$CdAs_2$ Structure: A2B_tI12_98_f_a-001

This structure originally had the label `A2B_tI12_98_f_a`. Calls to that address will be redirected here.

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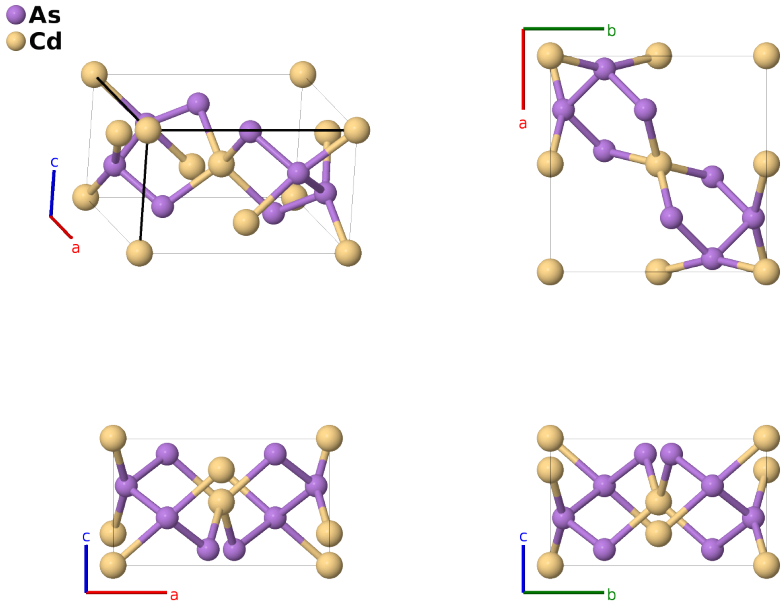
https://aflow.org/p/G4QQ

https://aflow.org/p/A2B_tI12_98_f_a-001

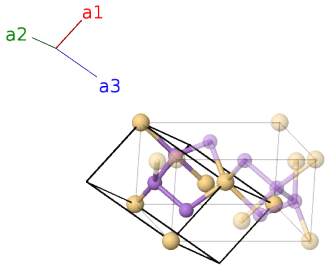


Prototype	As_2Cd
AFLOW prototype label	A2B_tI12_98_f_a-001
ICSD	609931
Pearson symbol	tI12
Space group number	98
Space group symbol	$I4_122$
AFLOW prototype command	`aflow --proto=A2B_tI12_98_f_a-001 --params=`$a, c/a, x_2$

Other compounds with this structure
$CdAs_{2-x}P_x$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cd I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Cd I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B_4}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B_5}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8f)	As I

References

[1] V. A. Rubtsov, E. M. Smolarenko, V. M. Trukhan, V. N. Yakimovich, and L. K. Orlik, *Phase diagram of the CdP_2-$CdAs_2$ system*, Phys. Stat. Solidi A **115**, K155–K158 (1989), doi:10.1002/pssa.2211150238.

[2] V. N. Yakimovich, V. A. Rubtsov, and V. M. Trukhan, *Phase Relationships in the CdP_4-ZnP_2-$CdAs_2$-$ZnAs_2$ System*, Inorg. Mater. **32**, 579–582 (1996).

Found in

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