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

This structure previously used the label(s) `AB2_hP6_186_b_ab`. Calls to these addresses will be redirected here.

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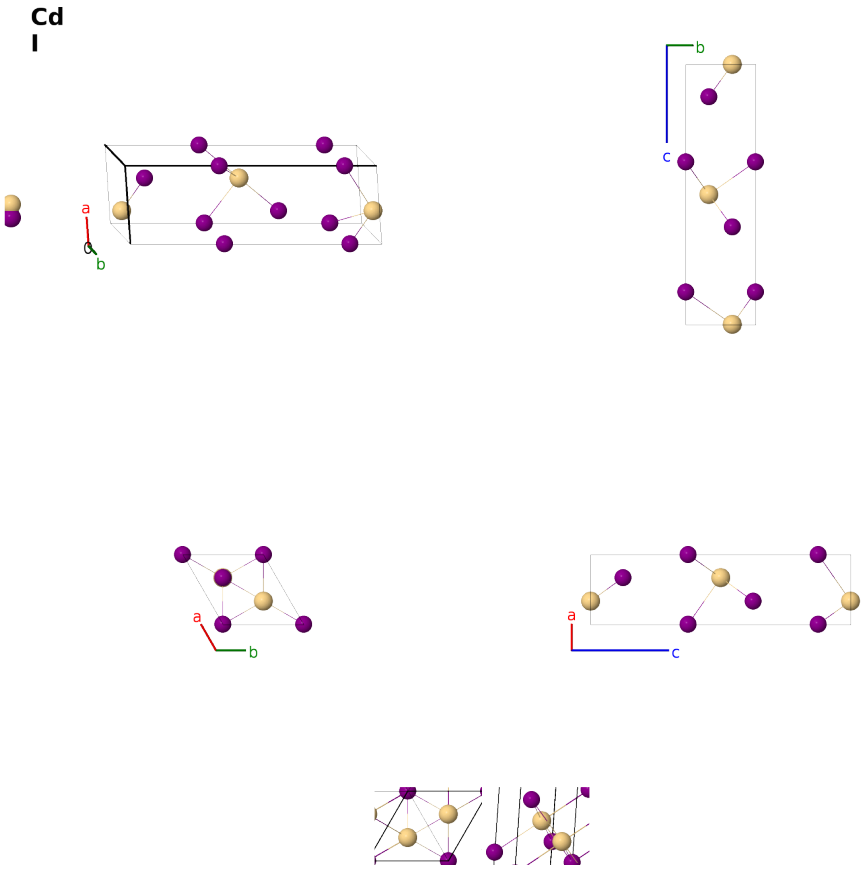
https://aflow.org/prototype-encyclopedia/G4EJ

https://aflow.org/prototype-encyclopedia/AB2_hP6_186_b_ab-001



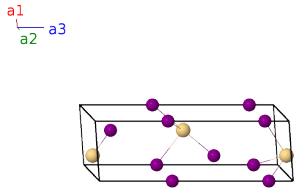
Prototype	CdI_2
AFLOW prototype label	AB2_hP6_186_b_ab-001
***Strukturbericht* designation**	*C*27
ICSD	38116
CCDC	1608838
Pearson symbol	hP6
Space group number	186
Space group symbol	$P6_3mc$

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 $C6$ (ω 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).

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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

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[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

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