Room Temperature AgC_4N_3 Structure: AB4C3_oI32_46_b_2bc_bc-001

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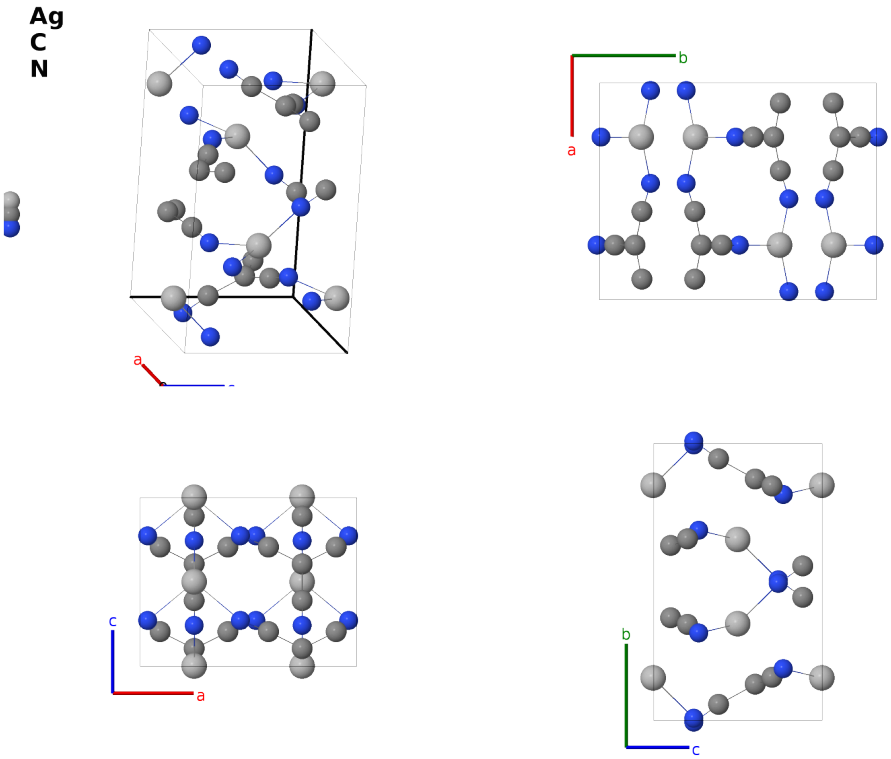
https://aflow.org/prototype-encyclopedia/77VH

https://aflow.org/prototype-encyclopedia/AB4C3_oI32_46_b_2bc_bc-001

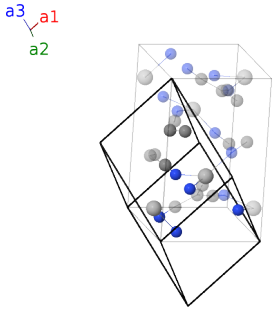


Prototype	AgC_4N_3
AFLOW prototype label	AB4C3_oI32_46_b_2bc_bc-001
ICSD	43823
CCDC	1613281
Pearson symbol	oI32
Space group number	46
Space group symbol	$Ima2$
AFLOW prototype command	`aflow --proto=AB4C3_oI32_46_b_2bc_bc-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- This is the room temperature structure of AgC_4N_3. Around 100K it undergoes a significatn change in structure which does not change the space group or Wyckoff positions. (Hodgson, 2014). This can be found on the low temperature AgC_4N_3 structure page.
- In chemical literature this is often referred to as Ag(tcm), where tcm is an abbreviation for tricyanomethanide.
- (Konnert, 2014) swapped the x- and z-axes compared to the standard setting of space group $Ima2$ #46. We used AFLOW to transform this to the standard orientation.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(y_1+z_1)\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 + \left(y_1+\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4b)	Ag I
$\mathbf{B_2}$	=	$-(y_1-z_1)\,\mathbf{a}_1 + \left(z_1+\frac{3}{4}\right)\mathbf{a}_2 - \left(y_1-\frac{3}{4}\right)\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4b)	Ag I
$\mathbf{B_3}$	=	$(y_2+z_2)\,\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\mathbf{a}_2 + \left(y_2+\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	C I
$\mathbf{B_4}$	=	$-(y_2-z_2)\,\mathbf{a}_1 + \left(z_2+\frac{3}{4}\right)\mathbf{a}_2 - \left(y_2-\frac{3}{4}\right)\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	C I
$\mathbf{B_5}$	=	$(y_3+z_3)\,\mathbf{a}_1 + \left(z_3+\frac{1}{4}\right)\mathbf{a}_2 + \left(y_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	C II
$\mathbf{B_6}$	=	$-(y_3-z_3)\,\mathbf{a}_1 + \left(z_3+\frac{3}{4}\right)\mathbf{a}_2 - \left(y_3-\frac{3}{4}\right)\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	C II
$\mathbf{B_7}$	=	$(y_4+z_4)\,\mathbf{a}_1 + \left(z_4+\frac{1}{4}\right)\mathbf{a}_2 + \left(y_4+\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	N I
$\mathbf{B_8}$	=	$-(y_4-z_4)\,\mathbf{a}_1 + \left(z_4+\frac{3}{4}\right)\mathbf{a}_2 - \left(y_4-\frac{3}{4}\right)\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	N I
$\mathbf{B_9}$	=	$(y_5+z_5)\,\mathbf{a}_1 + (x_5+z_5)\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	C III
$\mathbf{B_{10}}$	=	$-(y_5-z_5)\,\mathbf{a}_1 - (x_5-z_5)\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	C III
$\mathbf{B_{11}}$	=	$-(y_5-z_5)\,\mathbf{a}_1 + \left(x_5+z_5+\frac{1}{2}\right)\mathbf{a}_2 + \left(x_5-y_5+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	C III
$\mathbf{B_{12}}$	=	$(y_5+z_5)\,\mathbf{a}_1 + \left(-x_5+z_5+\frac{1}{2}\right)\mathbf{a}_2 + \left(-x_5+y_5+\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	C III

$\mathbf{B_{13}}$	$=$	$(y_6 + z_6)\ \mathbf{a}_1 + (x_6 + z_6)\ \mathbf{a}_2 + (x_6 + y_6)\ \mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	N II
$\mathbf{B_{14}}$	$=$	$-(y_6 - z_6)\ \mathbf{a}_1 - (x_6 - z_6)\ \mathbf{a}_2 - (x_6 + y_6)\ \mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	N II
$\mathbf{B_{15}}$	$=$	$-(y_6 - z_6)\ \mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	N II
$\mathbf{B_{16}}$	$=$	$(y_6 + z_6)\ \mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	N II

References

[1] J. Konnert and D. Britton, *The Crystal Structure of $AgC(CN)_3$*, Inorg. Chem. **5**, 1191–1196 (1966), doi:10.1021/ic50041a026.

[2] S. A. Hodgson, J. Adamson, S. J. Hunt, M. J. Cliffe, A. B. Cairns, A. L. Thompson, M. G. Tucker, N. P. Funnell, and A. L. Goodwin, *Negative area compressibility in silver(I) tricyanomethanide*, Chem. Commun. **50**, 5264–5266 (2014), doi:10.1039/C3CC47032F.

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