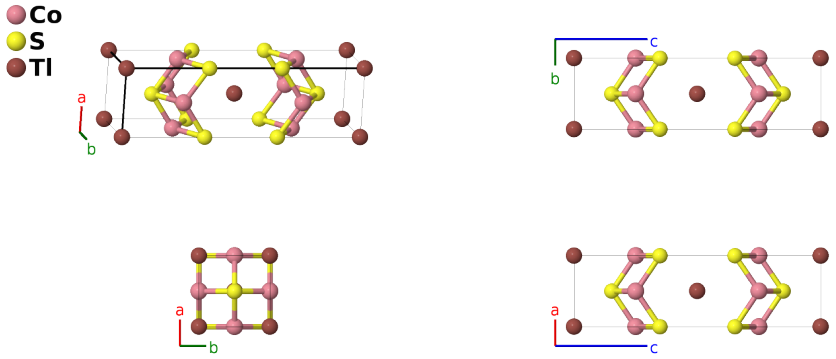
$TlCo_2S_2$ Structure: A2B2C_tI10_139_d_e_a-002

This structure originally had the label `A2B2C_tI10_139_d_e_a.TlCo2S2`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/D85X

https://aflow.org/p/A2B2C_tI10_139_d_e_a-002



Prototype	Co_2S_2Tl
AFLOW prototype label	A2B2C_tI10_139_d_e_a-002
ICSD	100438
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B2C_tI10_139_d_e_a-002 --params=`$a, c/a, z_3$

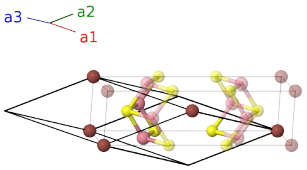
Other compounds with this structure

$BaCr_2As_2$, $BaFe_2As_2$, $BaMn_2Bi_2$, BaP_2Zn_2, $BaSr_2As_2$, $BaCo_2As_2$, $BiCe_2O_2$, $BiTh_2N_2$, BiU_2N_2, $CaCo_2As_2$, $SrCo_2As_2$, $EuCo_2As_2$, $EuFe4_2As_2$, $CsCo_2Se_2$, KCo_2As_2, KCo_2P_2, KCo_2Se_2, KFe_2As_2, KFe_2P_2, KRh_2As_2, KRh_2P_2, $RbCo_2Se_2$, $RbFe_2As_2$, $RbNi_2Se_2$, $SbTh_2N_2$, SbU_2N_2, $SeBi_2O_2$, $SeBi_2O_2$, $TeBi_2O_2$, $TeCe_2O_2$, $TeDy_2O_2$, $TeEr_2O_2$, $TeLu_2O_2$, $TeTb_2O_2$, TeY_2O_2, $TeTh_2N_2$, TeU_2N_2, $TlCo_2Se_2$, $TlCu_2S_2$, $TlCu_2Se_2$, $TlCu_2Te_2$, $TlFe_2S_2$, $TlFe_2Se_2$, $TlNi_2S_2$, $TlNi_2Se_2$, $Cl(Li_{0.25}Be_{0.75})_2O_2$, $Cl(Na_{0.25}Be_{0.75})_2O_2$, $EuFe_2(As_{0.8}P_{0.2})_2$

- This is a ternary form of the $D1_3$ ($BaAl_4$) structure. It differs from the $ThCr_2Si_2$ structure in that here $c/a > 3$.
- Other authors designate $TlCu_2Se_2$ or $Cl(Li_{0.25}Be_{0.75})_2O_2$ as the prototype for this structure, but (Klepp, 1978) give complete structural information for $TlCo_2S_2$, so we use that as the prototype.

Body-centered Tetragonal primitive vectors

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



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 $ThCr_2Si_2$-Struktur*, Monatsh. Chem. **109**, 1049–1057 (1978), doi:10.1007/BF00913007.

Found in

[1] R. Berger and C. F. van Bruggen, *$TlCu_2Se_2$: A p-type metal with a layer structure*, J. Less-Common Met. **99**, 113–123 (1984), doi:10.1016/0022-5088(84)90340-0.