$BaFe_2Al_9$ Structure: A9BC2_hP12_191_fm_a_c-001

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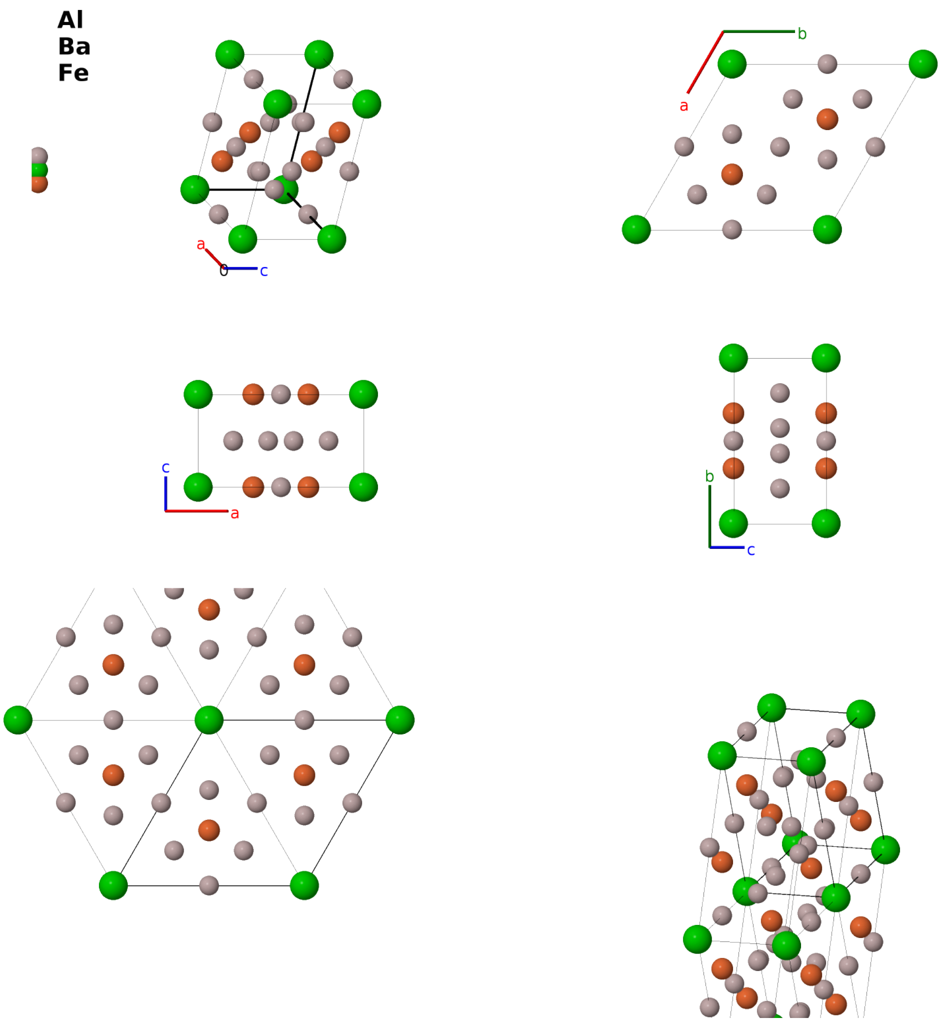
https://aflow.org/prototype-encyclopedia/CSJ8

https://aflow.org/prototype-encyclopedia/A9BC2_hP12_191_fm_a_c-001



Prototype	Al_9BaFe_2
AFLOW prototype label	A9BC2_hP12_191_fm_a_c-001
ICSD	57518
CCDC	1621573
Pearson symbol	hP12
Space group number	191

Space group symbol $P6/mmm$

AFLOW prototype command `aflow --proto=A9BC2_hP12_191_fm_a_c-001 --params=`$a, c/a, x_4$

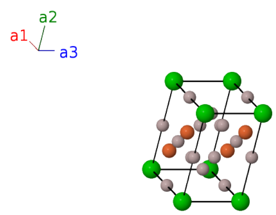
Other compounds with this structure

$BaCo_2Al_9$, $BaIr_2In_9$, $BaNi_2Al_9$, $CaCo_2Al_9$, $EuCo_2Al_9$, KCo_2In_9, KNi_2In_9, $SrCo_2Al_9$, $SrNi_2Al_9$

- The ICSD designates $SrCo_2Al_9$ as the representative for this structure type.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Fe I
$\mathbf{B_3}$	=	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_5}$	=	$\frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_6}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3f)	Al I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II
$\mathbf{B_8}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II
$\mathbf{B_{11}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	Al II

References

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