K_2CdPb Structure: AB2C_oC16_40_a_2b_b-001

This structure originally had the label `AB2C_oC16_40_a_2b_b`. Calls to that address will be redirected here.

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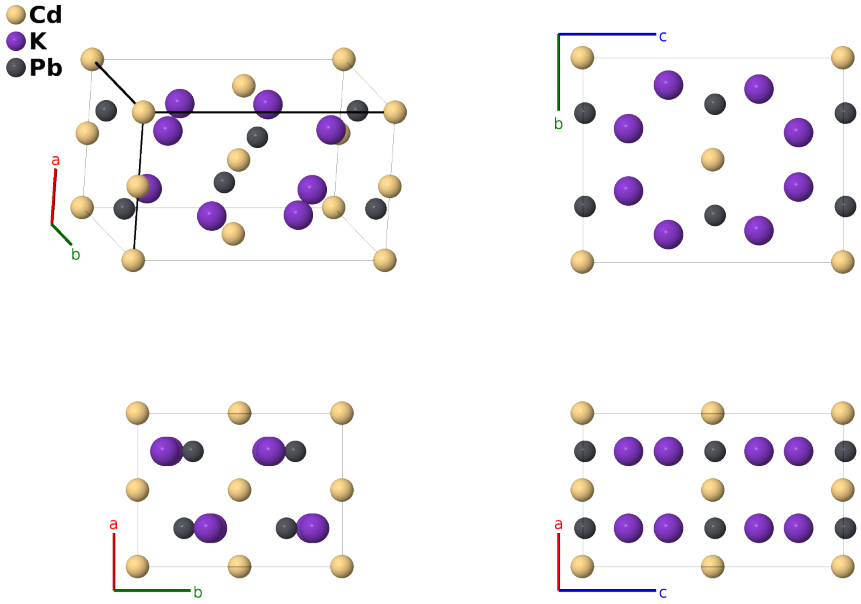
https://aflow.org/p/K8N1

https://aflow.org/p/AB2C_oC16_40_a_2b_b-001



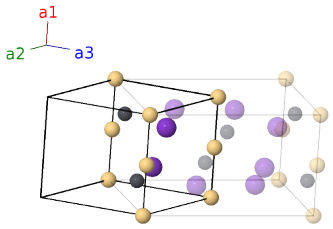
Prototype	CdK_2Pb
AFLOW prototype label	AB2C_oC16_40_a_2b_b-001
ICSD	10041
Pearson symbol	oC16
Space group number	40
Space group symbol	$Ama2$
AFLOW prototype command	`aflow --proto=AB2C_oC16_40_a_2b_b-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4$

Other compounds with this structure
K_2CdSn

- Space group $Ama2$ #40 allows an arbitrary choice of the origin of the z-axis. We use this to place the cadmium (4a) atom at the origin.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + (y_2 - z_2)\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - (y_2 + z_2)\,\mathbf{a}_2 - (y_2 - z_2)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	K II
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	K II
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Pb I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Pb I

References

[1] R. Matthes and H.-U. Schuster, *Synthese und Struktur der Phasen K_2CdSn und K_2CdPb*, Z. Naturforsch. B **34**, 541–543 (1979), doi:10.1515/znb-1979-0403.

Found in

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