Brownmillerite ($Ca_2(Fe_{2-x}Al_x)O_5$) Structure: AB2CD5_oI36_46_b_c_a_b2c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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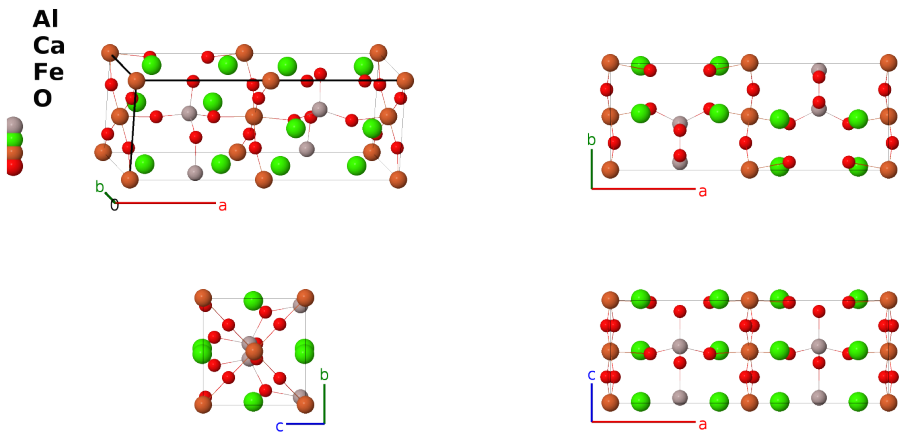
https://aflow.org/prototype-encyclopedia/UJW7

https://aflow.org/prototype-encyclopedia/AB2CD5_oI36_46_b_c_a_b2c-001



Prototype	$AlCa_2FeO_5$
AFLOW prototype label	AB2CD5_oI36_46_b_c_a_b2c-001
Mineral name	brownmillerite
ICSD	98831
CCDC	1658065
Pearson symbol	oI36
Space group number	46
Space group symbol	$Ima2$
AFLOW prototype command	`aflow --proto=AB2CD5_oI36_46_b_c_a_b2c-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

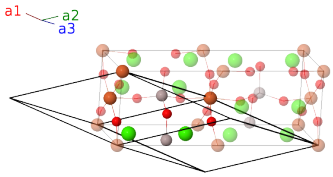
$(Ca_xSr_{1-x})_2FeCoO_5$, $Ca_2(Al_{2-x}Mn_x)O_5$, $Ca_2(Fe_{2-x}Cu_x)O_5$, $Ca_2Cr_2O_5$, Mn_2LaSrO_5, Mn_2NdSrO_5, $Sr_2Fe_2O_5$, Sr_2GaScO_5, $Sr_2In_2O_5$

- The Fe (4a) and Al (4b) sites are alloyed. In the current sample the (4a) site is 84.9% iron and 15.1% aluminum, while the (4b) site is 56.1% iron and 43.9% aluminum. We label the (4b) site as aluminium to separate it from the (4a) site.
- When x < 0.56 the structure transforms into a simple orthorhombic structure (Redhammer, 2004), while the stoichiometric (x = 0) structure transforms to this structure above 950K (Shaula, 2006).

- (Redhammer, 2004) give this structure in the $I2mb$ setting of space group #46. We use AFLOW to transform it into the standard $Ima2$ setting.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Al I
$\mathbf{B_4}$	=	$-(y_2 - z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Al I
$\mathbf{B_5}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_6}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_7}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca I
$\mathbf{B_8}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca I
$\mathbf{B_9}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4 - y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca I
$\mathbf{B_{10}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Ca I
$\mathbf{B_{11}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{12}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{13}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{14}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_5 + y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{15}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{16}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O III

$\mathbf{B_{17}}$	=	$-\left(y_6 - z_6\right)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{18}}$	=	$\left(y_6 + z_6\right)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O III

References

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First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).