$CdCl_2$ Structure: AB2_hR3_166_a_c-004

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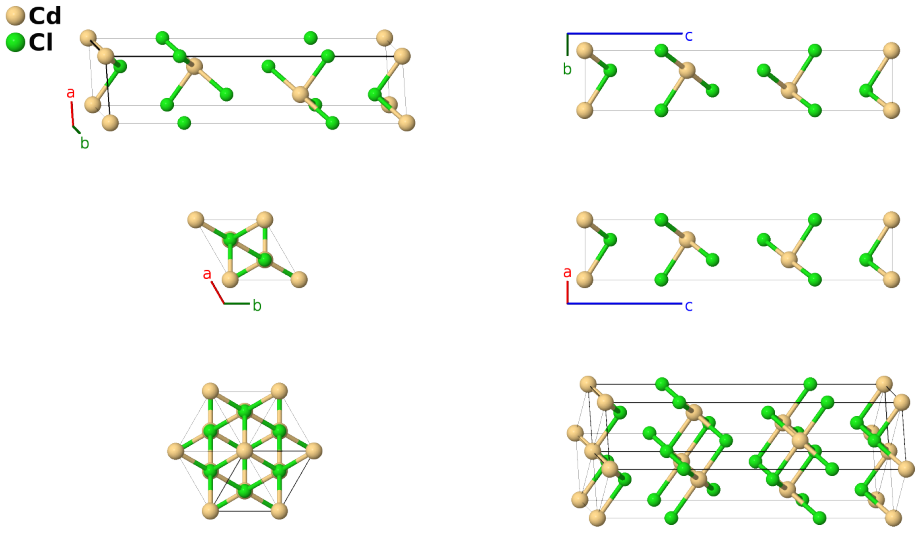
https://aflow.org/p/TKCJ

https://aflow.org/p/AB2_hR3_166_a_c-004



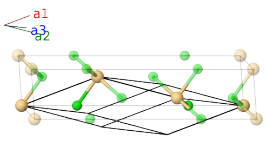
Prototype	$CdCl_2$
AFLOW prototype label	AB2_hR3_166_a_c-004
ICSD	30255
Pearson symbol	hR3
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB2_hR3_166_a_c-004 --params=`$a, c/a, x_2$

Other compounds with this structure
NbS_2, OCs_2, $TaSe_2$

- This is the binary form of the α-Sm ($C19$) structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cd I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Cl I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Cl I

References

[1] L. Pauling and J. L. Hoard, *The Crystal Structure of Cadmium Chloride*, Z. Krystallogr. **74**, 546–551 (1930), doi:10.1524/zkri.1930.74.1.546.