In ($A6$) Structure: A_tI2_139_a-001

This structure originally had the label `A_tI2_139_a.In`. Calls to that address will be redirected here.

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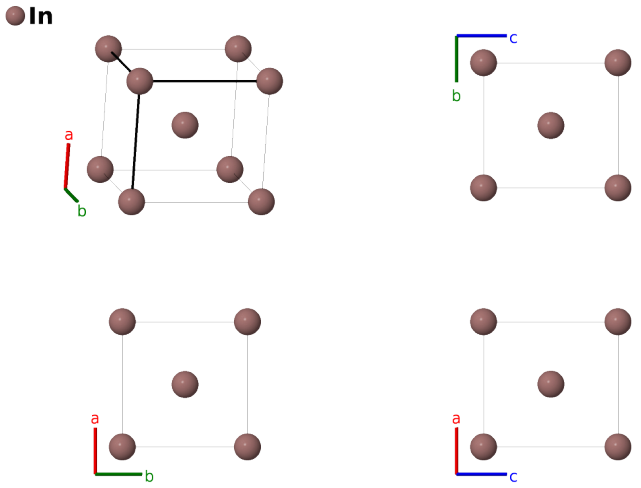
https://aflow.org/p/F5BG

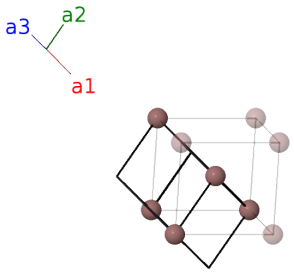
https://aflow.org/p/A_tI2_139_a-001



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

- 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



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

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	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).