ω Phase (CdI_2, $C6$) Structure: AB2_hP3_164_a_d-001

This structure originally had the label `AB2_hP3_164_a_d`. Calls to that address will be redirected here.

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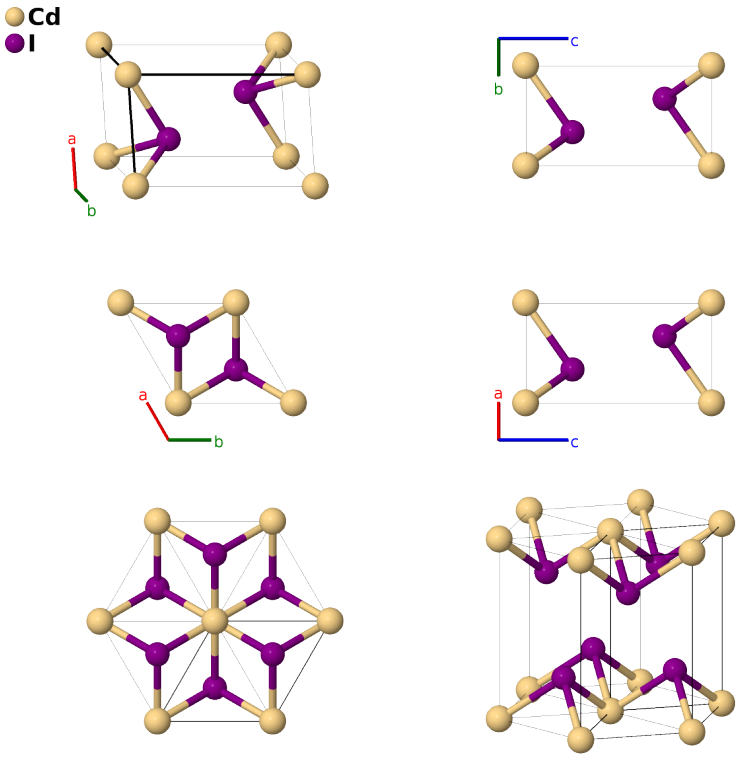
https://aflow.org/p/32EZ

https://aflow.org/p/AB2_hP3_164_a_d-001



Prototype	CdI_2
AFLOW prototype label	AB2_hP3_164_a_d-001
***Strukturbericht* designation**	$C6$
ICSD	53983
Pearson symbol	hP3
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=AB2_hP3_164_a_d-001 --params=`$a, c/a, z_2$

Other compounds with this structure

Ti, Zr, Hf, ZrNb, TiNb, TiV, α-W_2C, Cd_2Ce, Cd_2La, Cd_2Pr, Cd_2Y, Cl_2Fe (HP), Ge_2Eu, γ-I_2Hg, S_2Hf, S_2Pt, S_2Sn (berndtite), S_2Ta, S_2Ti, S_2Zr, Se_2Hf, Se_2Pt, Se_2Sn, Se_2Ti, Se_2V, Se_2Zr, Te_2Co, Te_2Ir, Te_2Pd, Te_2Rh, Te_2Ti, Te_2V, Te_2Zn, Te_2Zr, NiSeTe, PdSeTe, SSeSn, $(OH)_2Cd$

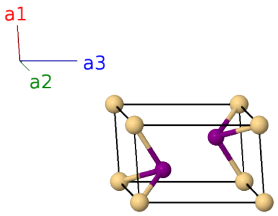
- The ω phase can be either hexagonal ($C32$) or trigonal (shown here). The trigonal ω phase transforms into several high-symmetry structures under certain conditions:

$\mathbf{c}/a$	$\mathbf{z}$	**Lattice**
Arbitrary	$\frac{1}{2}$	Ideal Omega ($C32$)
$\sqrt{\frac{3}{8}}$	$\frac{1}{6}$	Body-Centered Cubic ($A2$)
$\sqrt{\frac{3}{2}}$	$\frac{1}{6}$	Simple Cubic (A_h)
$\sqrt{6}$	$\frac{1}{6}$	Face-Centered Cubic ($A1$)
Arbitrary	0	Simple Hexagonal Structure (A_f)

- For more details about the omega phase and materials which form in the omega phase, see (Sikka, 1982) . As noted there, most omega phase intermetallic alloys are disordered. Although the "ω" label comes from ω-CrTi, (Ewald, 1931) lists the prototype for *Strukturbericht* designation $C6$ as CdI_2.
- Alternative stackings for CdI_2 have been proposed, including a $6H$ stacking and the questionable $C27$ structure.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	I I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	I I

References

[1] R. M. Bozorth, *The Crystal Structure of Cadmium Iodide*, J. Am. Chem. Soc. **44**, 2232–2236 (1922), doi:10.1021/ja01431a019.

[2] S. K. Sikka, Y. K. Vohra, and R. Chidambaram, *Omega Phase in Materials*, Prog. Mater. Sci. **27**, 245–310 (1982), doi:10.1016/0079-6425(82)90002-0.

Found in

[1] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).