$D1_3$ ($BaAl_4$) Structure: A4B_tI10_139_de_a-001

This structure originally had the label `A4B_tI10_139_de_a`. Calls to that address will be redirected here.

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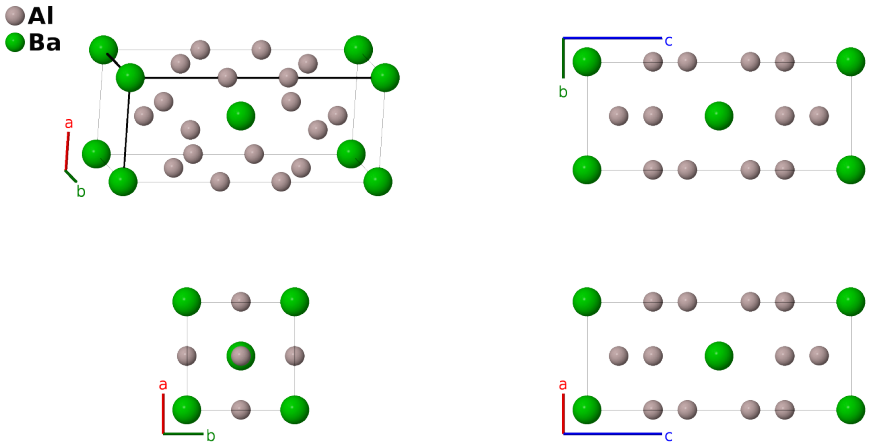
https://aflow.org/p/676C

https://aflow.org/p/A4B_tI10_139_de_a-001



Prototype	Al_4Ba
AFLOW prototype label	A4B_tI10_139_de_a-001
***Strukturbericht* designation**	$D1_3$
ICSD	57513
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A4B_tI10_139_de_a-001 --params=`$a, c/a, z_3$

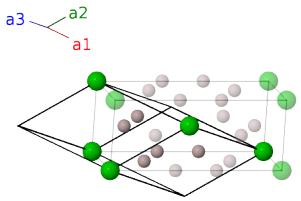
Other compounds with this structure

$BaGa_4$, $BaIn_4$, $CaAl_4$, $CaGa_4$, $CeAl_4$, $EuAl_4$, $EuGa_4$, KIn_4, $LaAl_4$, $NdAl_4$, $PrAl_4$, $SmAl_4$, $SrAl_4$, $SrGa_4$, $ThZn_4$, $TlGa_4$, YAl_4

- $BaAl_4$ is the parent structure of a number of ternary compounds (Shatruk, 2019):
- $ThCr_2Si_2$, space group $I4/mmm$ #139, with $c/a < 3$.
- $TlCo_2S_2$, also in space group $I4/mmm$ #139 but with $c/a > 3$.
- $CaBe_2Ge_2$, space group $P4/nmm$ #129.
- $BaNiSn_3$, space group $I4mm$ #107.

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)	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, *$ThCr_2Si_2$ 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.