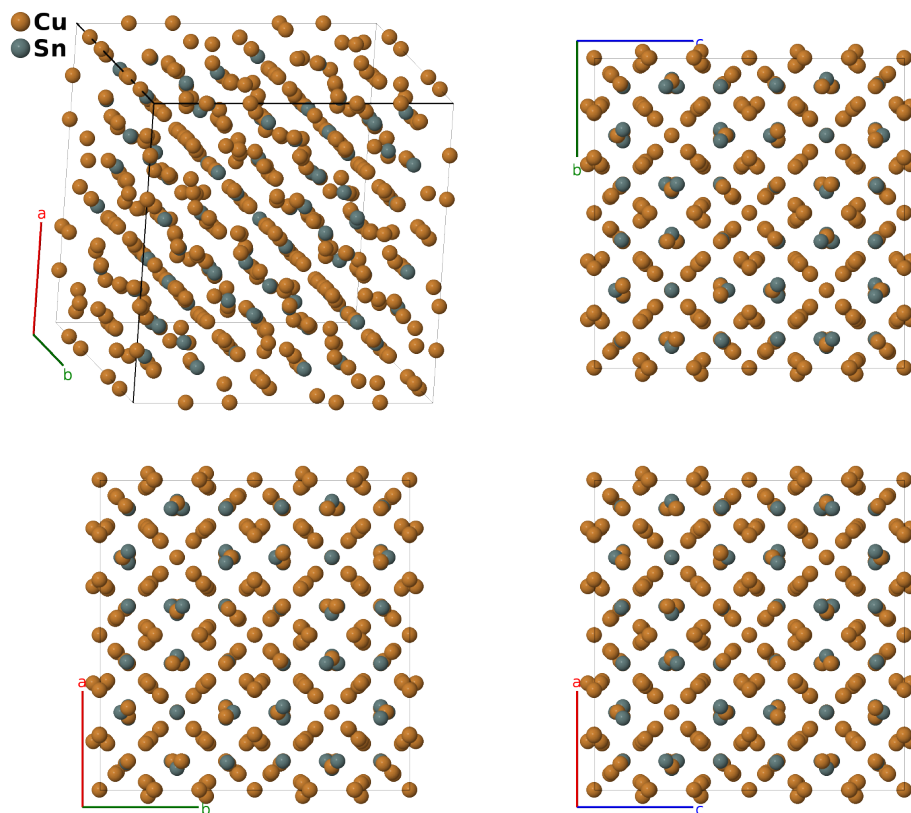


# $\delta$ -Cu<sub>41</sub>Sn<sub>11</sub> Structure: A41B11\_cF416\_216\_7e2fg3h\_egh-001

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<https://afLOW.org/p/1MZW>

[https://afLOW.org/p/A41B11\\_cF416\\_216\\_7e2fg3h\\_egh-001](https://afLOW.org/p/A41B11_cF416_216_7e2fg3h_egh-001)



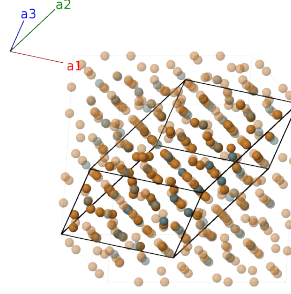
<b>Prototype</b>	Cu <sub>41</sub> Sn <sub>11</sub>
<b>AFLOW prototype label</b>	A41B11_cF416_216_7e2fg3h_egh-001
<b>ICSD</b>	none
<b>Pearson symbol</b>	cF416
<b>Space group number</b>	216
<b>Space group symbol</b>	$F\bar{4}3m$
<b>AFLOW prototype command</b>	<pre>afLOW --proto=A41B11_cF416_216_7e2fg3h_egh-001 --params=a, x1, x2, x3, x4, x5, x6, x7, x8, x9, x10, x11, x12, x13, z13, x14, z14, x15, z15, x16, z16</pre>

- This is designated as the  $\delta$  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).

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## Face-centered Cubic primitive vectors

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




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## Basis vectors

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





$$\begin{aligned}
\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}$$

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