Tl_3VS_4 Structure: A4B3C_cI16_217_c_b_a-001

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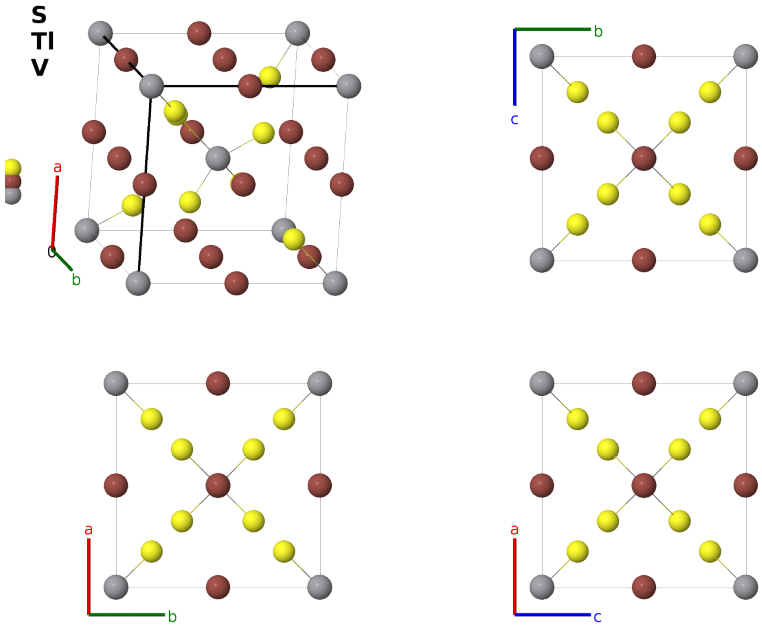
https://aflow.org/prototype-encyclopedia/Y0MN

https://aflow.org/prototype-encyclopedia/A4B3C_cI16_217_c_b_a-001



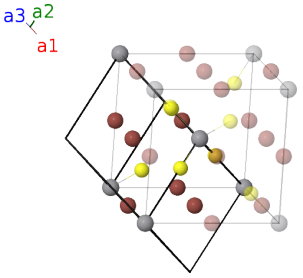
Prototype	S_4Tl_3V
AFLOW prototype label	A4B3C_cI16_217_c_b_a-001
ICSD	16572
CCDC	1597133
Pearson symbol	cI16
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	`aflow --proto=A4B3C_cI16_217_c_b_a-001 --params=`a, x_3

Other compounds with this structure
Tl_3NbS_4, Tl_3NbSe_4, Tl_3TaS_4, Tl_3TaSe_4, Tl_3VSe_4

- When $x_3 = 1/4$ all of the atoms are on the sites of a body-centered cubic lattice, and this structure becomes identical with our model $cI16$ ferrite structure.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	V I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6b)	Tl I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(6b)	Tl I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(6b)	Tl I
$\mathbf{B_5}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	S I
$\mathbf{B_6}$	=	$-2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	S I
$\mathbf{B_7}$	=	$-2x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	S I
$\mathbf{B_8}$	=	$-2x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	S I

References

[1] C. Crevecoeur, *Some ternary thallium chalcogenides*, Acta Cryst. **17**, 757 (1964), doi:10.1107/S0365110X64001864.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

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