

CaIn₂ Structure:

AB2_hP6_194_b_f-001

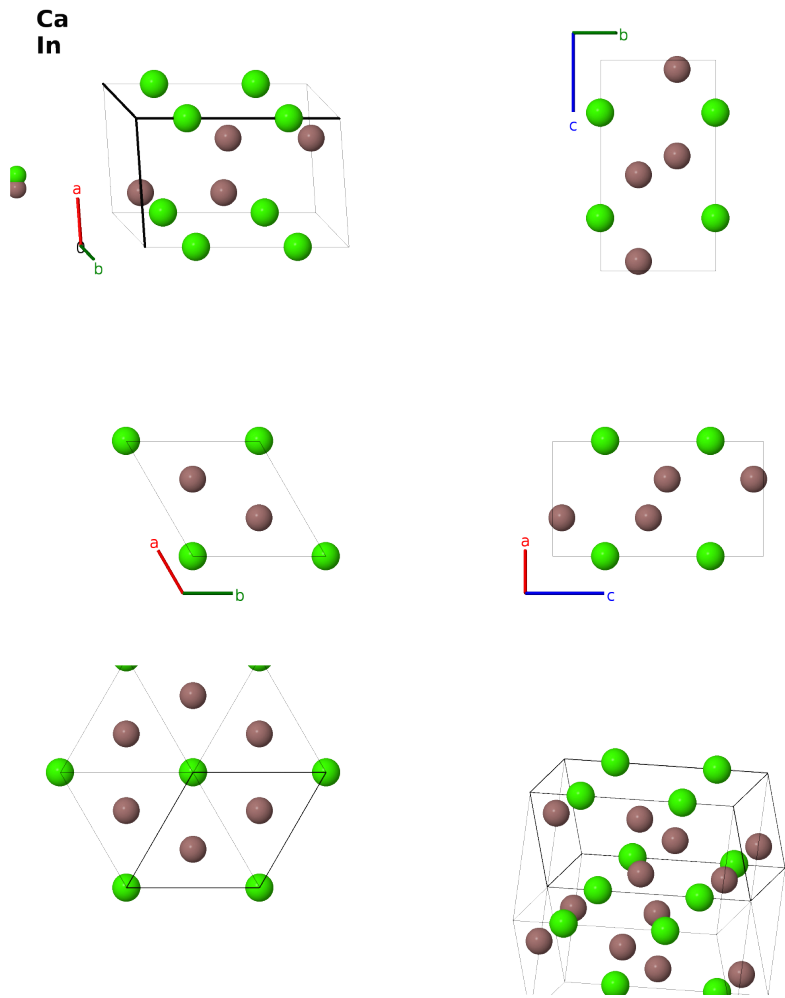
This structure previously used the label(s) **AB2_hP6_194_b_f**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/21YK>

https://aflow.org/prototype-encyclopedia/AB2_hP6_194_b_f-001



Prototype	CaIn ₂
AFLOW prototype label	AB2_hP6_194_b_f-001
ICSD	619376
CCDC	1748264
Pearson symbol	hP6

Space group number 194

Space group symbol $P6_3/mmc$

AFLOW prototype command `aflow --proto=AB2_hP6_194_b_f-001
--params=a, c/a, z2`

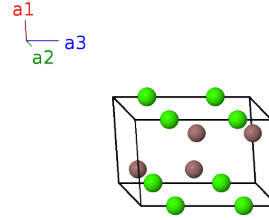
Other compounds with this structure

CaIn₂, EuIn₂, EuTl₂, SrIn₂, SrTl₂, YGa₂, YbIn₂

- (Iandelli, 1964) sets $z_2 = 0.205$, but the distances quoted in the paper are consistent with $z_2 = 1/4 - 0.205 = 0.045$. This value is confirmed in the quoted ICSD entry, attributed to (Bruzzone, 1964).
- When $z_2 = 0$ this structure reduces to the AlB₂ (C32), aka the hexagonal ω phase.
- CaIn₂ and hexagonal NbS₂ have the same AFLOW label, AB2_hP6_194_b.f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4f)	In I
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	In I
$\mathbf{B}_5$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4f)	In I
$\mathbf{B}_6$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	In I

References

- [1] A. Iandelli, *MX₂-Verbindungen der Erdalkali- und Seltenen Erdmetalle mit Gallium, Indium und Thallium*, Z. Anorganische und Allgemeine Chemie **330**, 221–232 (1964), doi:10.1002/zaac.19643300315.
- [2] G. Bruzzone and A. F. Ruggiero, *The Equilibrium Diagram of the Calcium-Indium System*, J. Less-Common Met. **7**, 368–372 (1964), doi:10.1016/0022-5088(64)90081-5.

Found in

- [1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017