$CaIn_2$ Structure: AB2_hP6_194_b_f-001

This structure originally had the label `AB2_hP6_194_b_f`. Calls to that address will be redirected here.

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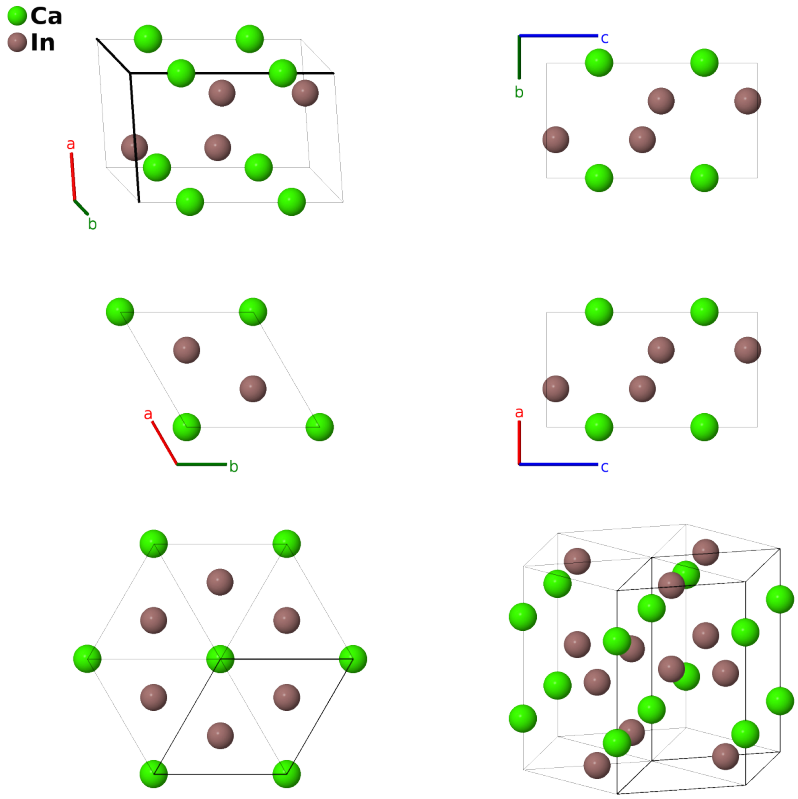
https://aflow.org/p/21YK

https://aflow.org/p/AB2_hP6_194_b_f-001



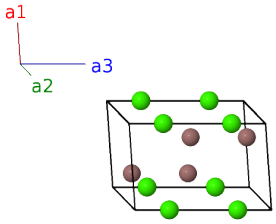
Prototype	$CaIn_2$
AFLOW prototype label	AB2_hP6_194_b_f-001
ICSD	619376
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB2_hP6_194_b_f-001 --params=`$a, c/a, z_2$

Other compounds with this structure
$CaIn_2$, $EuIn_2$, $EuTl_2$, $SrIn_2$, $SrTl_2$, YGa_2, $YbIn_2$

- (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 AlB_2 ($C32$), aka the hexagonal ω phase.
- $CaIn_2$ and hexagonal NbS_2 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	In I

References

[1] A. Iandelli, *MX_2-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, Tornoto, 1972).