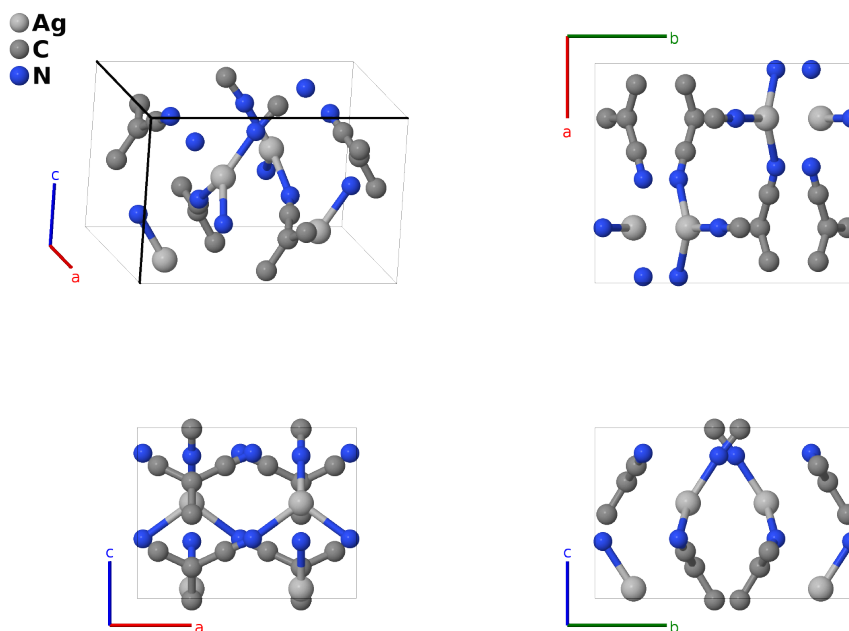


# Low Temperature $\text{AgC}_4\text{N}_3$ Structure: AB4C3\_oI32\_46\_b\_2bc\_bc-002

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/AS99>

[https://afLOW.org/p/AB4C3\\_oI32\\_46\\_b\\_2bc\\_bc-002](https://afLOW.org/p/AB4C3_oI32_46_b_2bc_bc-002)

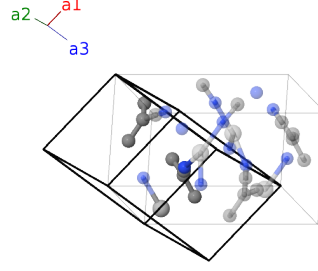


<b>Prototype</b>	$\text{AgC}_4\text{N}_3$
<b>AFLOW prototype label</b>	AB4C3_oI32_46_b_2bc_bc-002
<b>CCDC</b>	961476
<b>Pearson symbol</b>	oI32
<b>Space group number</b>	46
<b>Space group symbol</b>	$Ima2$
<b>AFLOW prototype command</b>	<pre>afLOW --proto=AB4C3_oI32_46_b_2bc_bc-002 --params=a, b/a, c/a, y1, z1, y2, z2, y3, z3, y4, z4, x5, y5, z5, x6, y6, z6</pre>

- This is the structure obtained by (Hodgson, 2014) on cooling to 100K. There is a considerable difference in the structure compared to the room temperature structure even though the space group and Wyckoff positions do not change.
- In chemical literature this is often referred to as  $\text{Ag}(\text{tcm})$ , where tcm is an abbreviation for tricyanomethanide.
- We use the ambient pressure structural data taken at 100K after heating.

## Body-centered Orthorhombic primitive vectors

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(y_1 + z_1) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 + (y_1 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Ag I
$\mathbf{B}_2$	$-(y_1 - z_1) \mathbf{a}_1 + (z_1 + \frac{3}{4}) \mathbf{a}_2 - (y_1 - \frac{3}{4}) \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Ag I
$\mathbf{B}_3$	$(y_2 + z_2) \mathbf{a}_1 + (z_2 + \frac{1}{4}) \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	C I
$\mathbf{B}_4$	$-(y_2 - z_2) \mathbf{a}_1 + (z_2 + \frac{3}{4}) \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	C I
$\mathbf{B}_5$	$(y_3 + z_3) \mathbf{a}_1 + (z_3 + \frac{1}{4}) \mathbf{a}_2 + (y_3 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	C II
$\mathbf{B}_6$	$-(y_3 - z_3) \mathbf{a}_1 + (z_3 + \frac{3}{4}) \mathbf{a}_2 - (y_3 - \frac{3}{4}) \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	C II
$\mathbf{B}_7$	$(y_4 + z_4) \mathbf{a}_1 + (z_4 + \frac{1}{4}) \mathbf{a}_2 + (y_4 + \frac{1}{4}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	N I
$\mathbf{B}_8$	$-(y_4 - z_4) \mathbf{a}_1 + (z_4 + \frac{3}{4}) \mathbf{a}_2 - (y_4 - \frac{3}{4}) \mathbf{a}_3$	=	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$-(y_5 - z_5) \mathbf{a}_1 + (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	C III
$\mathbf{B}_{12}$	$(y_5 + z_5) \mathbf{a}_1 + (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{15}$	$-(y_6 - z_6) \mathbf{a}_1 + (x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + (x_6 - y_6 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	N II

$$\mathbf{B}_{16} = \begin{pmatrix} (y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (8c) \quad \text{N II}$$

## References

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