# C27 ($CdI_2$) Structure (*Questionable*): AB2_hP6_186_b_ab-001

This structure originally had the label `AB2_hP6_186_b_ab`. Calls to that address will be redirected here.

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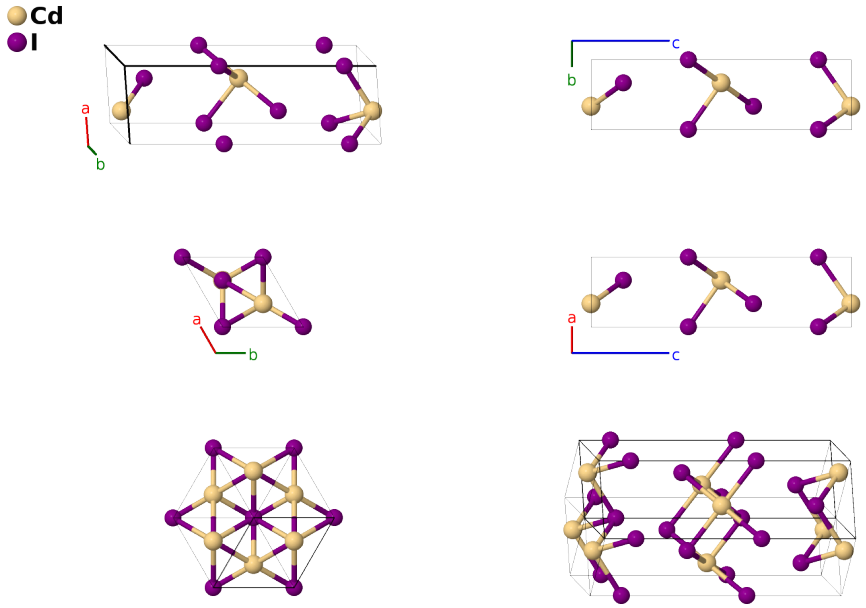
https://aflow.org/p/G4EJ

https://aflow.org/p/AB2_hP6_186_b_ab-001




| | |
|---|---|
| **Prototype** | $CdI_2$ |
| **AFLOW prototype label** | AB2_hP6_186_b_ab-001 |
| ***Strukturbericht* designation** | $C27$ |
| **ICSD** | 38116 |
| **Pearson symbol** | hP6 |
| **Space group number** | 186 |
| **Space group symbol** | $P6_3mc$ |
| **AFLOW prototype command** | `aflow --proto=AB2_hP6_186_b_ab-001 --params=`$a, c/a, z_1, z_2, z_3$ |

- This is a modification of the $C6$ ($\omega$ phase) $CdI_2$ structure proposed by (Hassel, 1933) to explain extra lines found in the x-ray spectra. This structure was never accepted by most researchers and does not appear in modern lists of *Strukturbericht* symbols, although (Parthé, 1993) lists it as a stacking varient of $CdI_2$. We include it here as part of the historical record.
- A ternary form does exist, the LiGaGe structure.

- Hassel originally placed a Cd atom at the origin, however both (Gottfried, 1937) and FINDSYM shift the origin as shown.
- There is no ICSD entry for (Hassell, 1933). The entry here is from (Smirnov, 1941).

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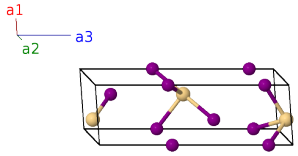
**Hexagonal primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (2a) | I I |
| $\mathbf{B_2}$ | = | $\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2a) | I I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$ | (2b) | Cd I |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2b) | Cd I |
| $\mathbf{B_5}$ | = | $\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$ | (2b) | I II |
| $\mathbf{B_6}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2b) | I II |

**References**


[1] O. Hassel, *Zur Kristallstruktur des Cadmiumjodids $CdJ_2$*, Z. physik. Chem. **22B**, 333–334 (1933), doi:10.1515/zpch-1933-2228.

[2] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

[3] L. Smirnov, A. Brager, and H. Zhdanov, *An X-ray examination of cadmium iodide*, Acta Physicochimica URSS **15**, 255–275 (1941).


**Found in**


[1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).