

CdCl₂ Structure:

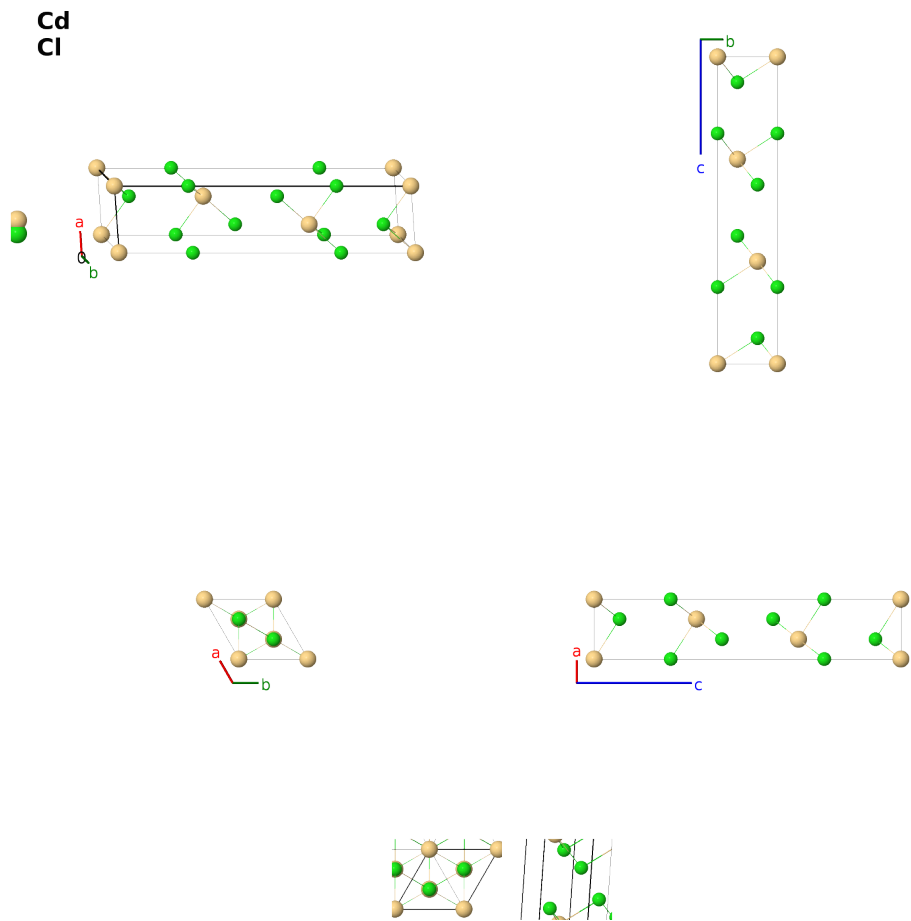
AB2_hR3_166_a_c-004

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/TKCJ>

https://aflow.org/prototype-encyclopedia/AB2_hR3_166_a_c-004



Prototype	CdCl ₂
AFLOW prototype label	AB2_hR3_166_a_c-004
ICSD	30255
CCDC	1604623
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= $a, c/a, x_2$`

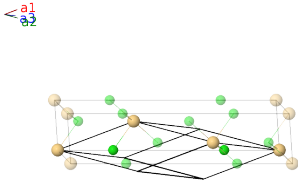
Other compounds with this structure

(Ag_xBi_{1-x})I₂, (Ag_xSb_{1-x})I₂, C(Sc_xY_{1-x})₂, CDy₂, CHo₂, CSc₂, CY₂, CdBr₂, CdCl₂, CoCl₂, FeCl₂, MgCl₂, MnBr₂, MnCl₂ (Sacchite), NbS₂, NiBr₂, NiCl₂, NiI₂, OCs₂, PbI₂, TaSe₂, ZnBr₂, ZnI₂

- This is the binary form of the α -Sm (*C*19) structure.
 - Hexagonal settings of this structure can be obtained with the option `--hex`.
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Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



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.

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