

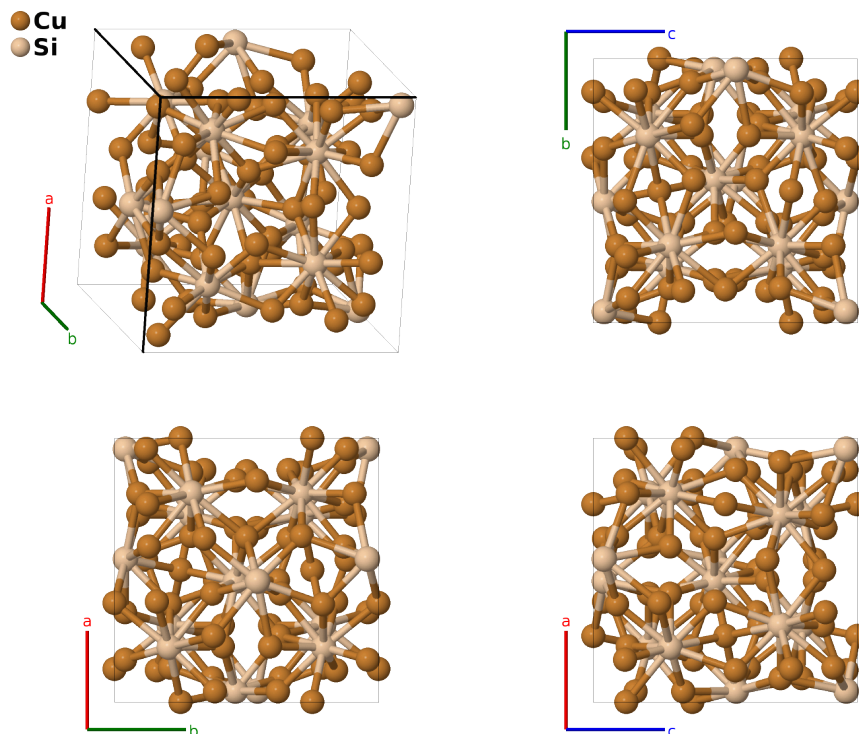
Cu₁₅Si₄ (*D*8₆) Structure: A15B4_cI76_220_ae_c-001

This structure originally had the label A15B4_cI76_220_ae_c. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/MVX2>

https://aflow.org/p/A15B4_cI76_220_ae_c-001



| | |
|------------------------------------|---|
| Prototype | Cu ₁₅ Si ₄ |
| AFLOW prototype label | A15B4_cI76_220_ae_c-001 |
| <i>Strukturbericht</i> designation | <i>D</i> 8 ₆ |
| ICSD | 629165 |
| Pearson symbol | cI76 |
| Space group number | 220 |
| Space group symbol | <i>I</i> $\bar{4}3d$ |
| AFLOW prototype command | <code>aflow --proto=A15B4_cI76_220_ae_c-001 --params=a, x₂, x₃, y₃, z₃</code> |

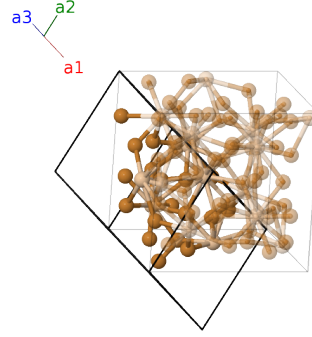
Other compounds with this structure

Cu₁₅As₄, Li₁₅Au₄, Li₁₅Ge₄, Li₁₅Si₄, Na₁₅Pb₄

- (Mattern, 2007) take their data from (Mukherjee, 1969), and we use the ICSD information from that reference.

Body-centered Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}a \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|--|-----|--|------------------|-----------|
| \mathbf{B}_1 | $= \frac{1}{4} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$ | $=$ | $\frac{3}{8}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$ | (12a) | Cu I |
| \mathbf{B}_2 | $= \frac{3}{4} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$ | $=$ | $\frac{1}{8}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{z}}$ | (12a) | Cu I |
| \mathbf{B}_3 | $= \frac{3}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$ | $=$ | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}}$ | (12a) | Cu I |
| \mathbf{B}_4 | $= \frac{1}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$ | $=$ | $\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}}$ | (12a) | Cu I |
| \mathbf{B}_5 | $= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$ | $=$ | $\frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}}$ | (12a) | Cu I |
| \mathbf{B}_6 | $= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$ | $=$ | $\frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$ | (12a) | Cu I |
| \mathbf{B}_7 | $= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_8 | $= \frac{1}{2} \mathbf{a}_1 - (2x_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_9 | $= -(2x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{10} | $= -(2x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$ | $=$ | $ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{11} | $= (2x_2 + \frac{1}{2}) \mathbf{a}_1 + (2x_2 + \frac{1}{2}) \mathbf{a}_2 + (2x_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{12} | $= \frac{1}{2} \mathbf{a}_1 - 2x_2 \mathbf{a}_3$ | $=$ | $-a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{13} | $= -2x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$ | $=$ | $a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{14} | $= -2x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$ | (16c) | Si I |
| \mathbf{B}_{15} | $= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$ | (48e) | Cu II |
| \mathbf{B}_{16} | $= (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$ | (48e) | Cu II |
| \mathbf{B}_{17} | $= (y_3 - z_3) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$ | (48e) | Cu II |
| \mathbf{B}_{18} | $= -(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (48e) | Cu II |
| \mathbf{B}_{19} | $= (x_3 + y_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (x_3 + z_3) \mathbf{a}_3$ | $=$ | $az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$ | (48e) | Cu II |
| \mathbf{B}_{20} | $= -(x_3 + y_3 - \frac{1}{2}) \mathbf{a}_1 + (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - z_3) \mathbf{a}_3$ | $=$ | $az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (48e) | Cu II |

$$\begin{aligned}
\mathbf{B}_{21} &= \begin{pmatrix} -x_3 + y_3 + \frac{1}{2} \\ y_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -az_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{22} &= \begin{pmatrix} x_3 - y_3 \\ x_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{23} &= \begin{pmatrix} x_3 + z_3 \\ y_3 + z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 + y_3 \\ y_3 + z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 + z_3 \\ y_3 + z_3 \end{pmatrix} \mathbf{a}_3 &= ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{24} &= \begin{pmatrix} -(x_3 - z_3) \\ x_3 + y_3 - \frac{1}{2} \\ -y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_3 + y_3 - \frac{1}{2} \\ -y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 + y_3 - \frac{1}{2} \\ -y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(x_3 + z_3 - \frac{1}{2}) \\ -x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 + z_3 - \frac{1}{2} \\ -x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_3 - z_3 \\ -x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{26} &= \begin{pmatrix} x_3 - z_3 + \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_3 + z_3 - \frac{1}{2} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -ay_3 \hat{\mathbf{x}} - a \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{27} &= \begin{pmatrix} x_3 + z_3 + \frac{1}{2} \\ y_3 + z_3 + \frac{1}{2} \\ x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_3 + z_3 + \frac{1}{2} \\ x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 + y_3 + \frac{1}{2} \\ x_3 + y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{28} &= \begin{pmatrix} -x_3 + z_3 + \frac{1}{2} \\ y_3 - z_3 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_3 - z_3 \\ x_3 + y_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_3 + y_3 \\ x_3 + y_3 \end{pmatrix} \mathbf{a}_3 &= -a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(x_3 + z_3) \\ y_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_3 - z_3 + \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_3 - y_3 \\ y_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{30} &= \begin{pmatrix} x_3 - z_3 \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_3 + z_3 \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 - y_3 + \frac{1}{2} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{31} &= \begin{pmatrix} y_3 + z_3 + \frac{1}{2} \\ x_3 + y_3 + \frac{1}{2} \\ x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 + y_3 + \frac{1}{2} \\ x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_3 + z_3 + \frac{1}{2} \\ x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{32} &= \begin{pmatrix} -(y_3 - z_3) \\ -x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_3 + y_3 \\ -x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_3 + z_3 + \frac{1}{2} \\ -x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{33} &= \begin{pmatrix} y_3 - z_3 + \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_3 - z_3 + \frac{1}{2} \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_3 + z_3 \\ x_3 - y_3 \end{pmatrix} \mathbf{a}_3 &= -a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{34} &= \begin{pmatrix} -(y_3 + z_3) \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 - y_3 + \frac{1}{2} \\ x_3 - z_3 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 - z_3 \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{35} &= \begin{pmatrix} x_3 + y_3 + \frac{1}{2} \\ x_3 + z_3 + \frac{1}{2} \\ y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 + z_3 + \frac{1}{2} \\ y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_3 + z_3 + \frac{1}{2} \\ y_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{36} &= \begin{pmatrix} -(x_3 + y_3) \\ -x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_3 + z_3 + \frac{1}{2} \\ y_3 - z_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_3 - z_3 \\ -x_3 + z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{37} &= \begin{pmatrix} -(x_3 - y_3) \\ y_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_3 + z_3 \\ y_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_3 + z_3 \\ y_3 - z_3 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II} \\
\mathbf{B}_{38} &= \begin{pmatrix} x_3 - y_3 + \frac{1}{2} \\ x_3 - z_3 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_3 - y_3 + \frac{1}{2} \\ x_3 - z_3 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_3 + z_3 \\ x_3 - z_3 \end{pmatrix} \mathbf{a}_3 &= -a \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{z}} & (48e) & \text{Cu II}
\end{aligned}$$

References

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