Appendix 1
Crystal Structure Descriptions

In this appendix, most of the crystal structure types introduced in the main text are formally described by means of their chemical formulas, StrukturBericht symbols, space groups, lattice parameters, special atom positions, etc. In addition, examples of actual compounds with these structures are given, along with their lattice parameters. All lattice parameters are stated in nm.

Structure types are listed in the order in which they appear in the text, and are sequentially numbered. Most of the structural data in this appendix was extracted from the following sources:


When consulting the tables on the following pages, one must be aware of the fact that many compounds can have multiple crystal structures; it is always a good idea to consult the original sources listed above (and others) to verify that the correct structure is obtained. In particular, the examples of structures of a given structure type will often include metastable structures, or high temperature/high pressure phases; we refer the reader to the original sources for those details. Furthermore, atom coordinates provided in this appendix have been used with the sole purpose of creating structure visualizations; this means that sites with partial occupancy will show up in a structure drawing as fully occupied sites. The reader who wishes to compute x-ray powder patterns for any of these structures should consult the original citations to make sure that all site occupancies are properly accounted for.

The compound names for intermetallics are listed in the same convention as in Pearson’s lists, namely an alphabetical ranking of all the elements in the compound, except for the prototype chemical formulas, for which we follow the list by J. Lima de Faria.
(J. Lima de Faria, *Structural Classification and Notation*, Chapter 1 in *Intermetallic Compounds, Vol. 3*, edited by J.H. Westbrook and R.L. Fleischer, John Wiley and Sons, New York (2002)). For instance, BiF$_3$ is the prototype for the D0$_3$ structure, which has Mg$_3$Pr and AlFe$_3$ as example compounds; note that the elements are listed alphabetically, so that the $AB_3$ compound is sometimes written as $B_3A$. The only exception will be when the conventional prototype name is not in alphabetical order, for instance ZnS, in which case we do not change the order to SZn.

The present version of this structures appendix was completed on October 1, 2009; updates containing corrections will be posted as needed.
Table A1.0. Alphabetical list of all prototype structures described in this appendix, along with the page number on which the complete description can be found. Note that for compounds, constituent elements are ranked alphabetically. If you know the structure number, then the page number is obtained simply by adding 3.

<table>
<thead>
<tr>
<th>Prototype</th>
<th>Page</th>
<th>Prototype</th>
<th>Page</th>
<th>Prototype</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>AgBa₂Ca₃Cu₄O₁₀</td>
<td>A1–87</td>
<td>Ca₂Mg₅(Si₄O₂₂)(OH)₃</td>
<td>A1–98</td>
<td>NaAlSi₂O₆</td>
<td>A1–96</td>
</tr>
<tr>
<td>Al₂SiO₅ (Kyanite)</td>
<td>A1–92</td>
<td>CaCl</td>
<td>A1–13</td>
<td>NiAs</td>
<td>A1–18</td>
</tr>
<tr>
<td>Al₂Si₂O₇(OH)₄</td>
<td>A1–99</td>
<td>Co₂Cr₂Mo₂</td>
<td>A1–43</td>
<td>Ni₁₇Th₂</td>
<td>A1–51</td>
</tr>
<tr>
<td>Al₂Zr₄</td>
<td>A1–33</td>
<td>Cr₃Si</td>
<td>A1–32</td>
<td>α-SiO₂</td>
<td>A1–100</td>
</tr>
<tr>
<td>As</td>
<td>A1–23</td>
<td>CuFeS₂</td>
<td>A1–16</td>
<td>β-SiO₂</td>
<td>A1–101</td>
</tr>
<tr>
<td>AuCu</td>
<td>A1–7</td>
<td>Cu₂Mg</td>
<td>A1–35</td>
<td>Sm₂Fe₁₇N₃</td>
<td>A1–56</td>
</tr>
<tr>
<td>AuCu₃</td>
<td>A1–8</td>
<td>Fe₂B</td>
<td>A1–59</td>
<td>Sm(Fe,Ti)₁₂N</td>
<td>A1–57</td>
</tr>
<tr>
<td>Ba₁₋₂K₂BiO₃</td>
<td>A1–71</td>
<td>Fe₅Zr₆</td>
<td>A1–60</td>
<td>Th₂Zn₁₇</td>
<td>A1–52</td>
</tr>
<tr>
<td>Ba₃Pb₁₋₂Bi₂O₃</td>
<td>A1–70</td>
<td>α-Ga</td>
<td>A1–27</td>
<td>Ti₂CS</td>
<td>A1–69</td>
</tr>
<tr>
<td>(Ba,Sr)CuO₄</td>
<td>A1–88</td>
<td>α-Hg</td>
<td>A1–26</td>
<td>TiO₂</td>
<td>A1–65</td>
</tr>
<tr>
<td>Be₂Al₂S₆O₁₈</td>
<td>A1–97</td>
<td>H₂O(Ic)</td>
<td>A1–106</td>
<td>TiBa₂CaCu₂O₇</td>
<td>A1–84</td>
</tr>
<tr>
<td>Be₃Nb</td>
<td>A1–49</td>
<td>In</td>
<td>A1–22</td>
<td>TiBa₂Ca₂Cu₃O₈</td>
<td>A1–85</td>
</tr>
<tr>
<td>BiF₃</td>
<td>A1–11</td>
<td>α-La</td>
<td>A1–20</td>
<td>TiBa₂Ca₃Cu₄O₁₁</td>
<td>A1–86</td>
</tr>
<tr>
<td>Bi₂Sr₂CuO₆₊ₓ</td>
<td>A1–75</td>
<td>La₂CuO₄</td>
<td>A1–72</td>
<td>Ti₂Ba₂Cu₂O₆₊ₓ</td>
<td>A1–79</td>
</tr>
<tr>
<td>Bi₂Sr₂Ca₂Cu₂O₈₊ₓ</td>
<td>A1–76</td>
<td>Mg</td>
<td>A1–6</td>
<td>Ti₂Ba₂CaCu₂O₆₊ₓ</td>
<td>A1–80</td>
</tr>
<tr>
<td>Bi₂Sr₂Ca₂Cu₃O₁₀₊ₓ</td>
<td>A1–77</td>
<td>MgAl₂O₄</td>
<td>A1–63</td>
<td>Ti₂Ba₂Ca₂Cu₃O₁₀₊ₓ</td>
<td>A1–81</td>
</tr>
<tr>
<td>Bi₂Sr₂Ca₂Cu₄O₁₂₊ₓ</td>
<td>A1–78</td>
<td>Mg₁₂₂(Al,Zn)₄₉</td>
<td>A1–81</td>
<td>Ti₂Ba₂Ca₃Cu₄O₁₂₊ₓ</td>
<td>A1–82</td>
</tr>
<tr>
<td>Ca₂(Al,Fe)Al₂Si₃O₁₃H</td>
<td>A1–94</td>
<td>MgZn₂</td>
<td>A1–36</td>
<td>W₁₇Fe₇</td>
<td>A1–40</td>
</tr>
<tr>
<td>Ca₂Al₂Si₃O₁₂₋₄H₂O</td>
<td>A1–103</td>
<td>Mn₁₂Th</td>
<td>A1–53</td>
<td>YBa₂Cu₃O₇₋ₓ</td>
<td>A1–74</td>
</tr>
<tr>
<td>Ca₂Cu₅</td>
<td>A1–50</td>
<td>Mn₂₁Th₆</td>
<td>A1–47</td>
<td>Zn(S/zinc-blende)</td>
<td>A1–14</td>
</tr>
<tr>
<td>ZrSiO₄</td>
<td>A1–91</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Crystal Structure Descriptions

A1–3
Structure 1  
Prototype: Cu  
SBS/PS: A1/cF4  
SG # 225: Fm3m (O_h^{3})  
Lattice complex: Cu @ 4a(0, 0, 0)

<table>
<thead>
<tr>
<th>Element</th>
<th>a</th>
<th>Element</th>
<th>a</th>
<th>Element</th>
<th>a</th>
<th>Element</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>0.3615</td>
<td>Ag</td>
<td>0.4086</td>
<td>Au</td>
<td>0.4078</td>
<td>Al</td>
<td>0.4049</td>
</tr>
<tr>
<td>Ni</td>
<td>0.3524</td>
<td>Pd</td>
<td>0.3891</td>
<td>Pt</td>
<td>0.3924</td>
<td>Pb</td>
<td>0.4950</td>
</tr>
</tbody>
</table>

Table A1.1. Representative elements for Structure 1. Pearson’s tables list 485 intermetallic compounds (mostly solid solutions) with this structure type.
Crystal Structure Descriptions

Structure 2  
Prototype: W
SBS/PS: A2/c12  
SG # 229: Im¯3m (O₆h)
Lattice complex: W @ 2a(0, 0, 0)

<table>
<thead>
<tr>
<th>Element</th>
<th>a</th>
<th>Element</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>W</td>
<td>3.1650</td>
<td>Fe</td>
<td>2.8664</td>
</tr>
<tr>
<td>Mo</td>
<td>3.1469</td>
<td>Ta</td>
<td>3.3026</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ba</td>
<td>5.0190</td>
</tr>
</tbody>
</table>

Table A1.2. Representative elements for Structure 2. Pearson’s tables list 333 intermetallic compounds (mostly solid solutions) with this structure type.
Structure 3
Prototype: Mg
SBS/PS: A3/hP2
SG # 194: P6₃/mmc (D₁₆h)
Lattice complex: Mg @ 2d(\(\frac{2}{3}, \frac{1}{3}, \frac{1}{4}\))

Table A1.3. Representative elements for Structure 3. Pearson’s tables list 120 intermetallic compounds (mostly solid solutions) with this structure type.
**Structure 4**  
Prototype: AuCu  
*SB/PS: L1₀/tP4 (or tP4 with centered cell)*  
*SG # 123: P4/mmm (D₄h)*  
*Lattice complex: Au @ 2c(0, 1/2, 1/2); Cu @ 1a(0, 0, 0) and 1c(1/2, 1/2, 0)*

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>(\frac{c}{a})</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>(\frac{c}{a})</th>
</tr>
</thead>
<tbody>
<tr>
<td>AuCu</td>
<td>0.3963</td>
<td>0.3671</td>
<td>0.926</td>
<td>AgTi</td>
<td>0.4104</td>
<td>0.4077</td>
<td>0.993</td>
</tr>
<tr>
<td>AlTi</td>
<td>0.3984</td>
<td>0.4065</td>
<td>1.020</td>
<td>CoPt</td>
<td>0.3806</td>
<td>0.3684</td>
<td>0.968</td>
</tr>
<tr>
<td>CrPd</td>
<td>0.3879</td>
<td>0.3802</td>
<td>0.980</td>
<td>FePd</td>
<td>0.3852</td>
<td>0.3723</td>
<td>0.966</td>
</tr>
<tr>
<td>MnNi</td>
<td>0.3690</td>
<td>0.3490</td>
<td>0.945</td>
<td>PtZn</td>
<td>0.4026</td>
<td>0.3474</td>
<td>0.863</td>
</tr>
</tbody>
</table>

Table A1.4. Representative compounds for Structure 4. Pearson’s tables list 97 intermetallic compounds with this structure type.
Structure 5  
Prototype: AuCu₃  
SBS/PS: L₁₂/cP₄  
SG # 221: Pm₃m \( (O_{h}^1) \)  
Lattice complex: Au @ 1a(0, 0, 0); Cu @ 3c\((0, \frac{1}{2}, \frac{1}{2}); \frac{1}{2}\)  

<table>
<thead>
<tr>
<th>Compound</th>
<th>( a )</th>
<th>Compound</th>
<th>( a )</th>
<th>Compound</th>
<th>( a )</th>
<th>Compound</th>
<th>( a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>AuCu₃</td>
<td>0.3749</td>
<td>AgPt₃</td>
<td>0.3900</td>
<td>AlNi₃</td>
<td>0.3572</td>
<td>TiZn₃</td>
<td>0.3932</td>
</tr>
<tr>
<td>AlPt₃</td>
<td>0.3876</td>
<td>Al₃Er</td>
<td>0.4215</td>
<td>Al₃U</td>
<td>0.4287</td>
<td>Pd₃Y</td>
<td>0.4074</td>
</tr>
</tbody>
</table>

Table A1.5. Representative compounds for Structure 5. Pearson’s tables list 436 intermetallic compounds with this structure type.
Structure 6  
Prototype: C (diamond)

\[ SBS/PS: \text{A4/cF8} \quad \text{SG \# 227: Fd\overline{3}m (O_h^7)} \]

Lattice complex: C @ 8a(0,0,0)

<table>
<thead>
<tr>
<th>Element</th>
<th>( a )</th>
<th>Element</th>
<th>( a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.356</td>
<td>Si</td>
<td>0.5431</td>
</tr>
<tr>
<td>Ge</td>
<td>0.5657</td>
<td>( \alpha )-Sn</td>
<td>0.6491</td>
</tr>
</tbody>
</table>

Table A1.6. Representative elements for Structure 6. Pearson’s tables list 16 intermetallic compounds with this structure type.
**Structure 7**  
*Prototype: NaCl (rock salt)*

*SG* # 225: *Fm\overline{3}m* (*O_\text{h}^3*)

*Table A1.7.*  
Representative compounds for Structure 7. Pearson’s tables list 799 intermetallic compounds with this structure type.

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaCl</td>
<td>0.5640</td>
<td>MgO</td>
<td>0.4213</td>
<td>FeO</td>
<td>0.4307</td>
</tr>
<tr>
<td>MgS</td>
<td>0.5200</td>
<td>BaSe</td>
<td>0.6600</td>
<td>CaTe</td>
<td>0.6356</td>
</tr>
<tr>
<td>LiF</td>
<td>0.4027</td>
<td>BrNa</td>
<td>0.5977</td>
<td>TiN</td>
<td>0.4240</td>
</tr>
</tbody>
</table>
Structure 8  Prototype: BiF₃
SBS/PS: D₀₃/cF16  SG # 225: Fm3m (O₃³)
Lattice complex: Bi @ 4a(0, 0, 0); F @ 4b (½, ½, ½) and 8c (1/4, 1/4, 1/4)

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiF₃</td>
<td>0.5865</td>
<td>BiLi₃</td>
<td>0.6722</td>
<td>Cd₃Pr</td>
<td>0.7200</td>
</tr>
<tr>
<td>CeMg₃Pr</td>
<td>0.7438</td>
<td>Cu₃Sb</td>
<td>0.6010</td>
<td>Fe₃Si</td>
<td>0.5662</td>
</tr>
<tr>
<td>Mg₃Pr</td>
<td>0.7430</td>
<td>AlFe₃</td>
<td>0.5780</td>
<td>Mn₃Si</td>
<td>0.5722</td>
</tr>
</tbody>
</table>

Table A1.8. Representative compounds for Structure 8. Pearson’s tables consider both D₀₃ and L2₁ structure types under the BiF₃ prototype, and list 394 intermetallic compounds with this structure type.
**Crystal Structure Descriptions**

**Structure 9**
Prototype: AlCu$_2$Mn (Heusler)

*SBS/PS: L2$_1$/cF16  SG # 225: Fm$\bar{3}$m ($O_h^5$)

Lattice complex: Cu @ 8c($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$); Al @ 4a(0, 0, 0); Mn @ 4b($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$)

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlCu$_2$Mn</td>
<td>0.5949</td>
<td>Cu$_2$MnSb</td>
<td>0.6097</td>
<td>Cu$_2$FeSn</td>
<td>0.5930</td>
</tr>
<tr>
<td>AlCu$_2$Hf</td>
<td>0.6172</td>
<td>AlNi$_2$Ti</td>
<td>0.5850</td>
<td>GaMnNi$_2$</td>
<td>0.xxxx</td>
</tr>
<tr>
<td>Co$_2$MnSn</td>
<td>0.5989</td>
<td>AlCo$_2$Nb</td>
<td>0.5946</td>
<td>AlCo$_2$Ta</td>
<td>0.5927</td>
</tr>
</tbody>
</table>

Table A1.9. Representative compounds for Structure 9. Pearson’s tables consider both D0$_3$ and L2$_1$ structure types under the BiF$_3$ prototype, and list 394 intermetallic compounds with this structure type.
**Structure 10**  
*Prototype: CsCl*  

*SBS/PS: B2/cP2*  

*SG # 221: Pm3m (O_{h}^{4})*  

*Lattice complex: Cs @ 1a(0, 0, 0); Cl @ 1b(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})*

<table>
<thead>
<tr>
<th>Compound</th>
<th>(a)</th>
<th>Compound</th>
<th>(a)</th>
<th>Compound</th>
<th>(a)</th>
<th>Compound</th>
<th>(a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CsCl</td>
<td>0.4123</td>
<td>BrCs</td>
<td>0.4286</td>
<td>AlCo</td>
<td>0.2862</td>
<td>AgMg</td>
<td>0.3280</td>
</tr>
<tr>
<td>CoTi</td>
<td>0.2986</td>
<td>CuZn</td>
<td>0.2945</td>
<td>FeTi</td>
<td>0.2976</td>
<td>NiTi</td>
<td>0.2972</td>
</tr>
</tbody>
</table>

Table A1.10. *Representative compounds for Structure 10. Pearson’s tables list 461 intermetallic compounds with this structure type.*
**Structure 11**  
*Prototype:* ZnS (zinc-blende)  
*SBS/PS:* B3/cF8  
*SG #216:* F43m (Td)  
*Lattice complex:* S @ 4a(0,0,0); Zn @ 4c(1/2,1/2,1/2)

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnS</td>
<td>0.5406</td>
<td>AlP</td>
<td>0.5415</td>
<td>BeSe</td>
<td>0.5070</td>
<td>SeZn</td>
<td>0.5667</td>
</tr>
<tr>
<td>TeZn</td>
<td>0.6103</td>
<td>GaP</td>
<td>0.5448</td>
<td>AsGa</td>
<td>0.5653</td>
<td>GaSb</td>
<td>0.6095</td>
</tr>
<tr>
<td>InP</td>
<td>0.5869</td>
<td>CdTe</td>
<td>0.6481</td>
<td>AlAs</td>
<td>0.5662</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table A1.11. *Representative compounds for Structure 11. Pearson’s tables list 247 intermetallic compounds with this structure type.*
Structure 12  
Prototype: CaF$_2$ (fluorite)  
SBS/PS: G1/cF12  
SG # 225: Fm$\overline{3}$m ($O_h^5$)  
Lattice complex: Ca @ 4a(0, 0, 0); F @ 8c($\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$)

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaF$_2$</td>
<td>0.5463</td>
<td>F$_2$Sr</td>
<td>0.5800</td>
<td>BaCl$_2$</td>
<td>0.7311</td>
</tr>
<tr>
<td>O$_2$Pb</td>
<td>0.5349</td>
<td>O$_2$U</td>
<td>0.5372</td>
<td>Li$_2$O</td>
<td>0.4611</td>
</tr>
<tr>
<td>Na$_2$Se</td>
<td>0.6823</td>
<td>K$_2$S</td>
<td>0.7406</td>
<td>ORb$_2$</td>
<td>0.6740</td>
</tr>
</tbody>
</table>

Table A1.12. Representative compounds for Structure 12. Pearson’s tables list 137 intermetallic compounds with this structure type.
**Structure 13**  
*Prototype: CuFeS$_2$ (chalcopyrite)*  

*SBS/PS: E1_{116}  
SG # 122: 142d ($D_{5d}^{12}$)*  

*Lattice complex: Cu $@ 4a(0,0,0)$; Fe $@ 4b(0,0,1/2)$; S $@ 8d(x,1/4,1/8)$ with $x = 1/4$*

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuFeS$_2$</td>
<td>0.524</td>
<td>1.03</td>
<td>Ag$_2$AlTe$_2$</td>
<td>0.6296</td>
<td>1.183</td>
</tr>
<tr>
<td>AlCuSe$_2$</td>
<td>0.5605</td>
<td>1.090</td>
<td>CdGeP$_2$</td>
<td>0.5738</td>
<td>1.0765</td>
</tr>
</tbody>
</table>

Table A1.13. Representative compounds for Structure 13. Pearson’s tables list 132 intermetallic compounds with this structure type.
Structure 14  
Prototype: ZnS (wurtzite)  

SG # 186: P6₃mc (C₄ᵥ)  
Lattice complex: Zn @ 2b(1/3, 2/3, z) with z = 0; S @ 2b(1/3, 2/3, z) with z = 3/8

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
<td>0.335</td>
<td>0.522</td>
<td>ZnS</td>
<td>0.381</td>
<td>0.623</td>
</tr>
<tr>
<td>BP</td>
<td>0.3562</td>
<td>0.590</td>
<td>GaN</td>
<td>0.3190</td>
<td>0.5189</td>
</tr>
</tbody>
</table>

Table A1.14. Representative compounds for Structure 14. Pearson’s tables list 86 intermetallic compounds with this structure type.
**Structure 15  
Prototype: NiAs**  
*SBS/PS: B8₁/hP4  
SG # 194: P6₃/mmc (D₄h₃)*  
*Lattice complex: Ni @ 2a(0, 0, 0); As @ 2c(\(\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\))*

<table>
<thead>
<tr>
<th>Compound</th>
<th>(a)</th>
<th>(c)</th>
<th>Compound</th>
<th>(a)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NiAs</td>
<td>0.36</td>
<td>0.501</td>
<td>AuSe</td>
<td>0.412</td>
<td>0.539</td>
</tr>
<tr>
<td>NbSb</td>
<td>0.4270</td>
<td>0.5447</td>
<td>CrS</td>
<td>0.3419</td>
<td>0.5550</td>
</tr>
</tbody>
</table>

Table A1.15. Representative compounds for Structure 15. Pearson’s tables list 217 intermetallic compounds with this structure type.
Crystal Structure Descriptions

Structure 16  
Prototype: Ni₃Sn

SG # 194: P6₃/mmc (D₄dh)

Lattice complex: Ni @ 2c(½, ½, ½); Sn @ 6h(x, 2x, ½) with x = 5/6

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni₃Sn</td>
<td>0.5275</td>
<td>0.4234</td>
<td>Fe₃Ga</td>
<td>0.520</td>
<td>0.426</td>
</tr>
<tr>
<td>InTi₃</td>
<td>0.589</td>
<td>0.476</td>
<td>Al₃Sm</td>
<td>0.6380</td>
<td>0.4597</td>
</tr>
</tbody>
</table>

Table A1.16. Representative compounds for Structure 16. Pearson’s tables list 106 intermetallic compounds with this structure type.
Structure 17  Prototype: $\alpha$-La
SBS/PS: A3’hP4  $SG \# 194$: P6$_3$/mmc ($D_{6h}^4$)
Lattice complex: La @ 2a(0, 0, 0) and 2c($\frac{1}{3}, \frac{2}{3}, \frac{1}{4}$)

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$-La</td>
<td>0.377</td>
<td>1.21596</td>
<td>Nd</td>
<td>0.36562</td>
<td>1.18056</td>
</tr>
<tr>
<td>Gd</td>
<td>0.3402</td>
<td>1.1047</td>
<td>Sm</td>
<td>0.3565</td>
<td>1.11456</td>
</tr>
</tbody>
</table>

Table A1.17. Representative compounds for Structure 17. Pearson’s tables list 34 intermetallic compounds with this structure type.
Structure 18  
Prototype: $\beta$-Sn 
SG # 141: $I4_1/amd$ ($D_{19}^{19}$)

Lattice complex: Sn @ 4$\alpha$(0, 0, 0) with origin (1) offset $(0, \frac{1}{4}, \frac{1}{8})$ from the center of symmetry

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$-Sn</td>
<td>0.58197</td>
<td>0.31750</td>
<td>Ge</td>
<td>0.49585</td>
<td>0.27463</td>
</tr>
</tbody>
</table>

Table A1.18. Representative compounds for Structure 18. Pearson’s tables list 20 intermetallic compounds with this structure type.
Structure 19  

Prototype: In  

SBS/PS: A6/tI2  

SG # 139: I4/mmm ($D_{4h}^{17}$)  

Lattice complex: In @ 2a(0, 0, 0)  

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>In</td>
<td>0.4598</td>
<td>0.4947</td>
<td>Pa</td>
<td>0.3925</td>
<td>0.3238</td>
</tr>
</tbody>
</table>

Table A1.19. Representative compounds for Structure 19. Pearson’s tables list 28 intermetallic compounds with this structure type.
**Structure 20**  
Prototype: As  
*SBS/PS: A7/hR2*  
SG # 166: R̅3m (D_{3d}^5)  
*Lattice complex: As @ 6c(0, 0, z) with z = 0.2271.*

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>As</td>
<td>0.3760</td>
<td>1.0547</td>
<td>Bi</td>
<td>0.4546</td>
<td>1.1862</td>
</tr>
</tbody>
</table>

Table A1.20. Representative compounds for Structure 20. Pearson’s tables list 21 intermetallic compounds with this structure type.
**Structure 21**  
*Prototype:* $\gamma$-Se  
*SG # 152:* $P\overline{3}121$ ($D_{3}^{1}$)  
*Lattice complex:* Se @ 3a(0.7364, 0, $\frac{1}{3}$)

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Se</td>
<td>0.4366</td>
<td>0.4959</td>
</tr>
<tr>
<td>Te</td>
<td>0.4527</td>
<td>0.5921</td>
</tr>
</tbody>
</table>

Table A1.21. *Representative compounds for Structure 21.*
Structure 22  
Prototype: C-graphite

SG # 194: P6\textsubscript{3}/mmc (D\textsubscript{6h})

Lattice parameters: \(a = 0.2464, c = 0.6711\)

Lattice complex: C@ 2b(0, 0, \(\frac{1}{4}\)), 2c(\(\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\)).
**Structure 23**  
Prototype: α-Hg  
*SBS/PS: A10/hR1*  
*Lattice parameters: a = 0.3464, c = 0.6677*  
*Lattice complex: α-Hg @ 1a(0, 0, 0)*  

SG # 166: R̅3m (D₃d)

![Diagram of α-Hg structure]
**Structure 24**  
*Prototype: α-Ga*  
*SBS/PS: A10/oC8*  
*SG # 64: Cmca (\(D_{18}^{2h}\))*  

Lattice parameters: \(a = 0.4517, b = 0.7645, c = 0.4511\)

Lattice complex: Ga @ 8f\((0, y, z)\) with \(y = 0.1525\) and \(z = 0.079\).
Structure 25  
Prototype: α-Mn  
SBS/PS: A12/cI58  
SG # 217: I43m ($T_d^3$)  

Lattice parameters: $a = 0.8894$

Lattice complex: Mn $\oplus 2a(0,0,0), 8c(x,x,x)$ with $x = 0.317$, $24g(x,x,z)$ with $(x,z)=(0.356,0.42)$ and $(0.089,0.278)$. 
**Structure 26**  
Prototype: β-Mn  
*SBS/PS: A13/cP20*  
*SG # 213: P4132 (O7)*  
Lattice parameters: $a = 0.6315$  
Lattice complex: Mn @ 8$c(x,x,x)$, $x = 0.0636$; and 12$d(\frac{1}{8},y,y+\frac{1}{4})$ with $y = 0.2022$. 
Structure 27  
Prototype: α-U  
SBS/PS: A20/oC4  
SG # 63: Cmcm (D\textsubscript{17}h)

Lattice parameters: \(a = 0.2854, b = 0.2854, c = 0.4955\)

Lattice complex: U @ 4c(0, y, \frac{1}{4}) with \(y = 0.1025\)
Structure 28  
Prototype: $\text{Al}_3\text{Ti}$

SG # 139: $\text{I}4/\text{mmm} (D_{4h}^{17})$

Lattice complex: $\text{Ti} @ 2a(0, 0, 0); \text{Al} @ 2b(0, 0, \frac{1}{2})$ and $4d(0, \frac{1}{2}, \frac{1}{2})$

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Al}_3\text{Ti}$</td>
<td>0.3836</td>
<td>0.8579</td>
<td>$\text{Al}_3\text{Ta}$</td>
<td>0.3837</td>
<td>0.8550</td>
</tr>
<tr>
<td>$\text{Al}_3\text{Hf}$</td>
<td>0.3928</td>
<td>0.8888</td>
<td>$\text{Ga}_3\text{Ta}$</td>
<td>0.3836</td>
<td>0.8579</td>
</tr>
<tr>
<td>$\text{Pt}_3\text{V}$</td>
<td>0.3839</td>
<td>0.7796</td>
<td>$\text{Pd}_3\text{V}$</td>
<td>0.3850</td>
<td>0.7750</td>
</tr>
</tbody>
</table>

Table A1.22. Representative compounds for Structure 28. Pearson's tables list 44 intermetallic compounds with this structure type.
**Structure 29**

Prototype: Cr₃Si

*SBS/PS: A15/cP8*  
*SG # 223: Pm\̅3n (O₃̅)*

*Lattice complex: Si @ 2a(0, 0, 0); Cr @ 6c(\(\frac{1}{4}, 0, \frac{1}{2}\))*

<table>
<thead>
<tr>
<th>Compound</th>
<th>(\alpha)</th>
<th>Compound</th>
<th>(\alpha)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr₃Si</td>
<td>0.4555</td>
<td>AuZr₃</td>
<td>0.5486</td>
</tr>
<tr>
<td>GeMo₃</td>
<td>0.4932</td>
<td>IrTi₃</td>
<td>0.50087</td>
</tr>
<tr>
<td>CoV₃</td>
<td>0.4676</td>
<td>Mo₃Os</td>
<td>0.49689</td>
</tr>
<tr>
<td>BiNb₃</td>
<td>0.5320</td>
<td>Re₇V₃</td>
<td>0.48783</td>
</tr>
<tr>
<td>Ti₄Ti</td>
<td>0.5256</td>
<td>Nb₃₈Si₂₄V₃₈</td>
<td>0.4915</td>
</tr>
</tbody>
</table>

Table A1.23. Representative compounds for Structure 29. The compounds with stoichiometry deviating from the nominal \(A₃B\) composition typically have defect arrangements (vacancies) accommodating the deviation. Pearson’s tables list 213 intermetallic compounds with this structure type.
Crystal Structure Descriptions

Structure 30  Prototype: $\text{Al}_3\text{Zr}_4$

$\text{SBS/PS: } \overline{\text{hP7}}$  $\text{SG } \# 174: \text{P6}(C_{15})$

Lattice complex: Zr @ $1b(0, 0, \frac{1}{2})$, $1f(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$ and $2h(\frac{1}{3}, \frac{2}{3}, 1)²$; Al @ $3j(\frac{1}{3}, \frac{1}{3}, 0)$

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Al}_3\text{Zr}_4$</td>
<td>0.5433</td>
<td>0.5390</td>
<td>$\text{Al}<em>{40}\text{Nb}</em>{10}\text{Zr}_{50}$</td>
<td>0.5368</td>
<td>0.5333</td>
</tr>
<tr>
<td>$\text{Al}_3\text{Hf}_4$</td>
<td>0.5331</td>
<td>0.5414</td>
<td>$\text{Al}<em>{33}\text{Cu}</em>{10}\text{Zr}_{57}$</td>
<td>0.5375</td>
<td>0.5390</td>
</tr>
</tbody>
</table>

Table A1.24. Representative compounds for Structure 30. Pearson’s tables list 4 intermetallic compounds with this structure type.
Structure 31  
Prototype: Al₂Zr₃

SBS/PS: —/tP20  
SG # 136: P4₂/mnm (D₁₄h)

Lattice complex: Zr @ 4d(0, 1/2, 1/4), 4f(x, x, 0) with x = 0.34 and 4g(x, x, 0) with x = 0.20; Al @ 8f(x, x, z) with x = 1/2 and z = 0.21.

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₂Zr₃</td>
<td>0.7630</td>
<td>0.6998</td>
<td>Al₂Dy₃</td>
<td>0.8281</td>
<td>0.7550</td>
</tr>
<tr>
<td>Ga₂Gd₃</td>
<td>0.8292</td>
<td>0.7530</td>
<td>Li₂Sr₃</td>
<td>0.9628</td>
<td>0.8550</td>
</tr>
<tr>
<td>Al₂Y₃</td>
<td>0.8239</td>
<td>0.7648</td>
<td>Ce₃Ga₂</td>
<td>0.83</td>
<td>0.764</td>
</tr>
</tbody>
</table>

Table A1.25.  Representative compounds for Structure 31. Pearson’s tables list 17 intermetallic compounds with this structure type.
Structure 32  Prototype: Cu$_2$Mg (Laves Phase)

SG # 227: Fd$ar{3}$m ($O_h^1$)

Lattice complex: Cu @ 16d($\frac{5}{8}$,$\frac{5}{8}$,$\frac{5}{8}$); Mg @ 8a(0,0,0)

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu$_2$Mg</td>
<td>0.7048</td>
<td>Be$_2$Ta</td>
<td>0.651</td>
<td>CaNi$_2$</td>
<td>0.7239</td>
</tr>
<tr>
<td>DyMn$_2$</td>
<td>0.756</td>
<td>EuPt$_2$</td>
<td>0.7714</td>
<td>Fe$_2$Tb</td>
<td>0.740</td>
</tr>
<tr>
<td>Li$_2$Pt</td>
<td>0.760</td>
<td>Mg$_2$Sn</td>
<td>0.6762</td>
<td>Mg$_2$Si</td>
<td>0.6352</td>
</tr>
</tbody>
</table>

Table A1.26. Representative compounds for Structure 32. Pearson’s tables list 1476 intermetallic compounds (many solid solutions) with this structure type.
Structure 33  Prototype: MgZn$_2$ (Laves Phase)

SBS/PS: C14/hP12  SG # 194: P6$_3$/mmc ($D_{6h}^4$)

Lattice complex: Mg @ 4f($\frac{1}{3}$, $\frac{2}{3}$, z) with z = 0.0629; Zn @ 2a(0, 0, 0) and 6h($x$, 2x, $\frac{1}{4}$) with $x$ = 0.8305

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgZn$_2$</td>
<td>0.5221</td>
<td>0.8567</td>
<td>Al$_2$Hf</td>
<td>0.524</td>
<td>0.868</td>
</tr>
<tr>
<td>BeV$_2$</td>
<td>0.4385</td>
<td>0.7130</td>
<td>Cu$_2$Yb</td>
<td>0.5260</td>
<td>0.8567</td>
</tr>
<tr>
<td>Co$_2$Nb</td>
<td>0.4835</td>
<td>0.7860</td>
<td>Mn$_3$SiW$_2$</td>
<td>0.476</td>
<td>0.775</td>
</tr>
</tbody>
</table>

Table A1.27. Representative compounds for Structure 33. Pearson’s tables list 497 intermetallic compounds (many solid solutions) with this structure type.
**Structure 34**  
**Prototype:** MgNi₂ (Laves Phase)  

[SBS/PS: C36/hP24]  
**SG # 194:** P6₃/mmc (D₄₆h)  

**Lattice complex:** Mg @ 4e(0, 0, z) with z = 0.094; 4f(1/3, 2/3, z) with z = 0.844; Ni @ 4f(1/3, 2/3, z) with z = 0.125; 6g(1/3, 0, 0); 6h(1/6, 1/3, 1/4)  

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgNi₂</td>
<td>0.4805</td>
<td>1.5770</td>
<td>EuNi₂</td>
<td>0.539</td>
<td>1.749</td>
</tr>
<tr>
<td>HfZn₂</td>
<td>0.519</td>
<td>1.689</td>
<td>Cr₂Ti</td>
<td>0.4932</td>
<td>1.601</td>
</tr>
<tr>
<td>HfMn₂</td>
<td>0.5016</td>
<td>1.637</td>
<td>Cr₂Zr</td>
<td>0.5100</td>
<td>1.661</td>
</tr>
</tbody>
</table>

Table A1.28. *Representative compounds for Structure 34. Pearson’s tables list 40 intermetallic compounds (many solid solutions) with this structure type.*
Structure 35  
Prototype: $B_2CoW_2$

$SBS/PS$: $\overline{1}a10$

$SG$ $\#71$: $I\text{mmm}$ $(D_{2d}^{25})$

Lattice complex: Co $\oplus 2a(0,0,0)$; W $\oplus 4f(x,\frac{1}{2},0)$ with $x = 0.205$; B $\oplus 4h(0,y,\frac{1}{2})$ with $y = 0.30$

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_2CoW_2$</td>
<td>0.7075</td>
<td>0.4561</td>
<td>0.3177</td>
</tr>
<tr>
<td>$AlGd_2Ni_2$</td>
<td>0.8416</td>
<td>0.5408</td>
<td>0.4186</td>
</tr>
<tr>
<td>$B_2NiW_2$</td>
<td>0.7077</td>
<td>0.4559</td>
<td>0.3186</td>
</tr>
<tr>
<td>$Cs_2PtTe_2$</td>
<td>1.1387</td>
<td>0.9250</td>
<td>0.3994</td>
</tr>
</tbody>
</table>

Table A1.29. Representative compounds for Structure 35. Pearson’s tables list 27 intermetallic compounds with this structure type.
**Structure 36**  
Prototype: CrFe (σ Phase)  
**SG # 136: P4_2/mmm (D_4h^4)**  
Lattice complex: M1 (metal atom 1) @ 2a(0, 0, 0); M2 @ 4f(x, x, 0) with x = 0.3981; M3 @ 8i(x, y, 0) with x = 0.4632 and y = 0.1316; M4 @ 8i(x, y, 0) with x = 0.7376 and y = 0.0653; M5 @ 4j(x, x, z) with x = 0.1823 and z = 0.2524

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>CrFe</td>
<td>0.87995</td>
<td>0.45442</td>
<td>FeV</td>
<td>0.894</td>
<td>0.462</td>
</tr>
<tr>
<td>FeMo</td>
<td>0.9218</td>
<td>0.4813</td>
<td>Mn_2Mo</td>
<td>0.910</td>
<td>0.474</td>
</tr>
<tr>
<td>PdTa_3</td>
<td>0.9978</td>
<td>0.5208</td>
<td>U</td>
<td>1.07589</td>
<td>0.56531</td>
</tr>
</tbody>
</table>

Table A1.30. Representative compounds for Structure 36. Pearson’s tables list 84 intermetallic compounds with this structure type.
Structure 37  
Prototype: \( \text{W}_6\text{Fe}_7 \) (\( \mu \) Phase)

*SG# 166: \( \text{R} \bar{3} \text{m} (D_{5d}^5) \)*

*SBS/PS: D8/hR13*

Lattice complex: hexagonal reference frame; Fe @ \( 3a(0, 0, 0) \) and \( 18h(x, \bar{x}, z) \) with \( x = 0.833 \) and \( z = 0.257 \); W @ \( 6c(0, 0, z) \) with \( z = 0.167 \), \( z = 0.346 \), \( z = 0.448 \)

<table>
<thead>
<tr>
<th>Compound</th>
<th>( a )</th>
<th>( c )</th>
<th>Compound</th>
<th>( a )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{W}_6\text{Fe}_7 )</td>
<td>0.4757</td>
<td>2.584</td>
<td>( \text{Co}_7\text{Nb}_6 )</td>
<td>0.501</td>
<td>2.650</td>
</tr>
<tr>
<td>( \text{Mn}_5\text{Si}_7 )</td>
<td>0.470</td>
<td>2.561</td>
<td>( \text{Ta}_7\text{Zn}_7 )</td>
<td>0.5035</td>
<td>2.7528</td>
</tr>
<tr>
<td>( \text{Al}_3\text{Nb}_5\text{Ni}_2 )</td>
<td>0.4993</td>
<td>2.7100</td>
<td>( \text{CuNiTa}_2 )</td>
<td>0.495</td>
<td>2.700</td>
</tr>
</tbody>
</table>

Table A1.31. Representative compounds for Structure 37. Pearson’s tables list 36 intermetallic compounds with this structure type.
Crystal Structure Descriptions

Structure 38  Prototype: $\text{Al}_3\text{Nb}_{10}\text{Ni}_9$ (M Phase)

$SBS/PS: \quad \text{—/oP52}  \quad \text{SG} \# 62: \text{Pnma} \left(D^{16}_{2h}\right)$

$Lattice parameters: \quad a = 0.9393, \quad b = 0.4933, \quad c = 1.6266$ \text{nm}

$Lattice complex: \quad \text{Nb} @ 4c(x, \frac{1}{4}, z) \text{ with } (x, z) \text{ equal to } (0.0593, 0.8506), (0.2996, 0.6016), (0.5242, 0.4590), (0.6164, 0.2932), (0.0144, 0.5518), \text{ and } (0.8388, 0.7062);$

$\text{Al \ and Ni are in solid solution on the following sites: } 4c(x, \frac{1}{4}, z) \text{ with } (x, z) \text{ equal to } (0.0714, 0.3775), (0.3255, 0.3303), \text{ and } (0.8168, 0.4222), \text{ and } 8d(x, y, z) \text{ with } (x, y, z) \text{ equal to } (0.1118, 0.0048, 0.7049) \text{ and } (0.2550, 0.9969, 0.4550)$
Structure 39  Prototype: Cr$_9$Mo$_{21}$Ni$_{20}$ (P Phase)

SBS/PS: —/αP56  

SG # 62: Pnma ($D_{2h}^{16}$)

Lattice parameters: $a = 1.6983$, $b = 0.4752$, $c = 0.9070$ nm

Lattice complex: the metal atoms are distributed over the following sites: $4c(x, \frac{1}{4}, z)$ with $(x, z)$ equal to $(0.1134, 0.0737)$, $(0.2547, 0.1363)$, $(0.1578, 0.3257)$, $(0.1819, 0.6058)$, $(0.3253, 0.6650)$, $(0.4536, 0.4746)$, $(0.4047, 0.1988)$, $(0.0780, 0.8152)$, $(0.3650, 0.9383)$, and $(0.0355, 0.5202)$; and $8d(x, y, z)$ with $(x, y, z)$ equal to $(0.5375, 0.9986, 0.2504)$ and $(0.2883, 0.0008, 0.3868)$. 
Structure 40  
Prototype: Co₅Cr₂Mo₃ (R Phase)

SBS/PS: —/hR53

SG # 148: R3 (C\(^3\))

Lattice parameters: \(a = 1.0903\), \(c = 1.9342\) nm

Lattice complex: the metal atoms are distributed over the following sites: 3b(0, 0, 1/2); 6c(0, 0, z) with z equal to 0.3044 and 0.0735; 18f\((x, y, z)\) with \((x, y, z)\) equal to (0.0509, 0.2790, 0.1000), (0.0212, 0.1393, 0.1962), (0.2250, 0.1969, 0.2685), (0.1759, 0.1265, 0.3969), (0.1132, 0.2687, 0.4652), (0.0330, 0.2579, 0.3183), (0.1596, 0.2470, 0.0020), and (0.2671, 0.2218, 0.1222)
**Structure 41**  
Prototype: Mg$_{32}$(Al,Zn)$_{49}$

*SBS/PS:* —/c1162  
*SG # 204:* Im$\overline{3}$ ($T_d^3$)

**Lattice complex:** Al, Zn @ 2$a(0, 0, 0)$; 24$q(0, y, z)$ with $y = 0.0908$ and $z = 0.1501$; 24$q(0, y, z)$ with $y = 0.1748$ and $z = 0.3007$; 48$h(x, y, z)$ with $y = 0.168$, $z = 0.1836$ and $z = 0.4031$; Mg @ 16$f(x, x, x)$ with $x = 0.1836$; 24$q(0, y, z)$ with $y = 0.2942$ and $z = 0.1194$; 12$e(x, 0, \frac{1}{2})$ with $x = 0.4002$; 12$e(x, 0, \frac{1}{2})$ with $x = 0.1797$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg$<em>{32}$(Al,Zn)$</em>{49}$</td>
<td>1.416</td>
</tr>
</tbody>
</table>

Table A1.32. *Representative compound for Structure 41.*
**Structure 42**  
*Prototype: α-Al-Mn-Si*

**SBS/PS:** —/cP138  
**SG # 200:** Pm3\( \bar{m} \) (\( T_1h \))

**Lattice complex:**  
- Mn @ 12\( j(y, z, 0) \) with \( y = 0.3271, z = 0.2006 \);  
- 12\( k(y, z, \frac{1}{2}) \) with \( y = 0.1797, z = 0.3085 \);  
- Al, Si @ 6\( e(x, 0, 0) \) with \( x = 0.3638 \);  
- 6\( h(x, \frac{1}{2}, \frac{1}{2}) \) with \( x = 0.1216 \);  
- 6\( f(x, 0, \frac{1}{2}) \) with \( x = 0.2897 \);  
- 12\( j(y, z, 0) \) with \( y = 0.1636 \) and \( z = 0.0997 \);  
- 12\( k(y, z, \frac{1}{2}) \) with \( y = 0.3342 \) and \( z = 0.399 \);  
- 12\( j(y, z, 0) \) with \( y = 0.3319 \), \( z = 0.4037 \);  
- 12\( k(y, z, \frac{1}{2}) \) with \( y = 0.1205 \), \( z = 0.1175 \);  
- 24\( l(x, y, z) \) with \( x = 0.1585 \), \( y = 0.1892 \), \( z = 0.298 \);  
- 24\( l(x, y, z) \) with \( x = 0.3897 \), \( y = 0.3127 \), \( z = 0.1955 \).

<table>
<thead>
<tr>
<th>Compound</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>α-Al-Mn-Si</td>
<td>1.268</td>
</tr>
</tbody>
</table>

Table A1.33. *Representative compound for Structure 42.*
Structure 43  
Prototype: AuBe$_5$

*SBS/PS: C15/cF24  
SG # 216: F43m (T$_d^3$)*

*Lattice complex: Au @ 3a(0, 0, 0); Be @ 4c($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) and 16e($\frac{7}{16}, \frac{5}{16}, \frac{5}{16}$)*

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AuBe$_5$</td>
<td>0.6085</td>
<td>Ni$_5$U</td>
<td>0.6780</td>
<td>Cu$_{35}$Gd</td>
<td>0.706</td>
</tr>
<tr>
<td>Cu$_5$Tm</td>
<td>0.6991</td>
<td>AgCu$_4$Gd</td>
<td>0.7163</td>
<td>Ni$<em>{66}$Zn$</em>{17}$Zr$_{17}$</td>
<td>0.6792</td>
</tr>
</tbody>
</table>

Table A1.34. Representative compounds for Structure 43. Pearson's tables list 97 intermetallic compounds with this structure type.
**Structure 44**

**Prototype:** Mn$_{23}$Th$_6$

*SBS/PS: D$_8$g/cF116  
SG # 225: Fm$\bar{3}$m ($O_6^h$)*

**Lattice complex:** Mn $@$ 4b($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$), 24d($0, \frac{1}{4}, \frac{1}{2}$), 32f($x, x, x$) with $x = 0.378$ and $x = 0.178$; Th $@$ 24e($x, 0, 0$) with $x = 0.203$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn$_{23}$Th$_6$</td>
<td>1.2523</td>
<td>Mn$_{23}$Sm$_6$</td>
<td>1.258</td>
<td>Ba$<em>6$Mg$</em>{23}$</td>
<td>1.521</td>
</tr>
<tr>
<td>Fe$_{23}$Tb$_6$</td>
<td>1.2007</td>
<td>Mn$<em>6$Ni$</em>{16}$Si$_7$</td>
<td>1.1063</td>
<td>Fe$<em>{10}$Ge$</em>{13}$Ti$_6$</td>
<td>1.1704</td>
</tr>
</tbody>
</table>

Table A1.35. Representative compounds for Structure 44. Pearson’s tables list 186 intermetallic compounds with this structure type.
Structure 45  
Prototype: NaZn$_{13}$  

SG # 226: Fm$\overline{3}c$ ($O_h$)  
Lattice complex: Na @ 8a($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$); Zn @ 8b(0, 0, 0) and 96i(0, y, z) with y = 0.178, z = 0.122

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaZn$_{13}$</td>
<td>1.22836</td>
<td>Co$_{13}$La</td>
<td>1.133</td>
<td>Be$_{13}$Mg</td>
<td>1.0166</td>
</tr>
<tr>
<td>Cd$_{13}$Cs</td>
<td>1.389</td>
<td>Ni$_7$Si$_6$Sm</td>
<td>1.112</td>
<td>Co$_{11}$Ga$_2$La</td>
<td>1.14694</td>
</tr>
</tbody>
</table>

Table A1.36. Representative compounds for Structure 45. Pearson’s tables list 93 intermetallic compounds with this structure type.
Structure 46  Prototype: Be$_3$Nb
SBS/PS: —/hR12  SG # 166: R$3$m ($D_3^5$)
Lattice complex: Be @ $3b(0, 0, \frac{1}{2})$, $6c(0, 0, z)$ with $z = 0.3344$ and $18b(x, \bar{x}, z)$ with $(x = 0.504, z = 0.0818)$; Nb @ $3a(0, 0, 0)$ and $6c(0, 0, z)$ with $z = 0.1402$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be$_3$Nb</td>
<td>0.4561</td>
<td>2.105</td>
<td>Co$_3$Sm</td>
<td>0.50584</td>
<td>2.4618</td>
</tr>
<tr>
<td>Ca$_2$Ni$_3$</td>
<td>0.5030</td>
<td>2.427</td>
<td>DyFe$_3$</td>
<td>0.5125</td>
<td>2.4578</td>
</tr>
<tr>
<td>Co$_2$GaY</td>
<td>0.5132</td>
<td>2.626</td>
<td>Co$_3$H$_2$Pr</td>
<td>0.5091</td>
<td>2.757</td>
</tr>
</tbody>
</table>

Table A1.37. Representative compounds for Structure 46. Pearson’s tables list 112 intermetallic compounds with this structure type.
Structure 47  Prototype: CaCu$_5$

SG # 191: P6/mmm ($D_{6h}^1$)

Lattice complex: Ca @ 1a(0,0,0); Cu @ 2c($\frac{1}{3},\frac{2}{3},0$) and 3g($\frac{1}{2},0,\frac{1}{2}$).

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaCu$_5$</td>
<td>0.5082</td>
<td>0.4078</td>
<td>Co$_5$Sm</td>
<td>0.50002</td>
<td>0.3964</td>
</tr>
<tr>
<td>Au$_5$Ba</td>
<td>0.558690</td>
<td>0.4542</td>
<td>NdPt$_5$</td>
<td>0.5345</td>
<td>0.4391</td>
</tr>
<tr>
<td>AlCu$_4$Er</td>
<td>0.5029</td>
<td>0.4139</td>
<td>GdRh$_3$Si$_2$</td>
<td>0.5505</td>
<td>0.3549</td>
</tr>
</tbody>
</table>

Table A1.38. Representative compounds for Structure 47. Pearson’s tables list 295 intermetallic compounds with this structure type.
Structure 48  Prototype: Ni$_{17}$Th$_2$

$SBS/PS$: $\overline{\overline{h}}$P38  
$SG\ #\ 194$: P6$_3$/mmc ($D_{6h}^4$)

Lattice complex: Ni @ 1$a(\frac{1}{3}, \frac{2}{3}, z)$ with $z = 0.110$, 6$b(\frac{1}{2}, 0, 0)$, 12$c(x, y, \frac{1}{4})$ with ($x = 0.333$, $y = 0.0$), and 12$d(x, 2x, z)$ with ($x = 0.167, z = 0.0$); Th @ 2$b(0, 0, \frac{1}{4})$ and 2$d(\frac{1}{3}, \frac{2}{3}, \frac{3}{4})$

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni$_{17}$Th$_2$</td>
<td>0.837</td>
<td>0.814</td>
<td>$\beta$-Co$_{17}$Sm$_2$</td>
<td>0.8384</td>
<td>0.8159</td>
</tr>
<tr>
<td>Be$_{17}$Ti$_2$</td>
<td>0.735</td>
<td>0.726</td>
<td>Dy$<em>2$Ni$</em>{17}$</td>
<td>0.8299</td>
<td>0.8037</td>
</tr>
<tr>
<td>Dy$_2$Ga$<em>5$Mn$</em>{12}$</td>
<td>0.8687</td>
<td>0.8616</td>
<td>Fe$_{34}$Sm$_3$Y$_3$</td>
<td>0.8502</td>
<td>0.8327</td>
</tr>
</tbody>
</table>

Table A1.39. Representative compounds for Structure 48. Pearson’s tables list 190 intermetallic compounds with this structure type.
**Structure 49**  
*Prototype: Th$_2$Zn$_{17}$*

*SBS/PS: —/hR19*  
*SGB # 166: R3m (D$_{3d}^5$)*

*Lattice complex:* Th $\oplus$ 6c$(0,0,z)$ with $z = 0.333$; Zn $\oplus$ 6c$(0,0,z)$ with $z = 0.097$,  
9$d(\frac{1}{2},0,\frac{1}{2}), 18f(x,0,0)$ with $x = 0.333$, and $18h(x,\bar{x},z)$ with $(x = 0.5, z = 0.167)$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Th$<em>2$Zn$</em>{17}$</td>
<td>0.903</td>
<td>1.320</td>
<td>$\alpha$-Co$_{17}$Sm$_2$</td>
<td>0.8420</td>
<td>1.2210</td>
</tr>
<tr>
<td>Ce$<em>2$Co$</em>{17}$</td>
<td>0.8378</td>
<td>1.2206</td>
<td>Ba$<em>{24}$Mg$</em>{17}$</td>
<td>1.0650</td>
<td>1.5587</td>
</tr>
<tr>
<td>Cu$_{12}$Dy$_2$Ga$_5$</td>
<td>0.8678</td>
<td>1.260</td>
<td>Fe$_{34}$SmTb$_3$</td>
<td>0.8519</td>
<td>1.2409</td>
</tr>
</tbody>
</table>

Table A1.40. *Representative compounds for Structure 49. Pearson’s tables list 223 intermetallic compounds with this structure type.*
**Structure 50**  
*Prototype: Mn$_{12}$Th*

*SG#  139: I4/mmm (D$_{4h}^{17}$)*  

*Lattice complex:*  
Th @ 2$a(0,0,0)$; Mn @ 8$f(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, 8$i(x, 0, 0)$ with $x = 0.361$,  
and 8$j(x, \frac{1}{2}, 0)$ with $x = 0.277$

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn$_{12}$Th</td>
<td>0.874</td>
<td>0.495</td>
<td>SmZn$_{12}$</td>
<td>0.8927</td>
<td>0.5215</td>
</tr>
<tr>
<td>Be$_{12}$Pd</td>
<td>0.7271</td>
<td>0.4251</td>
<td>CeMg$_{12}$</td>
<td>1.033</td>
<td>0.596</td>
</tr>
<tr>
<td>Fe$_6$Ga$_4$Yb</td>
<td>0.8648</td>
<td>0.5077</td>
<td>Fe$_5$Ga$_7$Sm</td>
<td>0.8671</td>
<td>0.5090</td>
</tr>
</tbody>
</table>

Table A1.41. *Representative compounds for Structure 50. Pearson’s tables list 338 intermetallic compounds with this structure type.*
Crystal Structure Descriptions

Structure 51  Prototype: BFe$_{14}$Nd$_2$

SG # 136: P4$_2$/mnm ($D_{4h}^{14}$)

Lattice complex: B @ 4f($x,x,0$) with $x = 0.3774$; Fe @ 4c(0, $\frac{1}{2}$, 0), 4e(0, 0, $z$) with $z = 0.3852$; 8j($x,x,z$) with ($x = 0.4021$, $z = 0.2955$) and ($x = 0.1824$, $z = 0.2543$), and 16k($x,y,z$) with ($x,y,z$) equal to (0.4627, 0.1404, 0.3237) and (0.7242, 0.0676, 0.3725); Nd 4f($x,x,0$) with $x = 0.1428$ and 4g($x,\bar{x},0$) with $x = 0.7302$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BFe$_{14}$Nd$_2$</td>
<td>0.8804</td>
<td>1.2205</td>
<td>B Dy$<em>2$Fe$</em>{14}$</td>
<td>0.8746</td>
<td>1.1977</td>
</tr>
<tr>
<td>C Ce$<em>2$Fe$</em>{14}$</td>
<td>0.87072</td>
<td>1.18956</td>
<td>C Er$<em>2$Fe$</em>{14}$</td>
<td>0.87213</td>
<td>1.17475</td>
</tr>
</tbody>
</table>

Table A1.42. Representative compounds for Structure 51. Pearson’s tables list 27 intermetallic compounds with this structure type.
Structure 52  Prototype: Fe$_{29}$Nd$_3$

$SG \# 12: \text{C}2/\text{m} (C^{3}_{2h})$

Lattice parameters: $a=1.06382$, $b=0.85892$, $c=0.97456$, $\beta = 96.93^\circ$

Lattice complex: Nd @ 2$a(0,0,0)$ and 4$i(x,0,z)$ with $x = 0.5975$, $z = 0.185$; Fe @ 4$i(x,0,z)$ with $(x,z)$= (0.1427, 0.2952), (0.2526, 0.5198), (0.8916, 0.2801), (0.707, 0.908); 8$j(x, y, z)$ with $(x, y, z)$= (0.7981, 0.7806, 0.0904), (0.625, 0.6436, 0.1832), (0.8018, 0.248, 0.3454), and (0.4037, 0.7466, 0.0633); 2$c(\frac{1}{2}, 0, 1)$, 4$e(0, \frac{1}{2}, \frac{1}{2})$, 4$g(0, y, 0)$ with $y = 0.3562$. 

\[ \text{C}2/\text{m} (C^{3}_{2h}) \]
Structure 53  Prototype: Sm$_2$Fe$_{17}$N$_3$

SBS/PS: —/hR22  SG # 166: R3m (D$_{3d}^5$)

Lattice parameters: a=0.87389, c=1.26528

Lattice complex: Fe @ 6c(0,0,z) with z = 0.0901, 9d($\frac{1}{2}$,0,$\frac{1}{2}$), 18f(x,0,0) with x = 0.2846, and 18h(x,$\bar{x}$,z), with x = 0.5063 and z = 0.1536; N @ 93($\frac{1}{2}$,0,0); Sm @ 6c(0,0,z) with z = 0.3441.
Structure 54  Prototype: Sm(Fe,Ti)$_{12}$N
SBS/PS: $\overline{1}$128  SG # 139: 14/mmm ($D_{4h}^{17}$)

Lattice parameters: $a = 0.85, c = 0.48$

Lattice complex: Fe @ 8$f(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, 8$i(x, 0, 0)$ with $x = 0.353$, 8$j(x, \frac{1}{2}, 0)$ with $x = 0.293$; N @ 2$b(0, 0, \frac{1}{2})$; Sm @ 2$a(0, 0, 0)$. 

Crystal Structure Descriptions
Structure 55  
Prototype: Fe$_3$C  
SBS/PS: —/aP16  
SG # 62: Pnma ($D_{2h}^{16}$)  

Lattice complex: Fe @ 2c($x, \frac{1}{2}, z$) with $x = 0.044$ and $z = 0.837$; and 8d($x, y, z$) with $x = 0.181, y = 0.063$, and $z = 0.337$; C @ 2c($x, \frac{1}{2}, z$) with $x = 0.881$ and $z = 0.431$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe$_3$C</td>
<td>0.50787</td>
<td>0.67297</td>
<td>0.45144</td>
</tr>
</tbody>
</table>

Table A1.43. Representative compound for Structure 55.
**Structure 56**  
Prototype: Fe$_2$B  

*SBS/PS*: $-\overline{1}12$  
*SG* # 140: I$4/mcm$ ($D_{4h}^{18}$)  

*Lattice complex*: Fe @ 8$h(x, \frac{1}{2} + x, 0)$ with $x = 0.1661$; and B @ 4$a(0, 0, \frac{1}{4})$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe$_2$B</td>
<td>0.5109</td>
<td>0.4249</td>
</tr>
</tbody>
</table>

Table A1.44. *Representative compound for Structure 56.*
Structure 57  Prototype: Fe$_{23}$Zr$_6$

SBS/PS: —cF116  
SG # 225: Fm$ar{3}$m ($O_h^5$)

Lattice complex: Fe @ 4b($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$); and 24d($0, \frac{1}{2}, \frac{1}{2}$); and 32f($x, x, x$) with $x = 0.378$ and $x = 0.178$; Zr @ 24e($x, 0, 0$) with $x = 0.203$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn$_{23}$Zr$_6$</td>
<td>1.2523</td>
</tr>
<tr>
<td>Fe$_{23}$Zr$_6$</td>
<td>1.169</td>
</tr>
</tbody>
</table>

Table A1.45. Representative compounds for Structure 57.
Structure 58  Prototype: $\text{Al}_2\text{O}_3$

\[ \text{SG} \# 167: \text{R}3\text{c} (D_{3d}^6) \]

\text{Lattice complex: A}1@ 12c(0, 0, z) with $z = 0.3521$; and O@ 18e($x, 0, 1/4$) with $x = 0.3065$;

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Al}_2\text{O}_3$</td>
<td>0.47617</td>
<td>1.29947</td>
</tr>
</tbody>
</table>

Table A1.46. \textit{Structural data for corundum: Structure 58.}
Structure 59  
Prototype: CaTiO$_3$  
SBS/PS: E21/cP5  
SG # 221: Pm3m ($O_h^3$)  
Lattice complex: Ti @ 1b($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$); and O @ 3d($\frac{1}{2}, \frac{1}{2}, 0$); and Ca @ 1a(0,0,0).

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaTiO$_3$</td>
<td>0.3795</td>
</tr>
<tr>
<td>MgSiO$_3$</td>
<td>0.348</td>
</tr>
</tbody>
</table>

Table A1.47. Structural data for Structure 59.
**Structure 60**  
*Prototype: MgAl$_2$O$_4*

SBS/PS: H1/cF56  
SG # 227: Fd3m ($O_h^6$)

*Lattice complex:*  
Mg@ 8$a$($\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$); and Al@ 16$d$($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$); and O@ 32(e$(x,x,x)$) with $x = 0.262$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>Compound</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgAl$_2$O$_4$</td>
<td>0.808</td>
<td>ZnAl$_2$O$_4$</td>
<td>0.812</td>
</tr>
<tr>
<td>Fe$_3$O$_4$</td>
<td>0.84</td>
<td>(Zn,Mn,Fe)(Fe,Mn)$_2$O$_4$</td>
<td>0.842</td>
</tr>
<tr>
<td>FeCr$_2$O$_4$</td>
<td>0.836</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table A1.48. *Structural data for Structure 60.*
**Structure 61**  
Prototype: CdI$_2$  
SBS/PS: C6/hP5  
SG # 164: P3m1 ($D_{3d}^3$)  

Lattice parameters: $a = 0.4224$, $c = 0.6859$

Lattice complex: Cd @ 1a(0, 0, 0); and I @ 2d($\frac{1}{3}$, $\frac{2}{3}$, z) with $z = 0.2492$. 
**Structure 62**  
Prototype: TiO$_2$  
SBS/PS: C4/P6  
SG #136: P4$_2$/mm (D$_{4h}^{14}$)  
Lattice complex: Ti @ 2a(0, 0, 0); and O @ 4f(x, x, 0) with x = 0.3053

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiO$_2$</td>
<td>0.4537</td>
<td>0.2958</td>
</tr>
</tbody>
</table>

Table A1.49. Structural data for Structure 62.
Structure 63  Prototype: BaFe$_{12}$O$_{19}$

SG # 194: P6$_3$/mmc ($D_{6h}$)

Lattice complex:  
- Ba @ 2d($\frac{1}{3}, \frac{1}{3}, 0$); Fe @ 2a(0, 0, 0); 2b(0, 0, $\frac{1}{3}$); 4f($\frac{1}{3}, \frac{2}{3}, 0$) with $z = 0.0028$; 12k($x, 2x, z$) with $x = 0.167$ and $z = 0.108$; O @ 4c(0, 0, 0) with $z = 0.150$; 4f($\frac{1}{3}, \frac{2}{3}, z$) with $z = -0.05$; 6h($x, 2x, \frac{1}{3}$) with $x = 0.5$; 12k($x, 2x, z$) with ($x, z$) = (0.167, 0.050) and (0.5, 0.150).

<table>
<thead>
<tr>
<th>Compound</th>
<th>a</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaFe$<em>{12}$O$</em>{19}$</td>
<td>0.5892</td>
<td>2.3183</td>
</tr>
<tr>
<td>Ba$<em>{0.68}$K$</em>{0.31}$Ti$<em>{0.68}$Fe$</em>{5.93}$Mg$<em>{0.69}$(Cr,Mn,Ni)$</em>{0.34}$O$_{19}$ (Haggertyite)</td>
<td>0.59369</td>
<td>2.32445</td>
</tr>
</tbody>
</table>

Table A1.50. Structural data for Structure 63.
**Structure 64**  
*Prototype:* PbBi$_2$Nb$_2$O$_9$  

*SBS/PS:* —/αA56  

*SG # 36:* Cmc2$_1$ (C$_{12}^{12}$v)  

**Lattice complex:**  
- Pb @ 4a($\frac{1}{4}$, $\frac{1}{2}$, $\frac{1}{2}$) with $y = 0.2693$;  
- Bi @ 8b(x, y, z) with $y = 0.2662$, $y = 0.742$ and $z = 0.2013$;  
- Nb @ 8b(x, y, z) with $x = 0.2776$, $y = 0.7435$ and $z = 0.4115$;  
- O @ 4a(x, y, 0) with $x = 0.3092$ and $y = 0.1936$;  
- 8b(x, y, z) with $(x, y, z) = (0.3034, y = 0.2751, z = 0.1593)$, $(0.5236, 0.4977, 0.2473)$, $(0.5283, 0.027, 0.5715)$, and $(0.5967, 0.5457, 0.5846)$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbBi$_2$Nb$_2$O$_9$</td>
<td>0.5503</td>
<td>0.5495</td>
<td>2.5531</td>
</tr>
</tbody>
</table>

Table A1.51. *Structural data for Structure 64.*
Structure 65  Prototype: ZnWO$_4$

Prototype: ZnWO$_4$

\begin{align*}
\text{SBS/PS: } & \text{ } -/\text{mP12} & \text{SG } \# 13: & \text{ P2} /c \text{ (C}_{4\text{h}})
\end{align*}

Lattice complex:  Zn @ 2f($\frac{1}{2}, y, \frac{1}{2}$) with $y = 0.674$; W @ 2e(0, $y, \frac{1}{2}$) with $y =$ 0.2662; O @ 4g($x, y, z$) with ($x, y, z$) = (0.22, 0.11, 0.95) and (0.26, 0.38, 0.39).

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnWO$_4$</td>
<td>0.472</td>
<td>0.57</td>
<td>0.495</td>
<td>90.15°</td>
</tr>
</tbody>
</table>

Table A1.52. Structural data for Structure 65.
**Structure 66**  
Prototype: Ti$_2$CS  

*SG# 194: P6$_3$/mmc (D$_{6h}$)*  

Lattice complex:  

\[ \text{Ti} @ 4e(0, 0, z) \text{ with } z = 0.1; \text{ C} @ 2a(0, 0, 0); \text{ S} @ 2d(\frac{1}{3}, \frac{2}{3}, \frac{1}{2}). \]

<table>
<thead>
<tr>
<th>Compound</th>
<th>( a )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti$_2$CS</td>
<td>0.321</td>
<td>1.12</td>
</tr>
</tbody>
</table>

Table A1.53. *Structural data for Structure 66.*
**Structure 67**  
*Prototype: BaPb$_{1-x}$Bi$_x$O$_3$ (0.05 < x < 0.30)*

*SBS/PS: —/015  
SG # 140: I4/mcm (D$_{4h}^{18}$)*

*Lattice parameters: a = 0.605, c = 0.8621*

*Lattice complex: Pb,Bi @ 4b(0, 1/2, 1/4); Ba @ 4c(0, 0, 0); O @ 4d(0, 1/2, 0) and 8e(1/4, 1/4, 1/4)*;
Structure 68  Prototype: \( \text{Ba}_{1-x}\text{K}_x\text{BiO}_3 \) (0.37 < \( x \) < 0.5)

\( SBS/PS: \rightarrow cP5 \)  \( SG \# 221: \ Pm3m \ (O_h^1) \)

Lattice parameters: \( a = 0.429 \)

\textit{Lattice complex:} \( \text{Bi} @ 1a(0.5, 0.5, 0.5); \text{Ba} @ 1b(0, 0, 0); \text{O} @ 3d(0.5, 0.5, 0); \)
Structure 69  
Prototype: La$_2$CuO$_4$

SG # 139: $I4/mmm$ ($D_{4h}^{17}$)

Lattice parameters: $a = 0.3783$, $c = 1.32883$

Lattice complex: La @ $xx(0, 0, z)$ with $z = 0.3606$; Cu @ $xx(0, 0, 0)$; O @ $xx(0, \frac{1}{2}, 0)$ and $xx(0, 0, z)$ with $z = 0.1828$. 
Structure 70  
Prototype: Nd₂CuO₄  
SBS/PS: —/t₁₅  
SG # 139: 14/mmm (D¹₇₄h)  
Lattice parameters: \( a = 0.395, c = 1.207 \)  
Lattice complex: Nd @ \((0, 0, z)\) with \( z = 0.3513 \); Cu @ \((0, 0, 0)\); O @ \((0, \frac{1}{2}, 0)\) and \((0, \frac{1}{2}, \frac{1}{4})\).
Structure 71  Prototype: YBa$_2$Cu$_3$O$_{7-x}$

SBS/PS: —/tI5  

SG # 47: Pmmm ($D_{2h}^1$)

Lattice parameters: $a = 0.38198$, $b = 0.38849$, $c = 1.16762$

Lattice complex: Y @ 1h($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$); Ba @ 2t($\frac{1}{2}$, $\frac{1}{2}$, z) with $z = 0.1843$; Cu @ 1a(0, 0, 0) and 2t($\frac{1}{2}$, $\frac{1}{2}$, z) with $z = 0.3556$; O @ 1e(0, $\frac{1}{2}$, 0), 2s($\frac{1}{2}$, 0, z) with $z = 0.3779$ and 2r(0, $\frac{1}{2}$, z) with $z = 0.379$. 
**Structure 72**  
Prototype: Bi$_2$Sr$_2$CuO$_{6+x}$  
SBS/PS: —/tI5  
SG # 139: I4/mmm ($D_{4h}^{17}$)  
Lattice parameters: $a = 0.3886$, $c = 2.4662$

*Lattice complex:*  
Bi @ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.202$;  
Sr @ $xx(0, 0, z)$ with $z = 0.083$;  
Cu @ $xx(\frac{1}{2}, \frac{1}{2}, 0)$;  
O @ $xx(0, \frac{1}{2}, 0)$;  
$xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.116$ and $z = 0.288$.  

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Crystal Structure Descriptions

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Structure 73  Prototype: Bi₂Sr₂CaCu₂O₈₊ₓ

SBS/PS: —/tI5  SG # 139: I₄/mmm (D₁₇)

Lattice parameters: \(a = 0.3828\), \(c = 3.089\)

Lattice complex: 
- Bi @ \(xx(\frac{1}{2}, \frac{1}{2}, z)\) with \(z = 0.2136\);
- Ca @ \(xx(0, 0, 0)\);
- Sr @ \(xx(0, 0, z)\) with \(z = 0.1218\);
- Cu @ \(xx(\frac{1}{2}, \frac{1}{2}, z)\) with \(z = 0.054\);
- O @ \(xx(0, \frac{1}{2}, z)\) with \(z = 0.0531, xx(\frac{1}{2}, \frac{1}{2}, z)\) with \(z = 0.1461, xx(x, \frac{1}{2}, z)\) with \(x = 0.604\) and \(z = 0.2815\).
Structure 74  
Prototype: Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+z}$

SBS/PS: —/tI5  
SG # 139: I4/mmm ($D_{4h}^{17}$)

Lattice parameters: $a = 0.38503$, $c = 3.70$

Lattice complex: Bi @ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.22$; Ca @ $xx(0, 0, z)$ with $z = 0.046$; Sr @ $xx(0, 0, z)$ with $z = 0.144$; Cu @ $xx(\frac{1}{2}, \frac{1}{2}, 0)$; $xx(\frac{1}{2}, 0, z)$ with $z = 0.089$; O @ $xx(\frac{1}{2}, 0, 0)$; $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.158$ and $z = 0.2724$; $xx(\frac{1}{2}, 0, z)$ with $z = 0.087$. 
**Structure 75**  
*Prototype: Bi$_2$Sr$_2$Ca$_3$Cu$_4$O$_{12+z}$*  
*SBS/PS: n15*  
*SG # 139: $Imm$ ($D_{4h}^{17}$)*

**Lattice parameters:** $a = 0.38503$, $c = 4.226$

**Lattice complex:** Bi @ $xx(\frac{1}{2},\frac{1}{2}, z)$ with $z = 0.224$; Ca @ $xx(0,0,0)$; $xx(0,0,z)$ with $z = 0.076$; Sr @ $xx(0,0,z)$ with $z = 0.138$; Cu @ $xx(\frac{1}{2},\frac{1}{2}, z)$ with $z = 0.038$ and $z = 0.136$; O @ $xx(\frac{1}{2},\frac{1}{2}, z)$ with $z = 0.136$ and $z = 0.268$; $xx(\frac{1}{2},0,z)$ with $z = 0.038$ and $z = 0.114$. 
Structure 76  Prototype: Tl\textsubscript{2}Ba\textsubscript{2}CuO\textsubscript{6+z}

SBS/PS: —/\textit{i}15  
SG # 139: I4/mmm ($D_{4h}^{17}$)

Lattice parameters: $a = 0.3866$, $c = 2.329$

Lattice complex: Tl @ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.202$; Ba @ $xx(0, 0, z)$ with $z = 0.083$; Cu @ $xx(\frac{1}{2}, \frac{1}{2}, 0)$; O @ $xx(0, \frac{1}{2}, 0); xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.116$ and $z = 0.288$. 
**Structure 77**  
Prototype: $\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_{8+x}$

$SG \# 139$: $\text{I4}/\text{mmm} (D_{4h}^{17})$

Lattice parameters: $a = 0.3855$, $c = 2.9318$

Lattice complex: Tl@ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.2136$; Ca@ $xx(0, 0, 0)$; Ba@ $xx(0, 0, z)$ with $z = 0.1218$; Cu@ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.054$; O@ $xx(0, \frac{1}{2}, z)$ with $z = 0.0531$; $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.1461$; $xx(x, \frac{1}{2}, z)$ with $x = 0.604$ and $z = 0.2815$. 
Structure 78  Prototype: Tl$_2$Ba$_2$Ca$_2$Cu$_3$O$_{10+x}$

SBS/PS: —/—/5

SG # 139: I4/mmm ($D_{4h}^{17}$)

Lattice parameters: $a = 0.38503$, $c = 3.588$

Lattice complex: Tl@ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.22$; Ca@ $xx(0, 0, z)$ with $z = 0.046$; Ba@ $xx(0, 0, z)$ with $z = 0.144$; Cu@ $xx(\frac{1}{2}, \frac{1}{2}, 0)$; $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.089$; O@ $xx(\frac{1}{2}, 0, 0)$; $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.158$ and $z = 0.2724$; $xx(\frac{1}{2}, 0, z)$ with $z = 0.087$. 
Structure 79  Prototype: Tl₂Ba₂Ca₃Cu₄O₁₂₊ₓ

SBS/PS: —/tI5  SG # 139: I4/mmm (D₁₇₄)

Lattice parameters: a = 0.38503, c = 4.226

Lattice complex: Tl @ xx(1/2, 1/2, z) with z = 0.224; Ca @ xx(0, 0, 0); xx(0, 0, z) with z = 0.076; Ba @ xx(0, 0, z) with z = 0.138; Cu @ xx(1/2, 1/2, z) with z = 0.038 and z = 0.136; O @ xx(1/2, 1/2, z) with z = 0.136 and z = 0.268; xx(1/2, 0, z) with z = 0.0.038 and z = 0.114.
Crystal Structure Descriptions

Structure 80  Prototype: TlBa$_2$CuO$_5$

SBS/PS: —/tI5

SG # 123: P4/mmm ($D_{4h}^1$)

Lattice parameters: $a = 0.385$, $c = 0.954$

Lattice complex: Tl@ $xx(\frac{1}{2}, \frac{1}{2}, 0)$; Ba@ $xx(0, 0, z)$ with $z = 0.298$; Cu@ $xx(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; O@ $xx(0, 0, 0)$; $xx(0, \frac{1}{2}, \frac{1}{2})$; $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.2078$. 
Structure 81 Prototype: TlBa$_2$CaCu$_2$O$_7$

Lattice parameters: $a = 0.38234$, $c = 1.2384$

Lattice complex: Tl@ $xx(0, 0, 0)$; Ba@ $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.2128$; Ca@ $xx(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; Cu@ $xx(0, 0, z)$ with $z = 0.3675$; O@ $xx(\frac{1}{2}, \frac{1}{2}, 0)$; $xx(0, 0, z)$ with $z = 0.164$; $xx(\frac{1}{2}, 0, z)$ with $z = 0.3749$.
Crystal Structure Descriptions

**Structure 82**  
**Prototype:** TlBa$_2$Ca$_2$Cu$_3$O$_9$

**SBS/PS:** —/tI5  
**SG # 123:** P4/mmm ($D_{4h}^1$)

**Lattice parameters:** $a = 0.38429$, $c = 1.5871$

**Lattice complex:** Tl at $xx(0, 0, 0)$; Ba at $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.176$; Ca at $xx(\frac{1}{2}, \frac{1}{2}, z)$ with $z = 0.397$; Cu at $xx(0, 0, \frac{1}{2})$; $xx(0, 0, z)$ with $z = 0.302$; O at $xx(\frac{1}{2}, \frac{1}{2}, 0)$; $xx(0, \frac{1}{2}, \frac{1}{2})$; $xx(0, \frac{1}{2}, z)$ with $z = 0.304$; $xx(0, 0, z)$ with $z = 0.132$.
Structure 83  
Prototype: TlBa$_2$Ca$_3$Cu$_4$O$_{11}$

SBS/PS: $\overline{4}i15$  
SG # 139: $I4/mmm (D^{17}_{4h})$

Lattice parameters: $a = 0.385, c = 1.915$

Lattice complex: Tl@$xx(0,0,0)$; Ba@$xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.150$; Ca@$xx(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; $xx(\frac{1}{2},\frac{1}{2},z)$ with $z = 0.3315$; Cu@$xx(0,0,z)$ with $z = 0.248$ and $z = 0.4151$; O@$xx(\frac{1}{2},\frac{1}{2},0); xx(0,0,z)$ with $z = 0.15; xx(\frac{1}{2},0,z)$ with $z = 0.248$ and $z = 0.4151$. 
Structure 84  Prototype: AgBa\textsubscript{2}Ca\textsubscript{3}Cu\textsubscript{4}O\textsubscript{10}

$SG \ # \ 83:\ P4/m \ (C_{4h})$

Lattice parameters: $a = 0.386$, $c = 1.81$

Lattice complex: Ag @ $xx(0,0,0)$; Ba @ $xx(1/2,1/2,z)$ with $z = 0.883$; Ca @ $xx(1/2,1/2,1/2)$; $xx(1/2,1/2,z)$ with $z = 0.677$; Cu @ $xx(0,0,0)$; $xx(0,0,z)$ with $z = 0.5884$ and $z = 0.7650$; O @ $xx(1/2,1/2,0)$; $xx(0,1/2,z)$ with $z = 0.5884$ and $z = 0.7650$; $xx(0,0,z)$ with $z = 0.8830$. 
Structure 85  
Prototype: (Ba,Sr)CuO$_4$

SBS/PS: —/015  
SG # 123: P4/mmm ($D_{4h}^1$)

Lattice parameters: $a = 0.393$, $c = 0.347$

Lattice complex: Ba,Sr @ $xx(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; Cu @ $xx(0,0,0)$; O @ $xx(0,\frac{1}{2},0)$. 

Crystal Structure Descriptions

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Prototype: (Ba,Sr)CuO$_4$

SBS/PS: —/015  
SG # 123: P4/mmm ($D_{4h}^1$)

Lattice parameters: $a = 0.393$, $c = 0.347$

Lattice complex: Ba,Sr @ $xx(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; Cu @ $xx(0,0,0)$; O @ $xx(0,\frac{1}{2},0)$. 

Crystal Structure Descriptions
**Structure 86**  
*Prototype: Forsterite: Mg$_2$SiO$_4$*

*SBS/PS: S1$_2$/oP28*  
*SG # 62: Pnma (D$^{16}_{2h}$)*

**Lattice parameters:** $a = 0.4762$, $b = 1.0225$, $c = 0.462$

**Lattice complex:**
- Mg @ 4$a$(0, 0, 0); and 4$c$(x, y, $\frac{1}{4}$) with $x = 0.9896$ and $y = 0.2776$
- O @ 4$c$(x, y, $\frac{1}{4}$) with $x = 0.7667$ and $y = 0.0918$; 4$c$(x, y, $\frac{1}{4}$) with $x = 0.2202$ and $y = 0.4477$; 8$d$(x, y, z) with $x = 0.2781$, $y = 0.1633$ and $z = 0.0337$
- Si @ 4$c$(x, y, $\frac{1}{4}$) with $x = 0.4226$ and $y = 0.5994$.
Structure 87  Prototype: Garnet: Ca$_3$Fe$_2$Si$_3$O$_{12}$

$SG # 230: \text{Ia\overline{3}d (O}^{10}_h)$

Lattice parameters: $a = 1.203$

Lattice complex: Ca@ 24c($\frac{1}{8}, 0, \frac{1}{4}$); Fe@ 16a(0, 0, 0); O@ 96h($x, y, z$) with $x = 0.0395, y = 0.0488$ and $z = 0.6556$; Si@ 24d($\frac{3}{8}, 0, \frac{1}{4}$).
**Structure 88**  
Prototype: Zircon ZrSiO$_4$

*SBS/PS:* 1/t124  
*SG # 141:* $I4_1/amd$ ($D_{19}^{19}$)

**Lattice parameters:** $a = 0.661$, $c = 0.6001$

**Lattice complex:**  
Zr@ 4a(0, $\frac{3}{4}$, $\frac{1}{8}$);  
O@ 16h(0, $y$, $z$) with $y = 0.0616$ and $z = 0.1967$;  
Si@ 4b($\frac{1}{4}$, $\frac{1}{4}$, $\frac{3}{8}$).
Structure 89  Prototype: Kyanite $\text{Al}_2\text{SiO}_5$

$SBS/PS$: —/tP16  $SG$ # 2: $\text{P}\overline{1}$ ($\text{C}_1^i$)

Lattice parameters: $a = 0.71262$, $b = 0.7852$, $c = 0.5724$, $\alpha = 89.99^\circ$, $\beta = 101.11^\circ$, $\gamma = 106.03^\circ$

Lattice complex: $\text{Al} @ 2i(x, y, z)$ with $(x, y, z) = (0.3254, 0.704, 0.4582)$, $(0.2974, 0.6989, 0.9505)$, $(0.0998, 0.3863, 0.6403)$, and $(0.112, 0.9175, 0.1649)$; $\text{O} @ 2i(x, y, z)$ with $(x, y, z) = (0.1095, 0.1468, 0.1288)$, $(0.123, 0.6856, 0.1812)$, $(0.2747, 0.4545, 0.9547)$, $(0.2831, 0.9354, 0.9353)$, $(0.1084, 0.152, 0.6669)$, $(0.1219, 0.6307, 0.6389)$, $(0.2822, 0.4453, 0.4288)$, $(0.2915, 0.9467, 0.4459)$, $(0.5008, 0.2749, 0.244)$ and $(0.5015, 0.2312, 0.7553)$; $\text{Si} @ 2i(x, y, z)$ with $(x, y, z) = (0.2962, 0.0649, 0.7066)$ and $(0.291, 0.3317, 0.1892)$. 
Structure 90  Prototype: Sillimanite Al$_2$SiO$_5$

SBS/PS: —/αP32  
SG # 62: Pnma ($D^{16}_{2d}$)

Lattice parameters: $a = 0.74883$, $b = 0.76808$, $c = 0.5774$

Lattice complex: Al @ 4a(0, 0, 0); and 4c($x$, $y$, $\frac{1}{2}$) with $x = 0.1417$ and $y = 0.3449$; O @ 4c($x$, $y$, $\frac{3}{4}$) with ($x$, $y$) = (0.3605, 0.4094), (0.4763, 0.0015) and (0.3569, 0.4341); 8d($x$, $y$, $z$) with ($x$, $y$, $z$) = (0.2747, 0.4545, 0.9547), (0.2831, 0.9354, 0.9353) and (0.1252, 0.223, 0.5145); Si @ 4c($x$, $y$, $\frac{3}{4}$) with $x = 0.1533$ and $y = 0.3402$;
Crystal Structure Descriptions

Structure 91  
Prototype: Epidote Ca₂(Al,Fe)Al₂Si₃O₁₃H  
SBS/PS: —/mP44  
SG # 11: P2₁/m (C2h)  

Lattice parameters: \( a = 0.8914, b = 0.564, c = 1.0162, \beta = 115.4^\circ \)  

Lattice complex:  
\( \text{Ca} \)@ 2\( e(x, \frac{1}{2}, z) \) with \((x, z) = (0.2438, 0.849)\) and \((0.3968, 0.579)\);  
\( \text{Al} \)@ 2\( a(0, 0, 0) \);  
\( \text{Fe} \)@ 2\( e(x, \frac{1}{2}, z) \) with \( x = 0.2946 \) and \( z = 0.2245 \);  
\( \text{O} \)@ 4\( f(x, y, z) \) with \((x, y, z) = (0.2339, 0.9923, 0.041), (0.304, 0.9809, 0.3554)\) and \((0.7957, 0.0152, 0.3382)\);  
\( \text{Si} \)@ 2\( e(x, \frac{1}{2}, z) \) with \((x, z) = (0.6604, 0.9527), (0.8156, 0.6811)\) and \((0.6851, 0.2744)\).
Structure 92  Prototype: Wollastonite-1T CaSiO$_3$

SBS/PS: —/tC40

SG # 2: $\overline{P}1$ ($C_i$)

Lattice parameters: $a = 1.0121$, $b = 1.107$, $c = 0.7312$, $\alpha = 99.51^\circ$, $\beta = 100.51^\circ$, $\gamma = 83.43^\circ$

Lattice complex: Ca @ 2i(x, y, z) with $(x, y, z) = (0.0208, 0.7807, 0.0772), (0.0171, 0.7806, 0.5709)$ and $(0.0144, 0.4885, 0.2504)$; O @ 2i(x, y, z) with $(0.1163, 0.5797, 0.0381), (0.1169, 0.5814, 0.5611), (0.1149, 0.3141, 0.7307), (0.1239, 0.8584, 0.8745), (0.123, 0.8577, 0.3669), (0.1152, 0.2864, 0.2267), (0.2211, 0.9963, 0.6785), (0.182, 0.0886, 0.3704)$ and $(0.1872, 0.0907, 0.0121)$; Si @ 2i(x, y, z) with $(x, y, z) = (0.2265, 0.9583, 0.8877), (0.2267, 0.9577, 0.4537)$, and $(0.2264, 0.1707, 0.2263)$. 

![Crystal Structure Diagram](image)
**Structure 93  Prototype: Jadeite NaAlSi$_2$O$_6$**

*SBS/PS: —/hP40  SG # 15: C2/c (C$^{6}_2$ih)*

Lattice parameters: $a = 0.9418$, $b = 0.8562$, $c = 0.5219$, $\beta = 107.58^\circ$

Lattice complex: Al @ 4e$(0, y, \frac{1}{2})$ with $y = -0.094$; Na @ 4e$(0, y, \frac{1}{2})$ with $y = 0.3009$; O @ 8f$(x, y, z)$ with $(x, y, z) = (0.109, 0.0763, 0.1277)$, $(0.3608, 0.263, 0.2929)$, and $(0.3433, 0.007, 0.0058)$; Si @ 8f$(x, y, z)$ with $x = 0.2906$, $y = 0.0934$ and $z = 0.2277$. 
Structure 94  Prototype: Beryl Be₃Al₂Si₆O₁₈
SBS/PS: —/hP40  SG # 192: P6/mmc (D₁₆h)
Lattice complex: a = 0.9212, c = 0.9236 Al @ 4c(2/3, 1/3, 1/2); Be @ 6f(1/2, 0, 1/4); Cs @
2a(0, 0, 1/4); Na @ 2b(0, 0, 0); O @ 12l(x, y, 0) with x = 0.3048 and y = 0.2352; and
24m(x, y, z) with x = 0.4983, y = 0.1473 and z = 0.1445; Si @ 12l(x, y, 0) with
x = 0.3892 and y = 0.1189.
Structure 95  
Prototype: Tremolite Ca\(_2\)Mg\(_5\)(Si\(_8\)O\(_{22}\))(OH)\(_3\)

SBS/PS: —/mC78  
SG # 12: C2/m (C\(_{2h}\))

Lattice complex: \(a = 0.9863\), \(b = 1.8048\), \(c = 0.5285\), \(\beta = 107.58^\circ\)  
Ca \(4h(0, y, \frac{1}{2})\) with \(y = 0.2779\); H \(4i(x, 0, z)\) with \(x = 0.2088\) and \(z = 0.7628\); Mg \(2a(0, 0, 0)\);  
Mg \(4h(0, y, \frac{1}{2})\) with \(y = 0.0883\); Na \(2b(0, \frac{1}{2}, 0)\);  
O \(8j(x, y, z)\) with \((x, y, z) = (0.1114, 0.0847, 0.2182), (0.1187, 0.1707, 0.725)\);  
Si \(8j(x, y, z)\) with \((x, y, z) = (0.338, 0.2921)\)

and \((0.3467, 0.1339, 0.0998)\) and \((0.3437, 0.1181, 0.591)\);  
Si \(8j(x, y, z)\) with \((x, y, z) = (0.2799, 0.0842, 0.2974)\) and \((0.2882, 0.1713, 0.8056)\).
Structure 96  Prototype: Kaolinite Al$_2$Si$_2$O$_5$(OH)$_4$

SBS/PS: —/tC26  SG # 1: P1 (C$1$

Lattice parameters: $a = 0.514, b = 0.893, c = 0.737, \alpha = 91.8^\circ, \beta = 104.5^\circ, \gamma = 90^\circ$

Lattice complex: All atoms in 1a($x, y, z$) positions: Al(0.502, 0.172, 0.003) and (0.002, 0.33, 0.002); O(0.754, 0.315, 0.155), (0.69, 0.004, 0.157), (0.791, 0.165, 0.482), (0.612, −0.12, 0.455) and (0.108, −0.058, 0.455); OH(0.778, 0.18, −0.14), (0.278, 0.32, −0.38), (0.316, −0.008, −0.136) and (0.248, 0.184, 0.155); Si(0.8, 0.322, 0.382) and (0.8, 0.0, 0.385).
Structure 97  
Prototype: α-Quartz SiO$_2$

$SG#154$: $P3_2121\ (D_6^3)$

Lattice parameters: $a = 0.49137$, $c = 0.54047$

Lattice complex: 
- O $6c(x, y, z)$ with $x = 0.4133$, $y = 0.2672$ and $z = 0.1188$
- Si $3a(x, 0, 0)$ with $x = 0.4697$

Origin offset by $(0, 0, -\frac{1}{3})$. 

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Crystal Structure Descriptions
**Structure 98**  
*Prototype: *β*-Quartz SiO$_2*  
*SBS/PS: —/hP9*  
*SG #171: P6$_2$ (C$1_2^1$)*  

**Lattice parameters:** $a = 0.49965$, $c = 0.54546$  

**Lattice complex:**  
O @ 6c$(x, y, z)$ with $x = 0.4157$, $y = 0.2078$ and $z = 0.1667$;  
Si @ 3a$(\frac{1}{2}, 0, 0)$; origin offset by $(0, 0, -\frac{1}{2})$.  

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*Crystal Structure Descriptions*  
A1–101
Structure 99  
Prototype: Na₄Al₃Si₃O₁₂CO

SG # 218: P43n (T₄)

Lattice parameters: a = 0.891

Lattice complex:  
Al @ 6e(1/4, 1/2, 0); Cl @ 2a(0, 0, 0); Na @ 8e(x, x, x); with x = 0.175; O @ 24i(x, y, z) with x = 0.15, y = 0.135 and z = 0.44; and Si @ 6c(1/4, 1/2, 0);
Structure 100  
Prototype: CaAl₂Si₄O₁₂·6H₂O
SBS/PS: —/hR74  
SG # 166: R3m (D₃d)
Lattice parameters: a = 0.937, α = 92.02°
Lattice complex: (dehydrated form) Ca @ 1a(0, 0, 0) with 0.6 site occupancy, 2c(x, x, x) with x = 0.169 and 0.35 site occupancy, 12i(x, y, z) with x = 0.09, y = 0.1609 and z = 0.47 and 0.16 site occupancy; O @ 6f(x, x, 0) with x = 0.284, 6g(x, x, 0.5) with x = 0.124, 6h(x, x, z) with x = 0.238 and z = 0.878, 6c(0, 0, z) with z = 0.255; Al, Si @ 12i(x, y, z) with x = 0.095, y = 0.328 and z = 0.864.
Structure 101  
Prototype: Fullerenoid Oxide Sr$_{33}$Bi$_{24+\delta}$Al$_{48}$O$_{141+\frac{24}{3}}$

SBS/PS: —/cF1784  
SG # 216: F$\bar{4}$3m ($T_d^3$)

Lattice parameters: $a = 2.509$

Lattice complex: Bi @ 16e($x, x, x$) with $x = 0.85$; 48h($x, x, z$) with ($x, z$) = (0.3, 0.5932) and (0.944475, 0.748866; occ.0.7); Sr @ 4c($\frac{3}{4},\frac{1}{4},\frac{3}{4}$); and 48h($x, x, z$) with ($x, z$) = (0.82763, 0.46345) and (0.17534, 0.99084); 16e($x, x, x$) with $x = 0.92946$ and $x = 0.587$; Al @ 48h($x, x, z$) with ($x, z$) = (0.0468, 0.1345), (0.0895, 0.2444), (0.7942, 0.1177) and (0.4545, 0.3661); O @ 16e($x, x, z$) with $x = 0.8269$ and $z = 0.1731$; 24f($0, 0, z$) with $z = 0.1121$; 24g($\frac{1}{2},\frac{1}{2}, z$) with $z = 0.1476$; 48h($x, z, z$) with $x = 0.0259$ and $y = 0.1083$, 48h($x, x, z$) with $x = 0.0772$ and $z = 0.312$; 48h($x, y, z$) with ($x, y, z$) = (0.51, 0.49, 0.345; occ.0.5) and (0.331, 0.372, 0.628; occ.1/3); 48h($x, y, x$) with ($x, y$) = (0.4047, 0.4853) and (0.796, 0.890; occ.0.6); 96i($x, y, z$) with ($x, y, z$) = (0.0421, 0.0585, 0.2042; occ.0.5), (0.1577, 0.0775, 0.2356), (0.9, 0.826, 0.9206; occ.0.5) and (0.273, 0.3597, 0.5388).
Structure 102  Prototype: Ice- I$_h$ H$_2$O

SG# 194: P6$_3$/mmc ($D_{6h}$)

Lattice parameters: $a = 0.45227$, $c = 0.73671$

Lattice complex: H @ 4f($\frac{1}{3}$, $\frac{2}{3}$, z) with $z = 0.173$; 12k(x, 2x, z) with $x = 0.437$ and $z = 0.024$; O @ 4f($\frac{1}{3}$, $\frac{2}{3}$, z) with $z = 0.0618$. 
Structure 103  Prototype: Ice-I, \( \text{H}_2\text{O} \)

SBS/PS: \(-/c\overline{F}24\)  

\(\text{SG} \ # \ 227: \ Fd\overline{3}m \ (O^7_h)\)  

Lattice parameters: \(a = 0.635\)  

Lattice complex: \(\text{H} @ 16c(\frac{1}{8}, \frac{1}{8}, \frac{1}{8}); \text{O} @ 8a(0,0,0)\).
Structure 104  Prototype: CO$_2$-Cubic

SBS/PS: $-\text{i}cP12$

$SG$ # 205: $\text{Pa}$\$\text{b} (T_b^6)$

Lattice parameters: $a = 0.5056$

Lattice complex: $\text{O}@ 8c(x, x, x)$ with $x = 0.1324$ and $x = -0.1324$; $\text{C}@ 4a(0, 0, 0)$. 
Structure 105  
Prototype: C₆H₆ 
SBS/PS: —/αP48  
SG # 61: Pbca (D¹⁺₅²₆)

Lattice parameters: \(a = 0.744, b = 0.955, c = 0.692\)

Lattice complex: All positions \(8\) \(c(x, y, z)\): C@ \((-0.0569, 0.1387, -0.0054), (-0.1335, 0.046, 0.1264)\) and \((-0.0774, -0.0925, 0.1295)\); H@ \((-0.0976, 0.2477, -0.0177), (-0.2409, 0.0794, 0.2218)\) and \((-0.1371, -0.1631, 0.2312)\).
Structure 106  
Prototype: Sr$_8$Ga$_{16}$Ge$_{30}$

SBS/PS: —/cP48  
SG # 223: Pm\bar{3}n (O$_h^4$)

Lattice complex:  
- Sr at $a = 1.0734$: Sr @ $2a(0,0,0); 24k(0,y,z)$ with $y = 0.2387$ and $z = 0.4623$;
- Ga at $6c(\frac{1}{2},0,0); 16i(x,x,x)$ with $x = 0.18459$;
- Ge at $16c(0,0,0); 24k(0,y,z)$ with $y = 0.30939$ and $z = 0.11770$. 
