

TlCo₂S₂ Structure: A2B2C_tI10_139_d_e_a-002

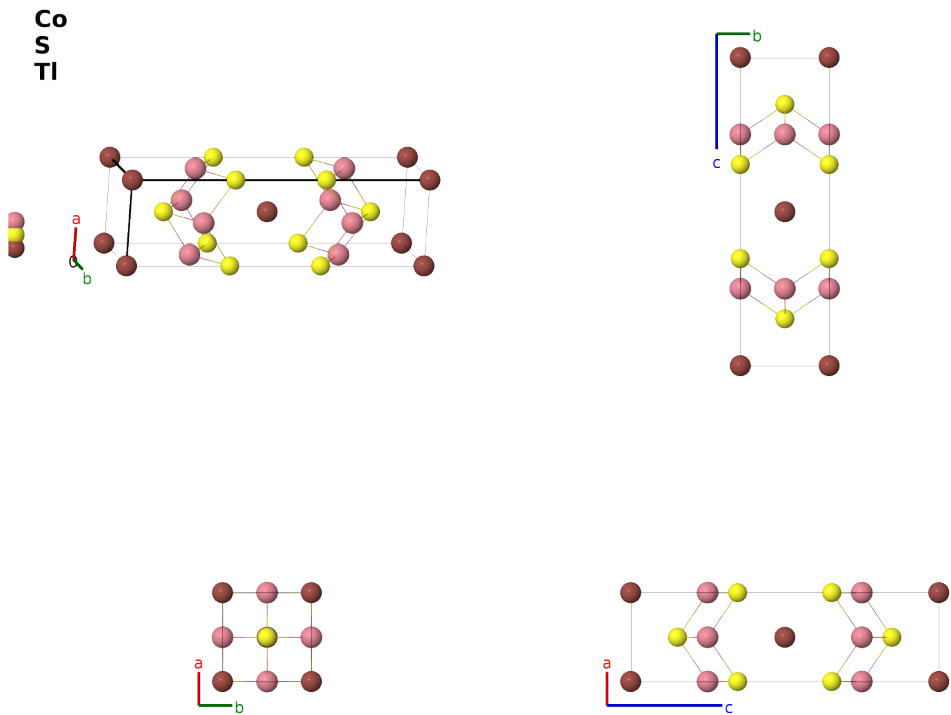
This structure previously used the label(s) **A2B2C.tI10_139_d_e_a.TlCo2S2**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/D85X>

https://aflow.org/prototype-encyclopedia/A2B2C_tI10_139_d_e_a-002



Prototype	Co ₂ S ₂ Tl
AFLOW prototype label	A2B2C_tI10_139_d_e_a-002
ICSD	100438
CCDC	1659572
Pearson symbol	tI10
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=A2B2C_tI10_139_d_e_a-002</code> <code>--params=a, c/a, z₃</code>

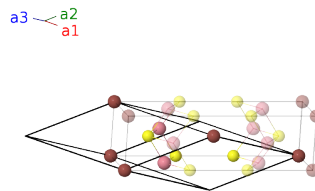
Other compounds with this structure

BaCr₂As₂, BaFe₂As₂, BaMn₂Bi₂, BaP₂Zn₂, BaSr₂As₂, BaCo₂As₂, BiCe₂O₂, BiTh₂N₂, BiU₂N₂, CaCo₂As₂, SrCo₂As₂, EuCo₂As₂, EuFe₄As₂, CsCo₂Se₂, KCo₂As₂, KCo₂P₂, KCo₂Se₂, KFe₂As₂, KFe₂P₂, KRh₂As₂, KRh₂P₂, RbCo₂Se₂, RbFe₂As₂, RbNi₂Se₂, SbTh₂N₂, SbU₂N₂, SeBi₂O₂, SeBi₂O₂, TeBi₂O₂, TeCe₂O₂, TeDy₂O₂, TeEr₂O₂, TeLu₂O₂, TeTb₂O₂, TeY₂O₂, TeTh₂N₂, TeU₂N₂, TlCo₂Se₂, TlCu₂S₂, TlCu₂Se₂, TlCu₂Te₂, TlFe₂S₂, TlFe₂Se₂, TlNi₂S₂, TlNi₂Se₂, Cl(Li_{0.25}Be_{0.75})₂O₂, Cl(Na_{0.25}Be_{0.75})₂O₂, EuFe₂(As_{0.8}P_{0.2})₂

- This is a ternary form of the $D1_3$ (BaAl₄) structure. It differs from the ThCr₂Si₂ structure in that here $c/a > 3$.
- Other authors designate TlCu₂Se₂ or Cl(Li_{0.25}Be_{0.75})₂O₂ as the prototype for this structure, but (Klepp, 1978) give complete structural information for TlCo₂S₂, so we use that as the prototype.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Tl I
$\mathbf{B}_2$	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d)	Co I
$\mathbf{B}_3$	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d)	Co I
$\mathbf{B}_4$	$z_3\mathbf{a}_1 + z_3\mathbf{a}_2$	$=$	$cz_3\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_5$	$-z_3\mathbf{a}_1 - z_3\mathbf{a}_2$	$=$	$-cz_3\hat{\mathbf{z}}$	(4e)	S I

References

- [1] K. Klepp and H. Boller, *Ternäre Thallium-Übergangsmetall-Chalkogenide mit ThCr₂Si₂-Struktur*, Monatsh. Chem. **109**, 1049–1057 (1978), doi:10.1007/BF00913007.

Found in

- [1] R. Berger and C. F. van Bruggen, *TlCu₂Se₂: A p-type metal with a layer structure*, J. Less-Common Met. **99**, 113–123 (1984), doi:10.1016/0022-5088(84)90340-0.

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