$Tl_2CdGeTe_4$ Structure: ABC4D2_tI16_121_a_b_i_c-001

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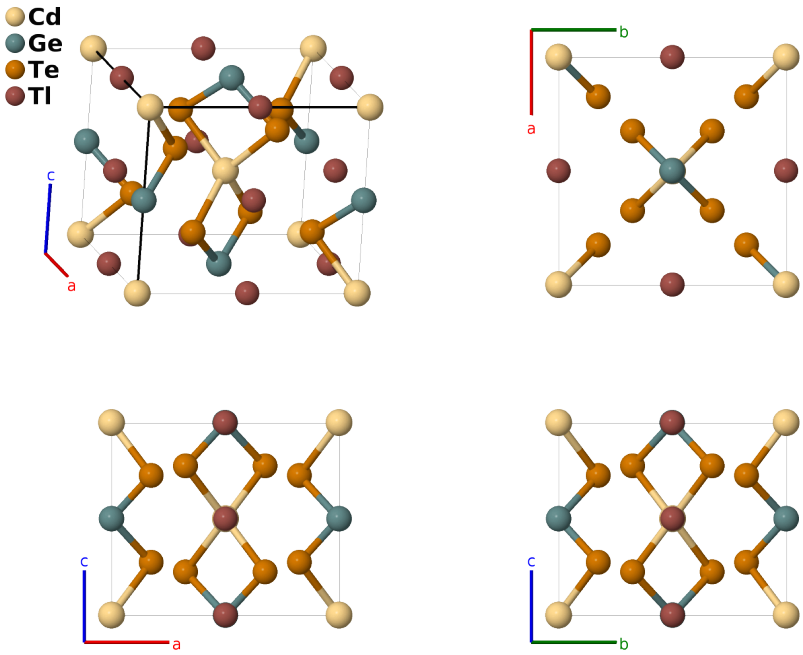
https://aflow.org/p/RB89

https://aflow.org/p/ABC4D2_tI16_121_a_b_i_c-001



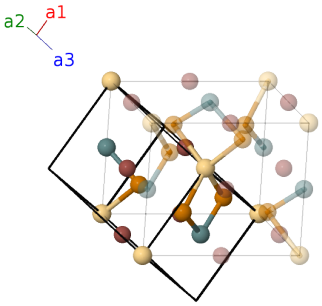
Prototype	$CdGeTe_4Tl_2$
AFLOW prototype label	ABC4D2_tI16_121_a_b_i_c-001
ICSD	172502
Pearson symbol	tI16
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	`aflow --proto=ABC4D2_tI16_121_a_b_i_c-001 --params=`$a, c/a, x_4, z_4$

Other compounds with this structure

$Tl_2CdSnTe_4$, $Tl_2HgGeTe_4$, $Tl_2HgSiSe_4$, $Tl_2HgSnSe_4$, $Tl_2HgSnTe_4$, $Tl_2MnGeTe_4$, $Tl_2MnSnTe_4$

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)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Tl I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Tl I
$\mathbf{B_5}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	Te I
$\mathbf{B_6}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	Te I
$\mathbf{B_7}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	Te I
$\mathbf{B_8}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	Te I

References

[1] M. A. McGuire, T. J. Scheidemantel, J. V. Badding, and F. J. DiSalvo, *Tl_2AXTe_4 (A = Cd, Hg, Mn; X = Ge, Sn): Crystal Structure, Electronic Structure, and Thermoelectric Properties*, Chem. Mater. **17**, 6186–6191 (2005), doi:10.1021/cm0518067.