</td>
<td>Cmcm</td>
<td>4.7246</td>
<td>1.1113</td>
</tr>
<tr>
<td>R2-n126</td>
<td>Cmcm</td>
<td>4.7254</td>
<td>1.1091</td>
</tr>
<tr>
<td>R2-n150</td>
<td>Cmcm</td>
<td>4.7589</td>
<td>1.1104</td>
</tr>
<tr>
<td>R2-n197</td>
<td>Cmcm</td>
<td>4.7673</td>
<td>1.1112</td>
</tr>
<tr>
<td>NaAlH$_4$-Cmcm</td>
<td>*Cmcm</td>
<td>5.0332</td>
<td>1.1048</td>
</tr>
<tr>
<td></td>
<td>$T = 360$ K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R3-n142</td>
<td>Fmm2</td>
<td>0.0000</td>
<td>1.1211</td>
</tr>
<tr>
<td>R3-n41</td>
<td>Fmm2</td>
<td>1.1412</td>
<td>1.1197</td>
</tr>
<tr>
<td>NaAlH$_4$</td>
<td>I4-1/a</td>
<td>1.1702</td>
<td>1.2995</td>
</tr>
<tr>
<td>R3-n175</td>
<td>Fmm2</td>
<td>1.2162</td>
<td>1.1195</td>
</tr>
<tr>
<td>NaAlH$_4$-Cmcm</td>
<td>*Cmcm</td>
<td>1.2915</td>
<td>1.1048</td>
</tr>
<tr>
<td>R3-n91</td>
<td>C2</td>
<td>1.3313</td>
<td>1.1034</td>
</tr>
<tr>
<td>R2-n199</td>
<td>P21/m</td>
<td>1.5772</td>
<td>1.1326</td>
</tr>
<tr>
<td>R2-n172</td>
<td>Fdd2</td>
<td>2.2281</td>
<td>0.9181</td>
</tr>
<tr>
<td>R2-n186</td>
<td>Fdd2</td>
<td>2.2866</td>
<td>0.9185</td>
</tr>
<tr>
<td>R3-n164</td>
<td>Cm</td>
<td>3.1307</td>
<td>1.1180</td>
</tr>
</tbody>
</table>

*Identical to the Wood-Marzari Cmcm structure (Ref. 6)
Table S7: All NaAlH₄ candidates with tetrahedral [AlH₄]⁻ structures are given below in ICSD format. The cell parameters are given as \(a, b, c, \alpha, \beta, \gamma\) in units of Å and degrees. The atom positions are fractional coordinates in \(x, y, z\).

<table>
<thead>
<tr>
<th>Structure label</th>
<th>C</th>
<th>(a) (Å)</th>
<th>(b) (Å)</th>
<th>(c) (Å)</th>
<th>(\alpha) (deg)</th>
<th>(\beta) (deg)</th>
<th>(\gamma) (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1-n104-I-42m.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>4.99990</td>
<td>4.99990</td>
<td>6.29473</td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
</tr>
<tr>
<td>A H1</td>
<td></td>
<td>0.813050</td>
<td>0.186950</td>
<td>0.652210</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td></td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td></td>
<td>0.0</td>
<td>0.0</td>
<td>0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1-n110-C2.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>8.07213</td>
<td>4.98705</td>
<td>6.32871</td>
<td>90.0</td>
<td>38.05023</td>
<td>90.0</td>
</tr>
<tr>
<td>A H1</td>
<td></td>
<td>0.688690</td>
<td>0.60980</td>
<td>0.461540</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td></td>
<td>0.187650</td>
<td>0.734960</td>
<td>0.160280</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td></td>
<td>0.0</td>
<td>0.923920</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td></td>
<td>0.0</td>
<td>0.922870</td>
<td>0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1-n140-Cm.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>9.90770</td>
<td>6.10813</td>
<td>5.57822</td>
<td>90.0</td>
<td>123.11984</td>
<td>90.0</td>
</tr>
<tr>
<td>A H1</td>
<td></td>
<td>0.630760</td>
<td>0.50</td>
<td>0.947190</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td></td>
<td>0.494240</td>
<td>0.50</td>
<td>0.387560</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H3</td>
<td></td>
<td>0.767810</td>
<td>0.283330</td>
<td>0.720220</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td></td>
<td>0.409460</td>
<td>0.50</td>
<td>0.939320</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td></td>
<td>0.666130</td>
<td>0.50</td>
<td>0.694740</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1-n197-Fmm2.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>7.05118</td>
<td>7.04847</td>
<td>6.32801</td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
</tr>
<tr>
<td>A H1</td>
<td></td>
<td>0.187740</td>
<td>0.50</td>
<td>0.524630</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td></td>
<td>0.50</td>
<td>0.687850</td>
<td>0.722720</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td></td>
<td>0.50</td>
<td>0.50</td>
<td>0.374050</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td></td>
<td>0.50</td>
<td>0.50</td>
<td>0.873660</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>R2-n107-I-42m.fsym.icsd</td>
<td>R2-n111-Pmn21.fsym.icsd</td>
<td>R2-n121-Cc.fsym.icsd</td>
<td>R2-n127-C2m.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------------</td>
<td>-------------------------</td>
<td>-------------------------</td>
<td>----------------------</td>
<td>-----------------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>A H1</td>
<td>A Na1</td>
<td>A Al1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.99081</td>
<td>0.812620</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.99081</td>
<td>0.187380</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.31024</td>
<td>0.348310</td>
<td>0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H1</td>
<td>0.812620</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Na1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Al1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.88173</td>
<td>0.1120</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.88173</td>
<td>0.578630</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.88173</td>
<td>0.513210</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.88173</td>
<td>0.916050</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.88173</td>
<td>0.442650</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H1</td>
<td>0.50</td>
<td>0.184840</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H2</td>
<td>0.307660</td>
<td>0.29330</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H3</td>
<td>0.50</td>
<td>0.82110</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Na1</td>
<td>0.50</td>
<td>0.604290</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Al1</td>
<td>0.50</td>
<td>0.142020</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.93257</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.93257</td>
<td>0.578630</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.93257</td>
<td>0.513210</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.93257</td>
<td>0.916050</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.93257</td>
<td>0.442650</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H1</td>
<td>0.917170</td>
<td>0.49450</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H2</td>
<td>0.234310</td>
<td>0.586570</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H3</td>
<td>0.98070</td>
<td>0.83840</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H4</td>
<td>0.093590</td>
<td>0.785450</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Na1</td>
<td>0.897920</td>
<td>0.160810</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Al1</td>
<td>0.04990</td>
<td>0.672050</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.763390</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.47460</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.521410</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.848260</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.718270</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6.74382</td>
<td>0.649160</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.84288</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.84288</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.84288</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.84288</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>66.84288</td>
<td>90.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H1</td>
<td>0.65720</td>
<td>0.50</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H2</td>
<td>0.15120</td>
<td>0.819970</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A H3</td>
<td>0.898740</td>
<td>0.50</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Na1</td>
<td>0.0</td>
<td>0.756010</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A Al1</td>
<td>0.714150</td>
<td>0.50</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.75025</td>
<td>0.233130</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.75025</td>
<td>0.704460</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.75025</td>
<td>0.721810</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.75025</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4.75025</td>
<td>0.5890</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R2-n129-P21.fsym.icsd</td>
<td>C</td>
<td>5.82016</td>
<td>9.81733</td>
<td>5.48658</td>
<td>90.0</td>
<td>62.48256</td>
<td>90.0</td>
</tr>
<tr>
<td>-----------------------</td>
<td>---</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>-------</td>
<td>----------</td>
<td>-------</td>
</tr>
<tr>
<td>A H1</td>
<td>0.982850</td>
<td>0.525620</td>
<td>0.506430</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td>0.651020</td>
<td>0.551960</td>
<td>0.301460</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H3</td>
<td>0.482810</td>
<td>0.471480</td>
<td>0.813710</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H4</td>
<td>0.63940</td>
<td>0.726520</td>
<td>0.677940</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td>0.355670</td>
<td>0.439940</td>
<td>0.247240</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td>0.690830</td>
<td>0.569740</td>
<td>0.574330</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R2-n138-C2.fsym.icsd</th>
<th>C</th>
<th>11.93810</th>
<th>4.79994</th>
<th>8.95182</th>
<th>90.0</th>
<th>44.88211</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A H1</td>
<td>0.927330</td>
<td>0.648620</td>
<td>0.206120</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td>0.822640</td>
<td>0.193620</td>
<td>0.187460</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H3</td>
<td>0.749580</td>
<td>0.664240</td>
<td>0.120920</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H4</td>
<td>0.615620</td>
<td>0.55030</td>
<td>0.509750</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td>0.450880</td>
<td>0.545420</td>
<td>0.853990</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td>0.775640</td>
<td>0.521770</td>
<td>0.261240</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R2-n140-Ama2.fsym.icsd</th>
<th>C</th>
<th>4.81943</th>
<th>7.97459</th>
<th>4.82184</th>
<th>90.0</th>
<th>116.64556</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A H1</td>
<td>0.189310</td>
<td>0.50</td>
<td>0.598590</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td>0.647110</td>
<td>0.669320</td>
<td>0.325270</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H3</td>
<td>0.785210</td>
<td>0.50</td>
<td>0.832930</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H4</td>
<td>0.304460</td>
<td>0.0</td>
<td>0.481090</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H5</td>
<td>0.539410</td>
<td>0.0</td>
<td>0.077420</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H6</td>
<td>0.031480</td>
<td>0.830660</td>
<td>0.939050</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td>0.521580</td>
<td>0.25050</td>
<td>0.8150</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td>0.821090</td>
<td>0.50</td>
<td>0.510540</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al2</td>
<td>0.216680</td>
<td>0.0</td>
<td>0.113130</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R2-n146-P4nbm.fsym.icsd</th>
<th>C</th>
<th>5.43599</th>
<th>5.43979</th>
<th>4.65884</th>
<th>90.0</th>
<th>90.0</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A H1</td>
<td>0.165770</td>
<td>0.334560</td>
<td>0.356730</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A H2</td>
<td>0.165860</td>
<td>0.665330</td>
<td>0.910870</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Na1</td>
<td>0.50</td>
<td>0.50</td>
<td>0.633760</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A Al1</td>
<td>0.0</td>
<td>0.50</td>
<td>0.133770</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

S8
<table>
<thead>
<tr>
<th>Structure</th>
<th>Atomic Positions</th>
<th>Lattice Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>R2-n159-Cmcm.fsym.icsd</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>7.07736</td>
<td>6.47337</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.314310</td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.50</td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.50</td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.50</td>
</tr>
<tr>
<td>R2-n160-P21.fsym.icsd</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>6.82994</td>
<td>4.90750</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.249420</td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.442280</td>
</tr>
<tr>
<td>A</td>
<td>H3</td>
<td>0.05990</td>
</tr>
<tr>
<td>A</td>
<td>H4</td>
<td>0.249870</td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.24880</td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.250580</td>
</tr>
<tr>
<td>R2-n165-C2221.fsym.icsd</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.16966</td>
<td>8.11419</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.638570</td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.77320</td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.50</td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.960120</td>
</tr>
<tr>
<td>R2-n172-Fdd2.fsym.icsd</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>12.86313</td>
<td>5.92218</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.414060</td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.445410</td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.750</td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.50</td>
</tr>
<tr>
<td></td>
<td>R2-n199-P21m.fsym.icsd</td>
<td></td>
</tr>
<tr>
<td>----------</td>
<td>------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>C</td>
<td>7.09028</td>
<td>4.91202</td>
</tr>
<tr>
<td>A H1</td>
<td>0.250170</td>
<td>0.174290</td>
</tr>
<tr>
<td>A H2</td>
<td>0.433320</td>
<td>0.692760</td>
</tr>
<tr>
<td>A H3</td>
<td>0.249910</td>
<td>0.822340</td>
</tr>
<tr>
<td>A H4</td>
<td>0.06690</td>
<td>0.693290</td>
</tr>
<tr>
<td>A Na1</td>
<td>0.75030</td>
<td>0.641170</td>
</tr>
<tr>
<td>A Al1</td>
<td>0.250110</td>
<td>0.848360</td>
</tr>
<tr>
<td></td>
<td>R2-n23-Cc.fsym.icsd</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>8.08816</td>
<td>5.27948</td>
</tr>
<tr>
<td>A H1</td>
<td>0.791810</td>
<td>0.765110</td>
</tr>
<tr>
<td>A H2</td>
<td>0.143270</td>
<td>0.658670</td>
</tr>
<tr>
<td>A H3</td>
<td>0.798730</td>
<td>0.786230</td>
</tr>
<tr>
<td>A H4</td>
<td>0.972240</td>
<td>0.103490</td>
</tr>
<tr>
<td>A Na1</td>
<td>0.605580</td>
<td>0.538420</td>
</tr>
<tr>
<td>A Al1</td>
<td>0.293030</td>
<td>0.45430</td>
</tr>
<tr>
<td></td>
<td>R2-n48-Pm.fsym.icsd</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.95449</td>
<td>7.85664</td>
</tr>
<tr>
<td>A H1</td>
<td>0.213810</td>
<td>0.50</td>
</tr>
<tr>
<td>A H2</td>
<td>0.831060</td>
<td>0.327320</td>
</tr>
<tr>
<td>A H3</td>
<td>0.645310</td>
<td>0.50</td>
</tr>
<tr>
<td>A H4</td>
<td>0.269390</td>
<td>0.172240</td>
</tr>
<tr>
<td>A H5</td>
<td>0.160920</td>
<td>0.0</td>
</tr>
<tr>
<td>A H6</td>
<td>0.756780</td>
<td>0.0</td>
</tr>
<tr>
<td>A Na1</td>
<td>0.44890</td>
<td>0.249290</td>
</tr>
<tr>
<td>A Al1</td>
<td>0.869880</td>
<td>0.50</td>
</tr>
<tr>
<td>A Al2</td>
<td>0.107960</td>
<td>0.0</td>
</tr>
</tbody>
</table>

S10
### R3-n103-Cm.fsym.icsd

<table>
<thead>
<tr>
<th>C</th>
<th>6.75196</th>
<th>20.55122</th>
<th>4.85912</th>
<th>90.0</th>
<th>134.50797</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>H1 0.997150</td>
<td>0.063160</td>
<td>0.408220</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2 0.434130</td>
<td>0.50</td>
<td>0.867340</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3 0.027010</td>
<td>0.50</td>
<td>0.830110</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H4 0.988090</td>
<td>0.731710</td>
<td>0.338880</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H5 0.03750</td>
<td>0.603940</td>
<td>0.329680</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H6 0.913490</td>
<td>0.663150</td>
<td>0.727020</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H7 0.021830</td>
<td>0.163710</td>
<td>0.961650</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1 0.847760</td>
<td>0.50</td>
<td>0.079920</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2 0.846450</td>
<td>0.834390</td>
<td>0.345990</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1 0.363490</td>
<td>0.50</td>
<td>0.124310</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2 0.855970</td>
<td>0.665280</td>
<td>0.341250</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### R3-n139-I222.fsym.icsd

<table>
<thead>
<tr>
<th>C</th>
<th>17.37998</th>
<th>4.75424</th>
<th>5.24636</th>
<th>90.0</th>
<th>90.0</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>H1 0.446750</td>
<td>0.213240</td>
<td>0.828990</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2 0.605420</td>
<td>0.752220</td>
<td>0.35230</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3 0.209850</td>
<td>0.348160</td>
<td>0.208410</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1 0.1650</td>
<td>0.0</td>
<td>0.50</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2 0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1 0.50</td>
<td>0.0</td>
<td>0.0</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2 0.153090</td>
<td>0.50</td>
<td>0.0</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### R3-n142-Fmm2.fsym.icsd

<table>
<thead>
<tr>
<th>C</th>
<th>7.07137</th>
<th>21.10304</th>
<th>6.43268</th>
<th>90.0</th>
<th>90.0</th>
<th>90.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>H1 0.185380</td>
<td>0.50</td>
<td>0.570760</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2 0.50</td>
<td>0.438830</td>
<td>0.766260</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3 0.313440</td>
<td>0.335860</td>
<td>0.062430</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H4 0.50</td>
<td>0.392110</td>
<td>0.374780</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H5 0.50</td>
<td>0.268180</td>
<td>0.349220</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1 0.50</td>
<td>0.666430</td>
<td>0.707190</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2 0.50</td>
<td>0.50</td>
<td>0.428540</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1 0.50</td>
<td>0.50</td>
<td>0.919410</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2 0.50</td>
<td>0.333170</td>
<td>0.211490</td>
<td>90.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>R3-n144-C2.fsym.icsd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>----------------------</td>
<td>-------------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>8.20916</td>
<td>5.15535</td>
<td>12.81860</td>
<td>90.0</td>
<td>67.03432</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.163230</td>
<td>0.825540</td>
<td>0.0710</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.058920</td>
<td>0.457710</td>
<td>0.888650</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3</td>
<td>0.977070</td>
<td>0.576310</td>
<td>0.328250</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H4</td>
<td>0.651150</td>
<td>0.497330</td>
<td>0.33760</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H5</td>
<td>0.22550</td>
<td>0.392890</td>
<td>0.45050</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H6</td>
<td>0.353160</td>
<td>0.406050</td>
<td>0.223920</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.208450</td>
<td>0.690880</td>
<td>0.164780</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2</td>
<td>0.0</td>
<td>0.716110</td>
<td>0.50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.0</td>
<td>0.645090</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2</td>
<td>0.794480</td>
<td>0.718130</td>
<td>0.334610</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>R3-n170-C2.fsym.icsd</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td></td>
<td>6.81756</td>
<td>6.980</td>
<td>10.73383</td>
<td>90.0</td>
<td>107.39228</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.066440</td>
<td>0.385070</td>
<td>0.70750</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.902610</td>
<td>0.68770</td>
<td>0.832820</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3</td>
<td>0.172120</td>
<td>0.380640</td>
<td>0.953380</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H4</td>
<td>0.410870</td>
<td>0.56670</td>
<td>0.834960</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H5</td>
<td>0.692520</td>
<td>0.625420</td>
<td>0.498160</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H6</td>
<td>0.936070</td>
<td>0.848230</td>
<td>0.372960</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.0</td>
<td>0.519470</td>
<td>0.50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2</td>
<td>0.790150</td>
<td>0.377520</td>
<td>0.831440</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.266260</td>
<td>0.379470</td>
<td>0.830590</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2</td>
<td>0.0</td>
<td>0.99010</td>
<td>0.50</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>R3-n172-P-4.fsym.icsd</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td></td>
<td>4.98076</td>
<td>4.98076</td>
<td>8.7042</td>
<td>90.0</td>
<td>90.0</td>
</tr>
<tr>
<td>A</td>
<td>H1</td>
<td>0.234410</td>
<td>0.146310</td>
<td>0.396880</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H2</td>
<td>0.339690</td>
<td>0.228130</td>
<td>0.71030</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>H3</td>
<td>0.705860</td>
<td>0.162850</td>
<td>0.922520</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na1</td>
<td>0.50</td>
<td>0.50</td>
<td>0.50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Na2</td>
<td>0.0</td>
<td>0.50</td>
<td>0.827410</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al1</td>
<td>0.0</td>
<td>0.0</td>
<td>0.50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Al2</td>
<td>0.50</td>
<td>0.0</td>
<td>0.809260</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Atomic Number</td>
<td>Element</td>
<td>Symbol</td>
<td>R3-n178-Cm.fsym.icsd</td>
<td>R3-n181-Cm.fsym.icsd</td>
<td>R3-n187-Cm.fsym.icsd</td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>---------</td>
<td>--------</td>
<td>-----------------------</td>
<td>-----------------------</td>
<td>-----------------------</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6.28079</td>
<td>5.92325</td>
<td>5.38058</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>0.819920</td>
<td>0.419190</td>
<td>0.015160</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.326160</td>
<td>0.360990</td>
<td>0.727670</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.928820</td>
<td>0.08790</td>
<td>0.044930</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.466830</td>
<td>0.50</td>
<td>0.50</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.968860</td>
<td>0.50</td>
<td>0.50</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7.07639</td>
<td>19.26351</td>
<td>19.0569</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>0.312710</td>
<td>0.566310</td>
<td>0.278120</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.50</td>
<td>0.50</td>
<td>0.274470</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.50</td>
<td>0.50</td>
<td>0.378620</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4.83798</td>
<td>5.37285</td>
<td>4.80547</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.588710</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>134.01271</td>
<td>110.47647</td>
<td>86.88332</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.588710</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.13401271</td>
<td>0.11047647</td>
<td>0.08683320</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.588710</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.013401271</td>
<td>0.11047647</td>
<td>0.08683320</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.588710</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.13401271</td>
<td>0.11047647</td>
<td>0.08683320</td>
<td></td>
</tr>
<tr>
<td>A 1</td>
<td>H1</td>
<td></td>
<td>90.0</td>
<td>90.0</td>
<td>90.0</td>
<td></td>
</tr>
<tr>
<td>A 2</td>
<td>H2</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 3</td>
<td>H3</td>
<td></td>
<td>0.588710</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td>A 4</td>
<td>Na1</td>
<td></td>
<td>0.963770</td>
<td>0.95570</td>
<td>0.336840</td>
<td></td>
</tr>
<tr>
<td>A 5</td>
<td>Al1</td>
<td></td>
<td>0.959690</td>
<td>0.959690</td>
<td>0.818740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>H4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 6</td>
<td>Na2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A 7</td>
<td>Al2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.013401271</td>
<td>0.11047647</td>
<td>0.08683320</td>
<td></td>
</tr>
</tbody>
</table>
Figure S1: Calculated isotropic chemical shifts of $^{27}$Al versus the Al-H coordination number of PEGS-generated structure prototypes. The shifts are referenced to NaAlH$_4$ (I4$_1$/a). Circles: Al nuclei in structures with composition Na$_n$Al$_n$H$_{4n}$, diamonds: structures with other compositions. **Coordination 6**: The non-linked [AlH$_6$]$^{3-}$ octahedrons have the most negative shift (range “a”, including Na$_3$AlH$_6$). In range “b” the octahedrons are corner sharing, sharing the hydrogens at two opposite corners with two different neighbouring octahedrons. In range “c” the octahedrons are also corner sharing, but now at 4 corners (e.g., the Amm2 structure in Fig. 1). In range “d” the octrahedrons are edge-sharing, also sharing 4 hydrogens with neighbors (e.g., the Pmc2$_1$ structure in Fig. 1). The number of shared hydrogens of the AlH$_6$ units increases from left to right. The AlH$_3$ (blue solid diamond, sharing all 6 hydrogens between octahedrons) does not fit this scheme. **Coordination 5**: $\delta_{\text{Al}} = -97$ ppm pertains to an isolated [AlH$_5$]$^{2-}$ unit. The data points around -50 ppm all belong to [AlH$_5$]$^{1-}$ units that share hydrogens at two opposite corners (e.g., the Cm structure in Fig. 1). The green diamonds at $\delta_{\text{Al}} = -19$ ppm are from a structure that is in-between 4 and 5-fold coordination. **Coordination 4**: All data points correspond to isolated [AlH$_4$]$^{-}$ units, except the ambiguous point at $\delta_{\text{Al}} = -19$ ppm and the point with $\delta_{\text{Al}} = 38$ ppm. The latter has two hydrogens shared with neighbors. For quadrupolar nuclei an additional shift is provided by second order quadrupolar effects. These shifts are field dependent and vanish as $B_0 \to \infty$. Taking the second order quadrupole-induced shift (QIS) into account, one obtains an isotropic shift of about 97.5 ppm, referenced to aqueous Al(NO$_3$)$_3$, for the $^{27}$Al in NaAlH$_4$ (I4$_1$/a) at zero field. The QIS are easily calculated from the EFGs and the $B_0$ field. They are always negative. For the $B_0$ field of 8.32 T used by Ref. 1, the QIS scrambles the data points with 4-fold coordination (cf. Figure 2) amongst themselves, but the 4-fold “cluster” of data points remains well-separated from the 5 and 6-fold “clusters”. Table S5 shows how the QIS affects the total shift for two values of $B_0$. 

S14
Figure S2: Simulated X-ray diffraction patterns for structures I4₁/a, Fmm2, and Cmcm for Cu Kα radiation.

References


(5) Dalton, a molecular electronic structure program, Release 2.0 (2005), see http://www.kjemi.uio.no/software/dalton/dalton.html.


(10) Sorte, E.; Conradi, M. Private communication. The reported line positions in our Table 1 were not calculated center-of-gravity values, \[ \frac{\int \omega f(\omega) d\omega}{\int f(\omega) d\omega}, \] and carry additional error due to the relatively low field strengths (350 and 500 MHz).