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

This structure originally had the label `AB2_hP9_156_b2c_3a2bc`. Calls to that address will be redirected here.

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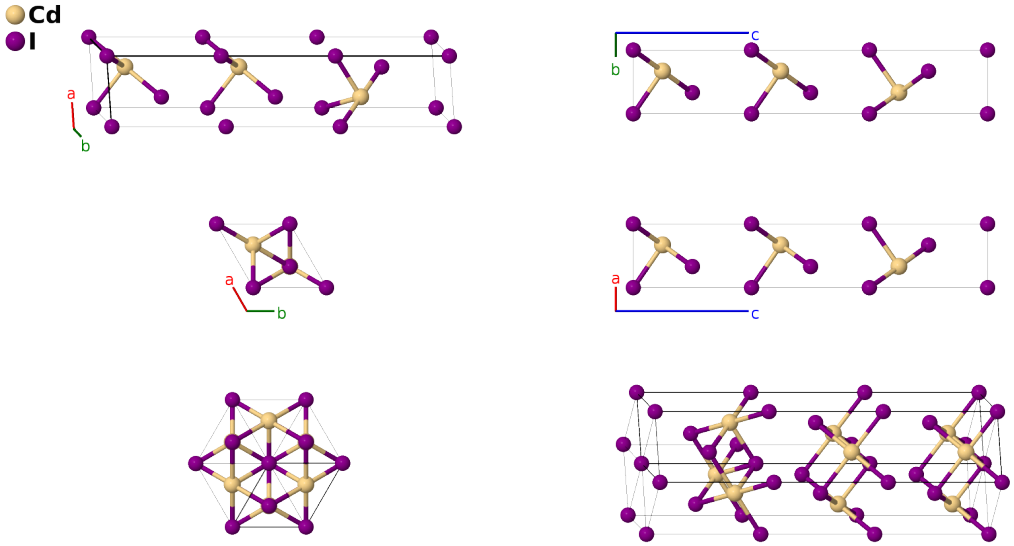
https://aflow.org/p/0FK1

https://aflow.org/p/AB2_hP9_156_2ab_a2b3c-001




| | |
|---|---|
| **Prototype** | $CdI_2$ |
| **AFLOW prototype label** | AB2_hP9_156_2ab_a2b3c-001 |
| **ICSD** | none |
| **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 $\omega$ ($C6$) 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.

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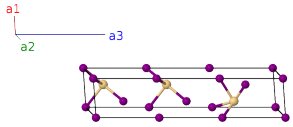
**Trigonal (Hexagonal) primitive vectors**

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$

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**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).