CdI_2 (Polytype $6H_1$) Structure: AB2_hP9_156_2ab_a2b3c-001

This structure previously used the label(s) `AB2_hP9_156_b2c_3a2bc`. Calls to these addresses will be redirected here.

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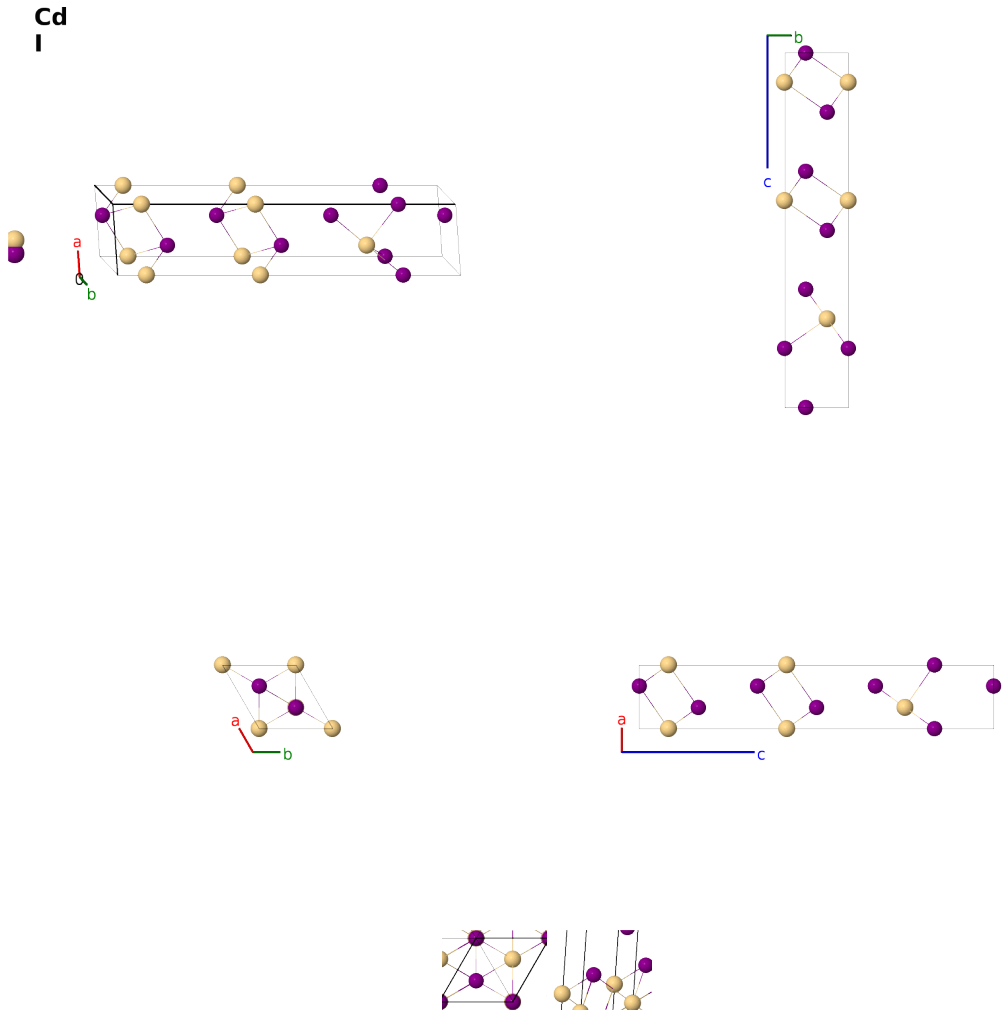
https://aflow.org/prototype-encyclopedia/0FK1

https://aflow.org/prototype-encyclopedia/AB2_hP9_156_2ab_a2b3c-001



Prototype	CdI_2
AFLOW prototype label	AB2_hP9_156_2ab_a2b3c-001
Pearson symbol	hP9
Space group number	156
Space group symbol	$P3m1$

AFLOW prototype command `aflow --proto=AB2_hP9_156_2ab_a2b3c-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9$

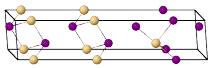
Other compounds with this structure

$PdTe_2$, $PtTe_2$, SnS_2 (berndtite)

- This is the $6H_{(a)}$ structure described by (Mitchell, 1956). He did not list the atomic positions, so the atoms are assumed to be evenly placed along the z-axis.
- This is an alternative stacking for CdI_2, which is usually found in the 2H ω ($C6$) phase.
- The $C27$ structure was also proposed as a structure of CdI_2, but this is now depreciated.
- (Mitchell, 1956) lists other possible stackings for CdI_2.
- Space group $P3m1$ #156 allows an arbitary choice for the origin of the z-axis. We exploit this to place the first iodine atom at the origin.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Cd I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	Cd II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1b)	Cd III
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(1b)	I II
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(1b)	I III
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(1c)	I IV
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(1c)	I V
$\mathbf{B_9}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(1c)	I VI

References

[1] R. S. Mitchell, *Polytypism of Cadmium Iodide and its Relationship to Screw Dislocations: I. Cadmium Iodide Polytypes*, Z. Kristallogr. **108**, 296–315 (1956), doi:10.1524/zkri.1956.108.3-4.296.

Found in

[1] P. Villars and K. Cenzual, *CdI2 Crystal Structure: Datasheet from "PAULING FILE Multinaries Edition – 2022"* (2022). SpringerMaterials (https://materials.springer.com/isp/crystallographic/docs/sd_1012215).

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