$KAg[CO_3]$ Structure: ABCD3_oI48_73_d_c_c_cf-001

This structure originally had the label `ABCD3_oI48_73_d_e_e_ef`. Calls to that address will be redirected here.

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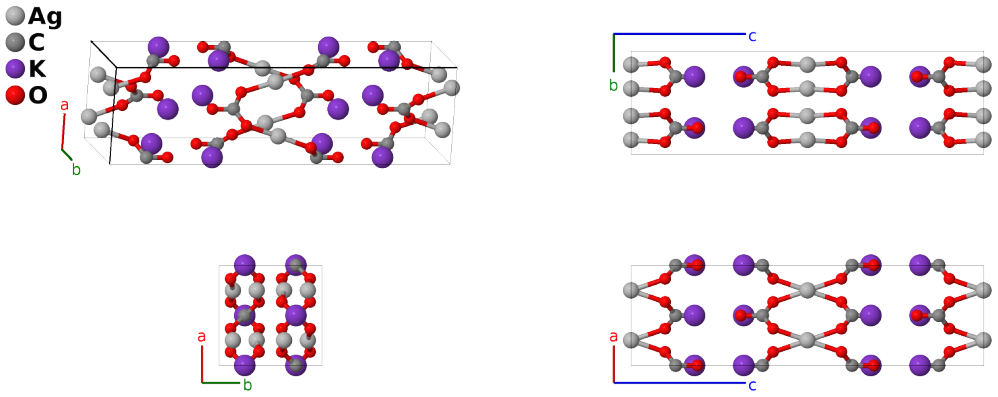
https://aflow.org/p/H0D0

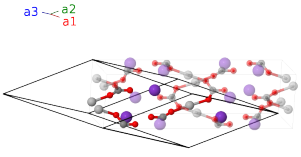
https://aflow.org/p/ABCD3_oI48_73_d_c_c_cf-001



Prototype	$AgCKO_3$
AFLOW prototype label	ABCD3_oI48_73_d_c_c_cf-001
ICSD	409484
Pearson symbol	oI48
Space group number	73
Space group symbol	*Ibca*
AFLOW prototype command	`aflow --proto=ABCD3_oI48_73_d_c_c_cf-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_4, x_5, y_5, z_5$

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
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \tfrac{1}{4}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \tfrac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	C I

$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(8d)	Ag I
$\mathbf{B_{14}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Ag I
$\mathbf{B_{15}}$	=	$-y_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$	(8d)	Ag I
$\mathbf{B_{16}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8d)	Ag I
$\mathbf{B_{17}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{18}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - \left(x_5 + y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{19}}$	=	$(y_5 - z_5)\,\mathbf{a}_1 - \left(x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_5 + y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{20}}$	=	$-\left(y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{21}}$	=	$-(y_5 + z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{22}}$	=	$\left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + \left(x_5 + y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{23}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{24}}$	=	$\left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16f)	O II

References

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.