

In (A6) Structure: A_tI2_139_a-001

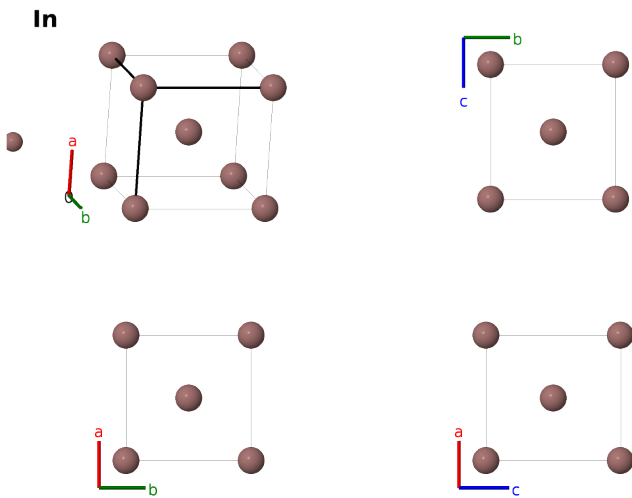
This structure previously used the label(s) **A.tI2.139.a.In**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/F5BG>

https://aflow.org/prototype-encyclopedia/A_tI2_139_a-001



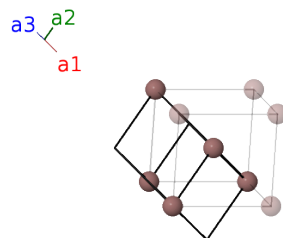
Prototype	In
AFLOW prototype label	A_tI2_139_a-001
<i>Strukturbericht</i> designation	A6
ICSD	639810
CCDC	1758964
Pearson symbol	tI2
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A_tI2_139_a-001 --params=a, c/a</code>

- This is an example of a “face”-centered tetragonal (fct) lattice, a distortion of the fcc lattice. This structure is actually a body-centered tetragonal lattice, since in the tetragonal system there is no distinction between face- and body-centered structures. In the $A6$ structure $c/a > 1$, while in the A_a structure $c/a < 1$.
- $A6$ and A_a structures have the same AFLOW prototype label, A_tI2.139.a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

- (Deshpande, 1969) give the lattice constants for indium using the fct description of the lattice. We have changed this to the bct description, dividing their lattice constant a by $\sqrt{2}$.
- The ICSD entry is from the earlier work of (Ridley, 1965).

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	=	0	=	0	(2a)
					In I

References

- [1] V. T. Deshpande and R. R. Pawar, *Anisotropic Thermal Expansion of Indium*, Acta Crystallogr. Sect. A **25**, 415–416 (1969), doi:10.1107/S0567739469000830.
- [2] N. Ridley, *Densities of some indium solid solutions*, J. Less-Common Met. **8**, 354–358 (1965), doi:10.1016/0022-5088(65)90071-8.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

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