

δ -Cu₄₁Sn₁₁ Structure:

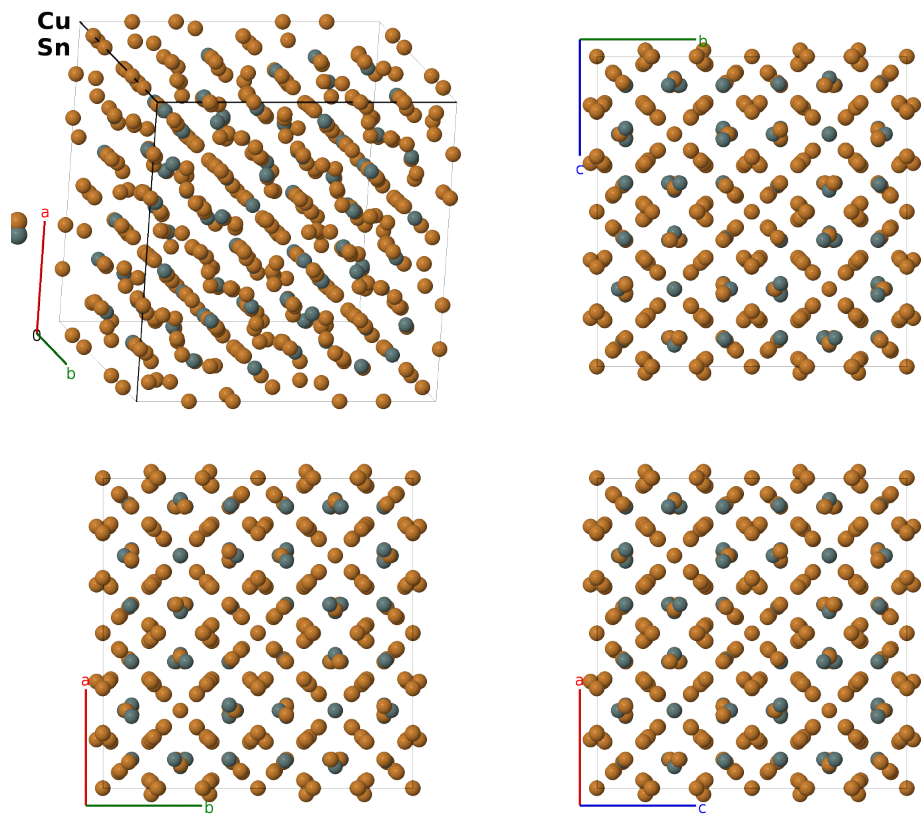
A41B11_cF416_216_7e2fg3h_egh-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/1MZW>

https://aflow.org/prototype-encyclopedia/A41B11_cF416_216_7e2fg3h_egh-001

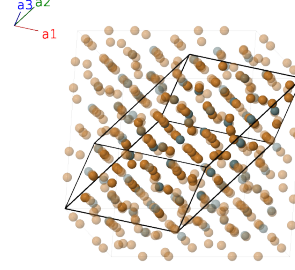


Prototype	Cu ₄₁ Sn ₁₁
AFLOW prototype label	A41B11_cF416_216_7e2fg3h_egh-001
ICSD	149164
CCDC	2047517
Pearson symbol	cF416
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A41B11_cF416_216_7e2fg3h_egh-001</code> <code>--params=a, x₁, x₂, x₃, x₄, x₅, x₆, x₇, x₈, x₉, x₁₀, x₁₁, x₁₂, x₁₃, z₁₃, x₁₄, z₁₄, x₁₅, z₁₅, x₁₆, z₁₆</code>

- This is designated as the δ phase in the Cu-Sn system. (Massalski, 1990)
- We have shifted the origin by $a(\hat{x} + \hat{y} + \hat{z})/4$ from that used by (Misra, 2021).
- There is considerable disorder in this system, we assign the atomic species at each Wyckoff position to the majority species. This means that the ICSD entry does not exactly match our atomic positions.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{x} + ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Cu I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - 3x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{x} - ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Cu I
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - 3x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{x} + ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Cu I
$\mathbf{B}_4$	$= -3x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{x} - ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Cu I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} + ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Cu II
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - 3x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} - ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Cu II
$\mathbf{B}_7$	$= x_2 \mathbf{a}_1 - 3x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} + ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Cu II
$\mathbf{B}_8$	$= -3x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} - ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Cu II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Cu III
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} - ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Cu III
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} + ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Cu III
$\mathbf{B}_{12}$	$= -3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Cu III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} + ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Cu IV
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} - ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Cu IV
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} + ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Cu IV
$\mathbf{B}_{16}$	$= -3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} - ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Cu IV
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} + ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Cu V
$\mathbf{B}_{18}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} - ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Cu V
$\mathbf{B}_{19}$	$= x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} + ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Cu V
$\mathbf{B}_{20}$	$= -3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} - ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Cu V
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{x} + ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Cu VI
$\mathbf{B}_{22}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{x} - ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Cu VI

$\mathbf{B}_{23} =$	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Cu VI
$\mathbf{B}_{24} =$	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Cu VI
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Cu VII
$\mathbf{B}_{26} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - 3x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Cu VII
$\mathbf{B}_{27} =$	$x_7 \mathbf{a}_1 - 3x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Cu VII
$\mathbf{B}_{28} =$	$-3x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Cu VII
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B}_{30} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - 3x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B}_{31} =$	$x_8 \mathbf{a}_1 - 3x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B}_{32} =$	$-3x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B}_{33} =$	$-x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}}$	(24f)	Cu VIII
$\mathbf{B}_{34} =$	$x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}}$	(24f)	Cu VIII
$\mathbf{B}_{35} =$	$x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{y}}$	(24f)	Cu VIII
$\mathbf{B}_{36} =$	$-x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{y}}$	(24f)	Cu VIII
$\mathbf{B}_{37} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{z}}$	(24f)	Cu VIII
$\mathbf{B}_{38} =$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{z}}$	(24f)	Cu VIII
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}}$	(24f)	Cu IX
$\mathbf{B}_{40} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}}$	(24f)	Cu IX
$\mathbf{B}_{41} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{y}}$	(24f)	Cu IX
$\mathbf{B}_{42} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{y}}$	(24f)	Cu IX
$\mathbf{B}_{43} =$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{z}}$	(24f)	Cu IX
$\mathbf{B}_{44} =$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{z}}$	(24f)	Cu IX
$\mathbf{B}_{45} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{46} =$	$x_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 -$ $(x_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{47} =$	$x_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{48} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 -$ $(x_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{49} =$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - (x_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{11} \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{50} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 +$ $x_{11} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(24g)	Cu X
$\mathbf{B}_{51} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{52} =$	$x_{12} \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 -$ $(x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{53} =$	$x_{12} \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 + x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{54} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 -$ $(x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{55} =$	$x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 - (x_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{56} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 - (x_{12} - \frac{1}{2}) \mathbf{a}_2 +$ $x_{12} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B}_{57} =$	$z_{13} \mathbf{a}_1 + z_{13} \mathbf{a}_2 + (2x_{13} - z_{13}) \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + az_{13} \hat{\mathbf{z}}$	(48h)	Cu XI
$\mathbf{B}_{58} =$	$z_{13} \mathbf{a}_1 + z_{13} \mathbf{a}_2 - (2x_{13} + z_{13}) \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} + az_{13} \hat{\mathbf{z}}$	(48h)	Cu XI

$$\begin{aligned}
\mathbf{B}_{89} &= z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Cu XIII} \\
\mathbf{B}_{90} &= z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = -ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Cu XIII} \\
\mathbf{B}_{91} &= -(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + (2x_{15} - z_{15}) \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Cu XIII} \\
\mathbf{B}_{92} &= (2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 - (2x_{15} + z_{15}) \mathbf{a}_3 = -ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Cu XIII} \\
\mathbf{B}_{93} &= z_{16} \mathbf{a}_1 + z_{16} \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} + az_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{94} &= z_{16} \mathbf{a}_1 + z_{16} \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} + az_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{95} &= (2x_{16} - z_{16}) \mathbf{a}_1 - (2x_{16} + z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} - az_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{96} &= -(2x_{16} + z_{16}) \mathbf{a}_1 + (2x_{16} - z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} - az_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{97} &= (2x_{16} - z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = az_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{98} &= -(2x_{16} + z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = az_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{99} &= z_{16} \mathbf{a}_1 + (2x_{16} - z_{16}) \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 = -az_{16} \hat{\mathbf{x}} - ax_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{100} &= z_{16} \mathbf{a}_1 - (2x_{16} + z_{16}) \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 = -az_{16} \hat{\mathbf{x}} + ax_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{101} &= z_{16} \mathbf{a}_1 + (2x_{16} - z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} + az_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{102} &= z_{16} \mathbf{a}_1 - (2x_{16} + z_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} + az_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{103} &= -(2x_{16} + z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + (2x_{16} - z_{16}) \mathbf{a}_3 = ax_{16} \hat{\mathbf{x}} - az_{16} \hat{\mathbf{y}} - ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III} \\
\mathbf{B}_{104} &= (2x_{16} - z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 - (2x_{16} + z_{16}) \mathbf{a}_3 = -ax_{16} \hat{\mathbf{x}} - az_{16} \hat{\mathbf{y}} + ax_{16} \hat{\mathbf{z}} & (48h) & \text{Sn III}
\end{aligned}$$

References

- [1] S. Misra, D. Pahari, S. Giri, F. Wang, S. Puravankara, and P. P. Jana, *The γ -brass type Cu-rich complex intermetallic phase $\text{Cu}_{41}\text{Sn}_{11}$: Structure and electrochemical study*, Solid State Sci. **119**, 106682 (2021), doi:10.1016/j.solidstatesciences.2021.106682.
- [2] T. B. Massalski, H. Okamoto, P. R. S., and L. Kacprzak, eds., *Binary Alloy Phase Diagrams* (ASM International, Materials Park, Ohio, USA, 1990), vol. 2, chap. Cu-Sn (Copper-Tin), pp. 1481–1483, 2nd edn.
- [3] U. Mizutani, *Hume-Rothery Rules for Structurally Complex Alloy Phases* (CRC Press, Boca Raton, London, New York, 2010).

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