Low Temperature UP_2 Structure: A2B_tI24_107_2abc_2ab-001

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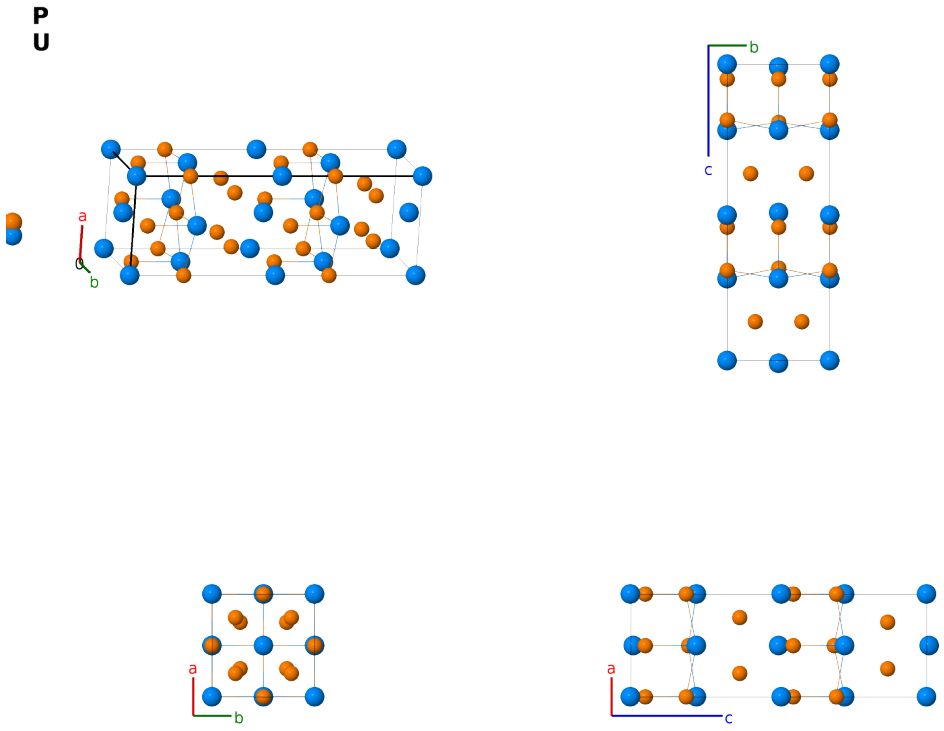
https://aflow.org/prototype-encyclopedia/3JHK

https://aflow.org/prototype-encyclopedia/A2B_tI24_107_2abc_2ab-001

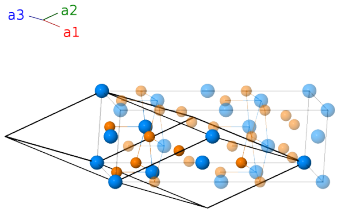


Prototype	P_2U
AFLOW prototype label	A2B_tI24_107_2abc_2ab-001
ICSD	87138
CCDC	1646965
Pearson symbol	tI24
Space group number	107
Space group symbol	$I4mm$
AFLOW prototype command	`aflow --proto=A2B_tI24_107_2abc_2ab-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, x_7, z_7$

- At temperatures above 83°C UP_2 transforms into its high-temperature structure. (Gerward, 1990)
- The current structure is very close to the Cu_2Sb ($C38$) structure. Indeed, if we allow an uncertainty of 0.3Å FINDSYM puts this in the $C38$ structure.
- The ICSD entry is from the earlier work of (Pietrasko, 1971).

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	P II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	U I
$\mathbf{B_4}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	U II
$\mathbf{B_5}$	=	$\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4b)	P III
$\mathbf{B_6}$	=	$z_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4b)	P III
$\mathbf{B_7}$	=	$\left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4b)	U III
$\mathbf{B_8}$	=	$z_6\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4b)	U III
$\mathbf{B_9}$	=	$(x_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	P IV
$\mathbf{B_{10}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	P IV
$\mathbf{B_{11}}$	=	$(x_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	P IV
$\mathbf{B_{12}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	P IV

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