$KAg(CN)_2$ ($F5_{10}$) Structure: AB2CD2_hP36_163_h_i_bf_i-001

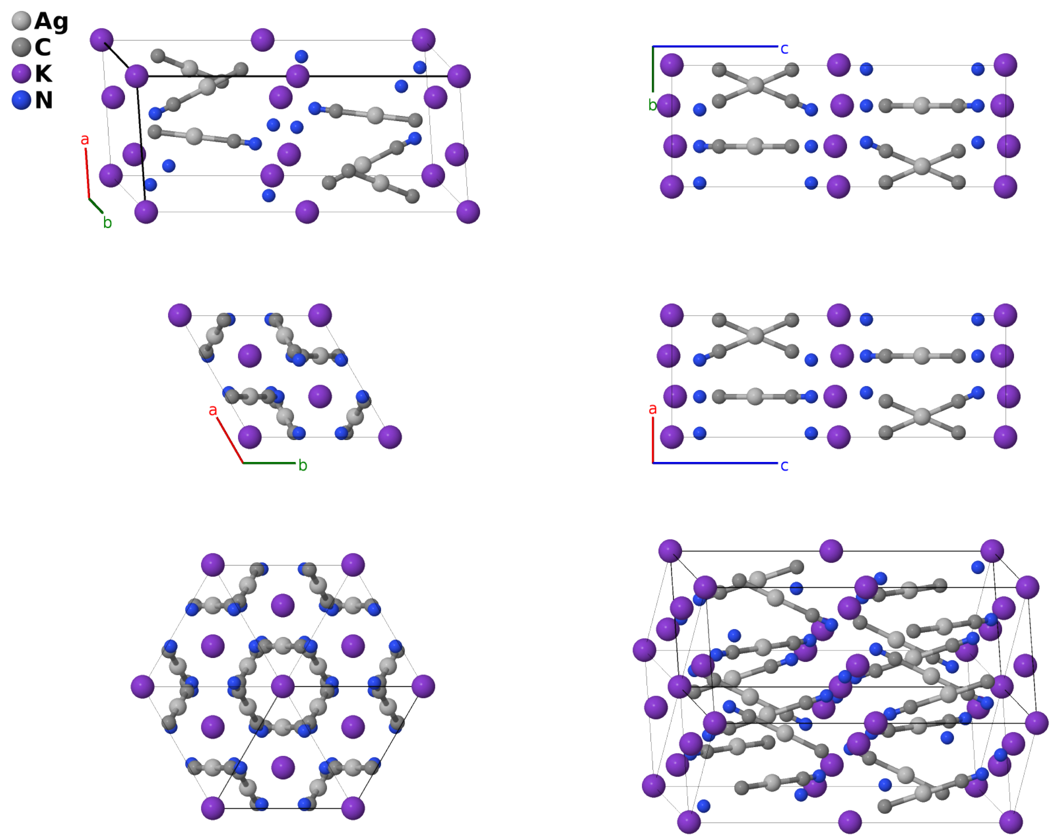
This structure originally had the label `AB2CD2_hP36_163_h_i_bf_i`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

---

https://aflow.org/p/JLGL

https://aflow.org/p/AB2CD2_hP36_163_h_i_bf_i-001



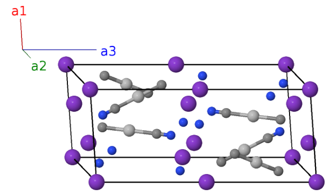
Prototype	AgC_2KN_2
AFLOW prototype label	AB2CD2_hP36_163_h_i_bf_i-001
***Strukturbericht* designation**	$F5_{10}$
ICSD	30275
Pearson symbol	hP36
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	`aflow --proto=AB2CD2_hP36_163_h_i_bf_i-001` `--params=`$a, c/a, z_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5$

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{\sqrt{3}}{2}a\,\mathbf{\hat{y}}$$

$$\mathbf{a_3} = c\,\mathbf{\hat{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\mathbf{\hat{z}}$	(2b)	K I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(4f)	K II
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4f)	K II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - cz_2\,\mathbf{\hat{z}}$	(4f)	K II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(4f)	K II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_9}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_{12}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_3\,\mathbf{\hat{y}} + \frac{3}{4}c\,\mathbf{\hat{z}}$	(6h)	Ag I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{15}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{16}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{17}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{21}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{22}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{23}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{24}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	C I
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{26}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - 2y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{27}}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{28}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I

$\mathbf{B_{29}}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{30}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{31}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{32}}$	=	$y_5\,\mathbf{a}_1 - \left(x_5 - y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{33}}$	=	$\left(x_5 - y_5\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{34}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{35}}$	=	$\left(x_5 - y_5\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - 2y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I
$\mathbf{B_{36}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - y_5\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	N I

References

[1] J. L. Hoard, *The Crystal Structure of Potassium Silver Cyanide*, Z. Krystallogr. **84**, 231–255 (1933), doi:10.1524/zkri.1933.84.1.231.

Found in

[1] P. Villars, *KAg(CN)$_2$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.