

Ag₃Te₂Tl Structure:

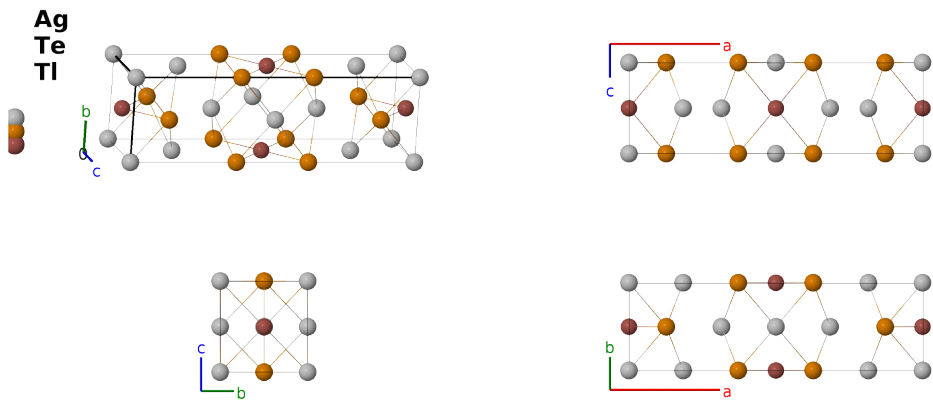
A3B2C_oC12_65_ah_g_c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/35VG>

https://aflow.org/prototype-encyclopedia/A3B2C_oC12_65_ah_g_c-001

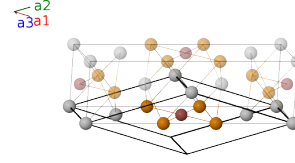


Prototype	Ag ₃ Te ₂ Tl
AFLOW prototype label	A3B2C_oC12_65_ah_g_c-001
ICSD	71081
CCDC	1631993
Pearson symbol	oC12
Space group number	65
Space group symbol	<i>Cmmm</i>
AFLOW prototype command	<code>aflow --proto=A3B2C_oC12_65_ah_g_c-001</code> <code>--params=a, b/a, c/a, x₃, x₄</code>

- (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

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



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.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.