SnIP Structure: ABC_mP42_13_e3g_e3g_f3g-001

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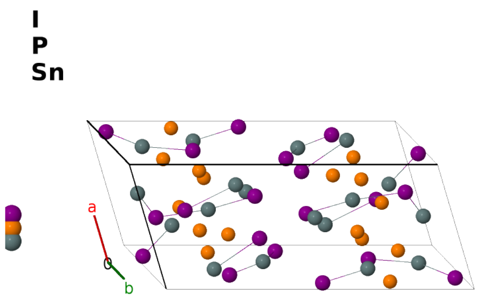
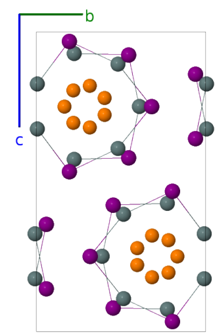
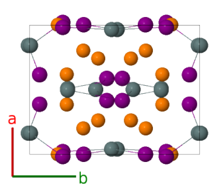
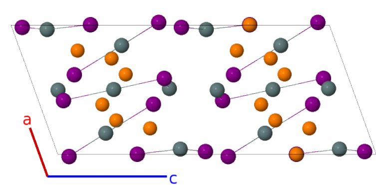
https://aflow.org/prototype-encyclopedia/BLJP

https://aflow.org/prototype-encyclopedia/ABC_mP42_13_e3g_e3g_f3g-001









Prototype	IPSn
AFLOW prototype label	ABC_mP42_13_e3g_e3g_f3g-001
ICSD	430054
CCDC	1789478
Pearson symbol	mP42
Space group number	13
Space group symbol	$P2/c$
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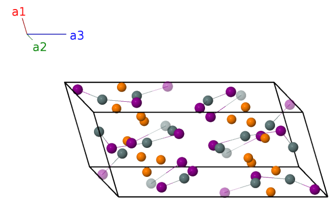
Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B_3}$	=	$y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	P I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	P I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{c\cos\beta}{4}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	Sn I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{3c\cos\beta}{4}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	Sn I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4g)	I II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4g)	I II
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4g)	I III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I III
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4g)	I III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I III
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4g)	I IV
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I IV
$\mathbf{B_{17}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4g)	I IV
$\mathbf{B_{18}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	I IV
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B_{21}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	P II
$\mathbf{B_{22}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	P II

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\begin{array}{llllll}
\mathbf{B_{23}} & = & x_8 \, \mathbf{a}_1 + y_8 \, \mathbf{a}_2 + z_8 \, \mathbf{a}_3 & = & \left(a x_8 + c z_8 \cos\beta\right) \, \mathbf{\hat{x}} + b y_8 \, \mathbf{\hat{y}} + c z_8 \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P III} \\
\mathbf{B_{24}} & = & -x_8 \, \mathbf{a}_1 + y_8 \, \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \, \mathbf{a}_3 & = & -\left(a x_8 + c \left(z_8 - \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} + b y_8 \, \mathbf{\hat{y}} - c \left(z_8 - \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P III} \\
\mathbf{B_{25}} & = & -x_8 \, \mathbf{a}_1 - y_8 \, \mathbf{a}_2 - z_8 \, \mathbf{a}_3 & = & -\left(a x_8 + c z_8 \cos\beta\right) \, \mathbf{\hat{x}} - b y_8 \, \mathbf{\hat{y}} - c z_8 \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P III} \\
\mathbf{B_{26}} & = & x_8 \, \mathbf{a}_1 - y_8 \, \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \, \mathbf{a}_3 & = & \left(a x_8 + c \left(z_8 + \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} - b y_8 \, \mathbf{\hat{y}} + c \left(z_8 + \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P III} \\
\mathbf{B_{27}} & = & x_9 \, \mathbf{a}_1 + y_9 \, \mathbf{a}_2 + z_9 \, \mathbf{a}_3 & = & \left(a x_9 + c z_9 \cos\beta\right) \, \mathbf{\hat{x}} + b y_9 \, \mathbf{\hat{y}} + c z_9 \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P IV} \\
\mathbf{B_{28}} & = & -x_9 \, \mathbf{a}_1 + y_9 \, \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \, \mathbf{a}_3 & = & -\left(a x_9 + c \left(z_9 - \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} + b y_9 \, \mathbf{\hat{y}} - c \left(z_9 - \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P IV} \\
\mathbf{B_{29}} & = & -x_9 \, \mathbf{a}_1 - y_9 \, \mathbf{a}_2 - z_9 \, \mathbf{a}_3 & = & -\left(a x_9 + c z_9 \cos\beta\right) \, \mathbf{\hat{x}} - b y_9 \, \mathbf{\hat{y}} - c z_9 \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P IV} \\
\mathbf{B_{30}} & = & x_9 \, \mathbf{a}_1 - y_9 \, \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \, \mathbf{a}_3 & = & \left(a x_9 + c \left(z_9 + \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} - b y_9 \, \mathbf{\hat{y}} + c \left(z_9 + \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{P IV} \\
\mathbf{B_{31}} & = & x_{10} \, \mathbf{a}_1 + y_{10} \, \mathbf{a}_2 + z_{10} \, \mathbf{a}_3 & = & \left(a x_{10} + c z_{10} \cos\beta\right) \, \mathbf{\hat{x}} + b y_{10} \, \mathbf{\hat{y}} + c z_{10} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn II} \\
\mathbf{B_{32}} & = & -x_{10} \, \mathbf{a}_1 + y_{10} \, \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \, \mathbf{a}_3 & = & -\left(a x_{10} + c \left(z_{10} - \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} + b y_{10} \, \mathbf{\hat{y}} - c \left(z_{10} - \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn II} \\
\mathbf{B_{33}} & = & -x_{10} \, \mathbf{a}_1 - y_{10} \, \mathbf{a}_2 - z_{10} \, \mathbf{a}_3 & = & -\left(a x_{10} + c z_{10} \cos\beta\right) \, \mathbf{\hat{x}} - b y_{10} \, \mathbf{\hat{y}} - c z_{10} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn II} \\
\mathbf{B_{34}} & = & x_{10} \, \mathbf{a}_1 - y_{10} \, \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \, \mathbf{a}_3 & = & \left(a x_{10} + c \left(z_{10} + \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} - b y_{10} \, \mathbf{\hat{y}} + c \left(z_{10} + \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn II} \\
\mathbf{B_{35}} & = & x_{11} \, \mathbf{a}_1 + y_{11} \, \mathbf{a}_2 + z_{11} \, \mathbf{a}_3 & = & \left(a x_{11} + c z_{11} \cos\beta\right) \, \mathbf{\hat{x}} + b y_{11} \, \mathbf{\hat{y}} + c z_{11} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn III} \\
\mathbf{B_{36}} & = & -x_{11} \, \mathbf{a}_1 + y_{11} \, \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \, \mathbf{a}_3 & = & -\left(a x_{11} + c \left(z_{11} - \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} + b y_{11} \, \mathbf{\hat{y}} - c \left(z_{11} - \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn III} \\
\mathbf{B_{37}} & = & -x_{11} \, \mathbf{a}_1 - y_{11} \, \mathbf{a}_2 - z_{11} \, \mathbf{a}_3 & = & -\left(a x_{11} + c z_{11} \cos\beta\right) \, \mathbf{\hat{x}} - b y_{11} \, \mathbf{\hat{y}} - c z_{11} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn III} \\
\mathbf{B_{38}} & = & x_{11} \, \mathbf{a}_1 - y_{11} \, \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \, \mathbf{a}_3 & = & \left(a x_{11} + c \left(z_{11} + \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} - b y_{11} \, \mathbf{\hat{y}} + c \left(z_{11} + \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn III} \\
\mathbf{B_{39}} & = & x_{12} \, \mathbf{a}_1 + y_{12} \, \mathbf{a}_2 + z_{12} \, \mathbf{a}_3 & = & \left(a x_{12} + c z_{12} \cos\beta\right) \, \mathbf{\hat{x}} + b y_{12} \, \mathbf{\hat{y}} + c z_{12} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn IV} \\
\mathbf{B_{40}} & = & -x_{12} \, \mathbf{a}_1 + y_{12} \, \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \, \mathbf{a}_3 & = & -\left(a x_{12} + c \left(z_{12} - \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} + b y_{12} \, \mathbf{\hat{y}} - c \left(z_{12} - \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn IV} \\
\mathbf{B_{41}} & = & -x_{12} \, \mathbf{a}_1 - y_{12} \, \mathbf{a}_2 - z_{12} \, \mathbf{a}_3 & = & -\left(a x_{12} + c z_{12} \cos\beta\right) \, \mathbf{\hat{x}} - b y_{12} \, \mathbf{\hat{y}} - c z_{12} \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn IV} \\
\mathbf{B_{42}} & = & x_{12} \, \mathbf{a}_1 - y_{12} \, \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \, \mathbf{a}_3 & = & \left(a x_{12} + c \left(z_{12} + \frac{1}{2}\right) \cos\beta\right) \, \mathbf{\hat{x}} - b y_{12} \, \mathbf{\hat{y}} + c \left(z_{12} + \frac{1}{2}\right) \sin\beta \, \mathbf{\hat{z}} & \text{(4g)} & \text{Sn IV} \\
\end{array}
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References

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Found in

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