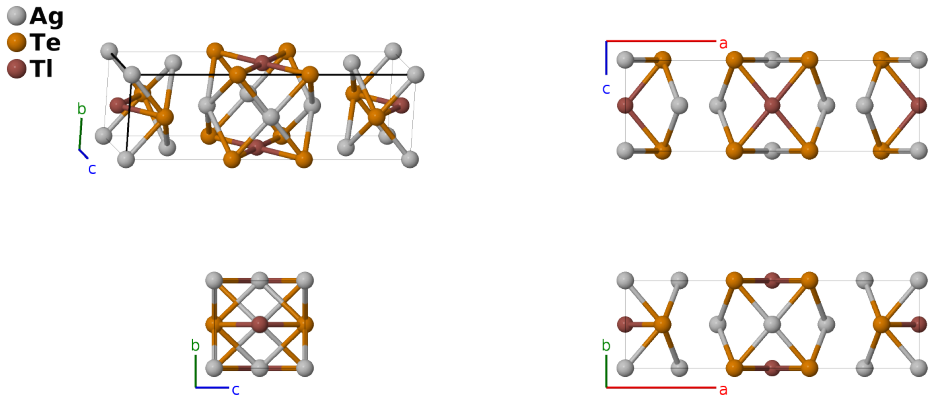
Ag_3Te_2Tl Structure: A3B2C_oC12_65_ah_g_c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/35VG

https://aflow.org/p/A3B2C_oC12_65_ah_g_c-001

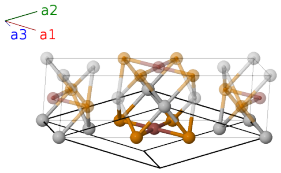


Prototype	Ag_3Te_2Tl
AFLOW prototype label	A3B2C_oC12_65_ah_g_c-001
ICSD	71081
Pearson symbol	oC12
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A3B2C_oC12_65_ah_g_c-001 --params=`$a, b/a, c/a, x_3, x_4$

- (Avilov, 1972) put this in space group $Pmna$ #51, with two formula units in the full orthorhombic cell. (Cenzual, 1991) showed that their coordinates actually described a system in space group $Cmmm$ #65, with one formula unit in the primitive cell.
- The ICSD entry references (Cenzual, 1991).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ag I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Tl I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Te I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Te I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ag II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ag II

References

[1] A. S. Avilov, R. M. Imamov, and Z. G. Pinsker, *Crystal structure of Ag_3TlTe_2*, Sov. Phys. Crystal. **17**, 237–239 (1972). Translated from Kristallografiya.

Found in

[1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.