$ThCr_2Si_2$ Structure: A2B2C_tI10_139_d_e_a-003

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

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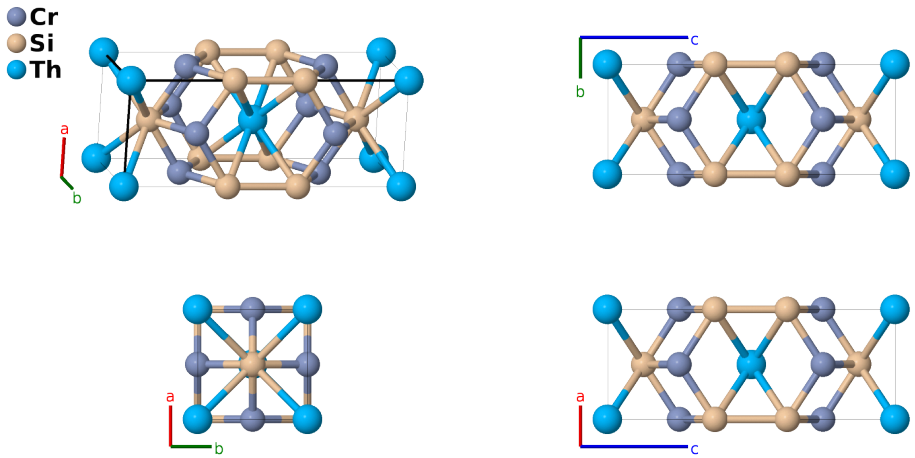
https://aflow.org/p/LS62

https://aflow.org/p/A2B2C_tI10_139_d_e_a-003



Prototype	Cr_2Si_2Th
AFLOW prototype label	A2B2C_tI10_139_d_e_a-003
ICSD	18157
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B2C_tI10_139_d_e_a-003 --params=`$a, c/a, z_3$

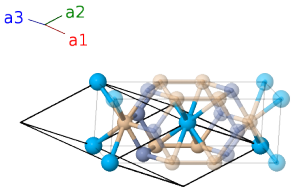
Other compounds with this structure

$BaAl_2Ge_2$, $BaFe_2As_2$, $BaFe_2P_2$, $BaMg_2Si_2$, $BaMg_2Ge_2$, $BaMn_2Ge_2$, $BaNi_2As_2$, $BaNi_2Ge_2$, $BaRh_2B_2$, $CaAl_2Zn_2$, $CaAu_2Si_2$, $CaFe_2As_2$, $CaMn_2Ge_2$, $CaNi_2Ge_2$, $CeAl_2Ga_2$, $CeCu_2Si_2$, $CeRh_2Si_2$, $CeRu_2Si_2$, $CsCo_2As_2$, $CsCo_2P_2$, $CsFe_2As_2$, $CsFe_2P_2$, $CsIr_2As_2$, $CsIr_2P_2$, $CsRh_2As_2$, $CsRh_2P_2$, $CsRu_2As_2$, $CsRu_2P_2$, $DyCr_2Si_2$, $EuCo_2As_2$, $EuCo_2P_2$, $EuFe_2P_2$, $EuRh_2P_2$, KNi_2S_2, KNi_2Se_2, $LaCo_2P_2$, $LaRu_2P_2$, $LuFe_2B_2$, $LuRu_2Si_2$, $PuCr_2Si_2$, $SrCo_2P_2$, $SrFe_2As_2$, $SrFe_2P_2$, $SrNi_2P_2$, $SrRh_2As_2$, $SrRh_2P_2$, $SrRu_2P_2$, $ThCr_2Si_2$, $ThCu_2Si_2$, $ThMn_2Ge_2$, $ThMn_2Si_2$, $ThNi_2Si_2$, $TlCu_2Se_2$, UCr_2Si_2, URu_2Si_2, YFe_2Ge_2, YNi_2Ge_2

- (Shatruk, 2019) refers to this as "the perovskite of intermetallics." The list of compounds below is by no means complete.
- This is a ternary form of the $D1_3$ ($BaAl_4$) structure.
- The structures generally identified as having prototype $ThCr_2Si_2$ actually divide up into two distinct regions, based on c/a ratio. We assign structures with $c/a \leq 3$ to the $ThCr_2Si_2$ structure, and those with $c/a > 3$ to the $TlCo_2S_2$ structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Th 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)	Cr 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)	Cr I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Si I

References

[1] Z. Ban and M. Sikirica, *The crystal structure of ternary silicides ThM_2Si_2 (M = Cr, Mn, Fe, Co, Ni and Cu)*, Acta Cryst. **18**, 594–599 (1964), doi:10.1107/S0365110X6500141X.

[2] M. Shatruk, *$ThCr_2Si_2$ structure type: The "perovskite" of intermetallics*, J. Solid State Chem. **272**, 198–209 (2019), doi:10.1016/j.jssc.2019.02.012.