Cd_8As_7Cl Structure: A7B12C_cP20_195_ag_3e_b-001

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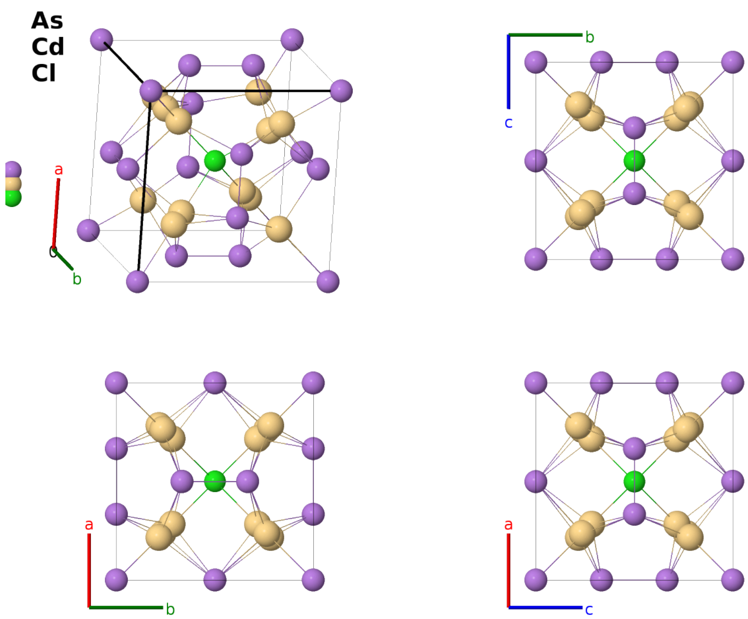
https://aflow.org/prototype-encyclopedia/J7FX

https://aflow.org/prototype-encyclopedia/A7B12C_cP20_195_ag_3e_b-001

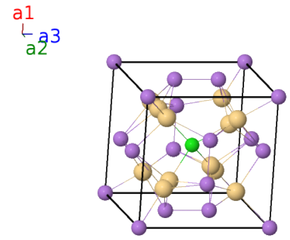


Prototype	As_7Cd_8Cl
AFLOW prototype label	A7B12C_cP20_195_ag_3e_b-001
ICSD	84983
CCDC	1644952
Pearson symbol	cP20
Space group number	195
Space group symbol	$P23$
AFLOW prototype command	`aflow --proto=A7B12C_cP20_195_ag_3e_b-001` `--params=`a, x_3, x_4, x_5, x_6

- The paired Cd-II and Cd-III sites are never simultaneously occupied. The Cd-II site is filled 53.5% of the time, and Cd-III 46.5%. For approximate first-principles calculations one could average the two positions.
- Space group $P23$ #195 is chiral, Sohncke Class III, so this structure could be found in a mirror image configuration in the same space group.

Simple Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= a\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	As I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Cl I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Cd I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Cd I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Cd I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Cd I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Cd II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Cd II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Cd II
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Cd II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(4e)	Cd III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(4e)	Cd III
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(4e)	Cd III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(4e)	Cd III
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	As II
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	As II
$\mathbf{B_{17}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(6g)	As II
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(6g)	As II
$\mathbf{B_{19}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(6g)	As II
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(6g)	As II

References

[1] A. V. Shevelkov, L. N. Reshetova, and B. A.Popovkin, *Cd_8As_7Cl: A Novel Pnictidohalide with a New Structure Type*, J. Solid State Chem. **134**, 282–285 (1997), doi:10.1006/jssc.1997.7555.

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