

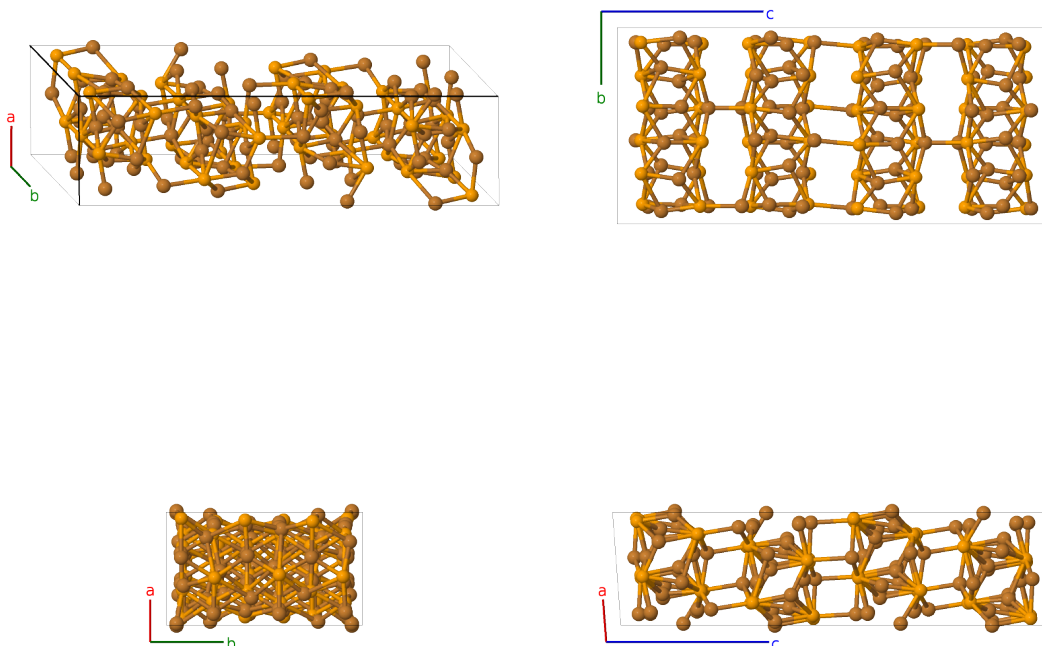
Low Temperature Cu₂Se Structure: A2B_mC144_15_12f_6f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/F9TK>

https://aflow.org/p/A2B_mC144_15_12f_6f-001

● Cu
● Se



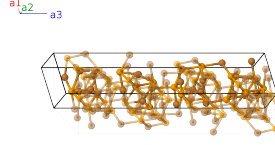
Prototype	Cu ₂ Se
AFLOW prototype label	A2B_mC144_15_12f_6f-001
ICSD	none
Pearson symbol	mC144
Space group number	15
Space group symbol	<i>C</i> 2/ <i>c</i>
AFLOW prototype command	<pre>aflow --proto=A2B_mC144_15_12f_6f-001 --params=a, b/a, c/a, β, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18</pre>

- Cu₂Se exists in two forms:

- This low-temperature layered monoclinic structure, and
 - a high-temperature (above $\approx 400\text{K}$) highly disordered superionic cubic structure.
- The data for the rhombohedral phase was taken at room temperature, while the high temperature structure was examined at 415 K.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu I
\mathbf{B}_2	$-(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu I
\mathbf{B}_3	$-(x_1 - y_1) \mathbf{a}_1 - (x_1 + y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu I
\mathbf{B}_4	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu I
\mathbf{B}_5	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu II
\mathbf{B}_6	$-(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu II
\mathbf{B}_7	$-(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu II
\mathbf{B}_8	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu II
\mathbf{B}_9	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu III
\mathbf{B}_{10}	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu III
\mathbf{B}_{11}	$-(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu III
\mathbf{B}_{12}	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu III
\mathbf{B}_{13}	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu IV
\mathbf{B}_{14}	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu IV
\mathbf{B}_{15}	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Cu IV
\mathbf{B}_{16}	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Cu IV

$$\begin{aligned}
\mathbf{B}_{17} &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu V} \\
\mathbf{B}_{18} &= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 = -(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu V} \\
\mathbf{B}_{19} &= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu V} \\
\mathbf{B}_{20} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu V} \\
\mathbf{B}_{21} &= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VI} \\
\mathbf{B}_{22} &= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 = -(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VI} \\
\mathbf{B}_{23} &= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3 = -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VI} \\
\mathbf{B}_{24} &= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VI} \\
\mathbf{B}_{25} &= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3 = (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VII} \\
\mathbf{B}_{26} &= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 = -(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VII} \\
\mathbf{B}_{27} &= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 = -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VII} \\
\mathbf{B}_{28} &= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VII} \\
\mathbf{B}_{29} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VIII} \\
\mathbf{B}_{30} &= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VIII} \\
\mathbf{B}_{31} &= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VIII} \\
\mathbf{B}_{32} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu VIII} \\
\mathbf{B}_{33} &= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 = (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu IX} \\
\mathbf{B}_{34} &= -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu IX} \\
\mathbf{B}_{35} &= -(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3 = -(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu IX} \\
\mathbf{B}_{36} &= (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu IX} \\
\mathbf{B}_{37} &= (x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu X} \\
\mathbf{B}_{38} &= -(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 = -(ax_{10} + c(z_{10} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu X} \\
\mathbf{B}_{39} &= -(x_{10} - y_{10}) \mathbf{a}_1 - (x_{10} + y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}} & (8f) & \text{Cu X}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{63} &= \begin{matrix} -(x_{16} - y_{16}) \mathbf{a}_1 - \\ (x_{16} + y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - \\ cz_{16} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se IV} \\
\mathbf{B}_{64} &= \begin{matrix} (x_{16} + y_{16}) \mathbf{a}_1 + \\ (x_{16} - y_{16}) \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{16} + c(z_{16} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + \\ c(z_{16} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se IV} \\
\mathbf{B}_{65} &= \begin{matrix} (x_{17} - y_{17}) \mathbf{a}_1 + \\ (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 \end{matrix} &= & (ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Se V} \\
\mathbf{B}_{66} &= \begin{matrix} -(x_{17} + y_{17}) \mathbf{a}_1 - \\ (x_{17} - y_{17}) \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{17} + c(z_{17} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - \\ c(z_{17} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se V} \\
\mathbf{B}_{67} &= \begin{matrix} -(x_{17} - y_{17}) \mathbf{a}_1 - \\ (x_{17} + y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - \\ cz_{17} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se V} \\
\mathbf{B}_{68} &= \begin{matrix} (x_{17} + y_{17}) \mathbf{a}_1 + \\ (x_{17} - y_{17}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{17} + c(z_{17} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + \\ c(z_{17} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se V} \\
\mathbf{B}_{69} &= \begin{matrix} (x_{18} - y_{18}) \mathbf{a}_1 + \\ (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 \end{matrix} &= & (ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Se VI} \\
\mathbf{B}_{70} &= \begin{matrix} -(x_{18} + y_{18}) \mathbf{a}_1 - \\ (x_{18} - y_{18}) \mathbf{a}_2 - (z_{18} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{18} + c(z_{18} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - \\ c(z_{18} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se VI} \\
\mathbf{B}_{71} &= \begin{matrix} -(x_{18} - y_{18}) \mathbf{a}_1 - \\ (x_{18} + y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - \\ cz_{18} \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se VI} \\
\mathbf{B}_{72} &= \begin{matrix} (x_{18} + y_{18}) \mathbf{a}_1 + \\ (x_{18} - y_{18}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{18} + c(z_{18} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + \\ c(z_{18} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} &(8f) & \text{Se VI}
\end{aligned}$$

References

- [1] L. Gulay, M. Daszkiewicz, O. Strok, and A. Pietraszko, *Crystal structure of Cu₂Se*, Chem. Met. Alloys **4**, 200–205 (2011), doi:10.30970/cma4.0184.