

TlCr₅Se₈ Structure:

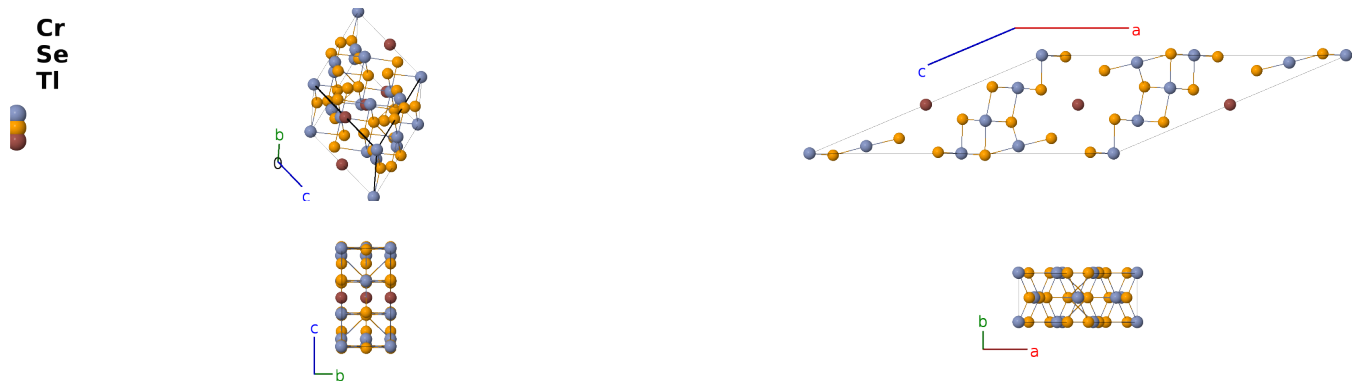
A5B8C_mC28_12_a2i_4i_c-001

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<https://aflow.org/prototype-encyclopedia/AFXE>

https://aflow.org/prototype-encyclopedia/A5B8C_mC28_12_a2i_4i_c-001



Prototype	Cr ₅ Se ₈ Tl
AFLOW prototype label	A5B8C_mC28_12_a2i_4i_c-001
ICSD	78157
CCDC	1638484
Pearson symbol	mC28
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A5B8C_mC28_12_a2i_4i_c-001</code> <code>--params=a, b/a, c/a, β, $x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8$</code>

Other compounds with this structure

Tl(V_{1-x}Cr_x)₅Se₈, CsCr₅S₈

- The chromium atoms may be replaced with arbitrary amounts of vanadium. We used the data for the stoichiometric compound.
- The data for CsCr₅S₈ was taken much earlier, and so it could be used as the prototype, but the data for TlCr₅Se₈ is more accessible.
- There is no ICSD or CCDC entry for (Maier, 2015), so we link to the earlier work of (Bensch, 1994).

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Cr I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Tl I
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Cr II
$\mathbf{B}_4$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Cr II
$\mathbf{B}_5$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Cr III
$\mathbf{B}_6$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Cr III
$\mathbf{B}_7$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Se I
$\mathbf{B}_8$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Se I
$\mathbf{B}_9$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Se II
$\mathbf{B}_{10}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Se II
$\mathbf{B}_{11}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Se III
$\mathbf{B}_{12}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Se III
$\mathbf{B}_{13}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Se IV
$\mathbf{B}_{14}$	$=$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Se IV

References

- [1] S. Maier, R. Lefèvre, X. Lin, R. Nunna, D. Berthebaud, S. Hèbert, A. Marb, and F. Gascoin, *The solid solution series $Tl(V_{1-x}Cr_x)_5Se_8$: crystal structure, magnetic and thermoelectric properties*, J. Mater. Chem. C **3**, 10509–10517 (2015), doi:10.1039/c5tc01766a.
- [2] W. Bensch, E. Wörner, M. Muhler, and U. Ruschewitz, *Single Crystal Structure, Magnetic Properties, and Electronic Structure of $Tl_xCr_5S_8$ ($x = 1.0$ and 0.7)*, J. Solid State Chem. **110**, 234–242 (1994), doi:10.1006/jssc.1994.1164.

First cited in

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