Low Temperature AgC_4N_3 Structure: AB4C3_oI32_46_b_2bc_bc-002

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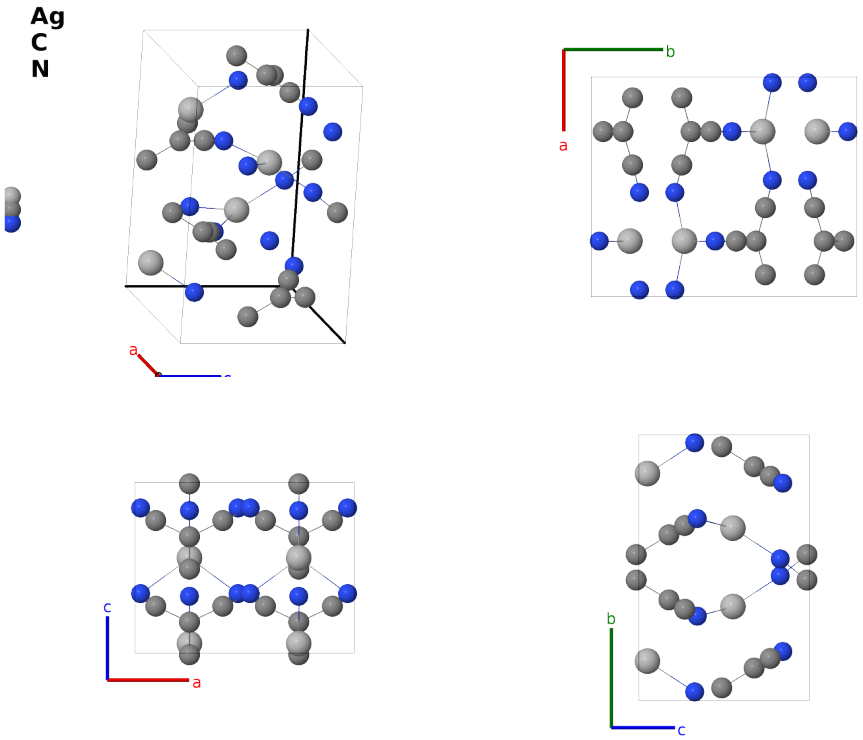
https://aflow.org/prototype-encyclopedia/AS99

https://aflow.org/prototype-encyclopedia/AB4C3_oI32_46_b_2bc_bc-002



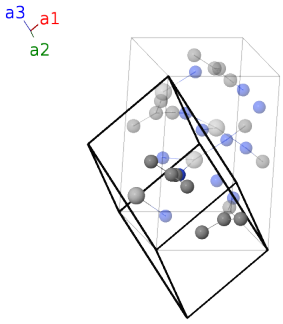
Prototype	AgC_4N_3
AFLOW prototype label	AB4C3_oI32_46_b_2bc_bc-002
CCDC	961476
Pearson symbol	oI32
Space group number	46
Space group symbol	$Ima2$
AFLOW prototype command	`aflow --proto=AB4C3_oI32_46_b_2bc_bc-002 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- This is the 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 Ag(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

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



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

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

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