

D_{13} (BaAl₄) Structure: A4B_tI10_139_de_a-001

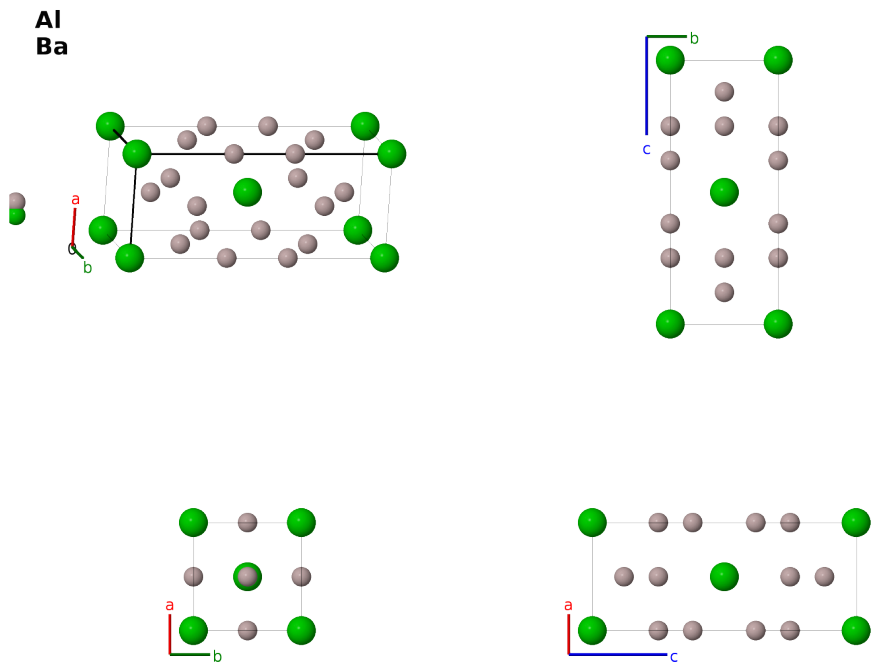
This structure previously used the label(s) **A4B_tI10_139_de_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/676C>

https://aflow.org/prototype-encyclopedia/A4B_tI10_139_de_a-001



Prototype	Al ₄ Ba
AFLOW prototype label	A4B_tI10_139_de_a-001
<i>Strukturbericht</i> designation	D_{13}
ICSD	57513
CCDC	1621570
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A4B_tI10_139_de_a-001 --params=a, c/a, z₃</code>

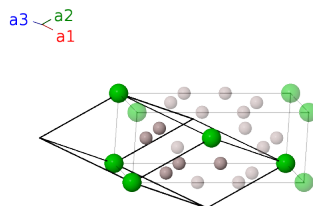
Other compounds with this structure

BaGa₄, BaIn₄, CaAl₄, CaGa₄, CeAl₄, EuAl₄, EuGa₄, KIn₄, LaAl₄, NdAl₄, PrAl₄, SmAl₄, SrAl₄, SrGa₄, ThZn₄, TlGa₄, YAl₄

- BaAl₄ is the parent structure of a number of ternary compounds (Shatruk, 2019):
- ThCr₂Si₂, space group $I4/mmm$ #139, with $c/a < 3$.
- TlCo₂S₂, also in space group $I4/mmm$ #139 but with $c/a > 3$.
- CaBe₂Ge₂, space group $P4/nmm$ #129.
- BaNiSn₃, space group $I4mm$ #107.

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
$\mathbf{B}_1$	=	0	=	0	(2a) Ba I
$\mathbf{B}_2$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d) Al I
$\mathbf{B}_3$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d) Al I
$\mathbf{B}_4$	=	$z_3\mathbf{a}_1 + z_3\mathbf{a}_2$	=	$cz_3\hat{\mathbf{z}}$	(4e) Al II
$\mathbf{B}_5$	=	$-z_3\mathbf{a}_1 - z_3\mathbf{a}_2$	=	$-cz_3\hat{\mathbf{z}}$	(4e) Al II

References

- [1] K. R. Andress and E. Alberti, *Röntgenographische Untersuchung der Legierungsreihe Aluminium-Barium*, Z. Metallkd. **27**, 126–128 (1935).
- [2] M. Shatruk, *ThCr₂Si₂ structure type: The “perovskite” of intermetallics*, J. Solid State Chem. **272**, 198–209 (2019), doi:10.1016/j.jssc.2019.02.012.

Found in

- [1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

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