Brownmillerite (Srebrodolskite) Brownmillerite ($Ca_2Fe_2O_5$) Structure: A2B2C5_oP36_62_d_ac_c2d-001

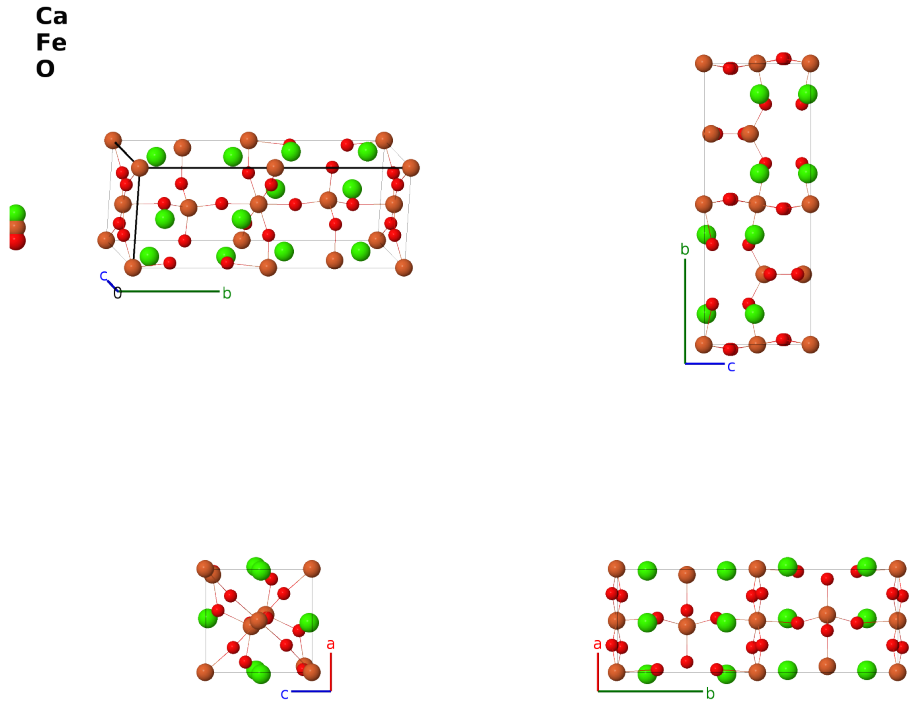
Cite this page as:

- 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.

---

https://aflow.org/prototype-encyclopedia/6H47

https://aflow.org/prototype-encyclopedia/A2B2C5_oP36_62_d_ac_c2d-001



Prototype	$Ca_2Fe_2O_5$
AFLOW prototype label	A2B2C5_oP36_62_d_ac_c2d-001
Mineral name	brownmillerite
ICSD	155632
CCDC	1672233
Pearson symbol	oP36
Space group number	62
Space group symbol	*Pnma*

AFLOW prototype command `aflow --proto=A2B2C5_oP36_62_d_ac_c2d-001 --params=`$a, b/a, c/a, x_2, z_2, x_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

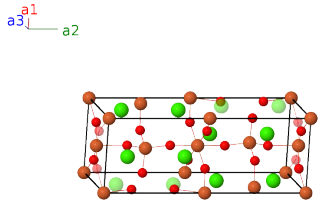
Other compounds with this structure

$Ca_2Al_2O_5$, $Sr_2Co_2O_5$, $Sr_2Fe_2O_5$

- Brownmillerite typically has the composition $Fe_{2-x}Al_xO_5$, but the pure compound, which the ICSD names Srebrodolskite, has been observed.
- Above 950K this structure transforms into a body-centered orthorhombic structure (Shaula, 2006). This transformation also occurs in the alloyed compounds when x > 0.56 (Redhammer, 2004).
- (Shaula, 2006) list the O3 Wyckoff position as (8d), but the coordinates are given for a (4c) site, which gives the proper stoichiometry.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Ca I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	Ca I

$$\mathbf{B_{16}} = \left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_4-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Ca I}$$

$$\mathbf{B_{17}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{Ca I}$$

$$\mathbf{B_{18}} = \left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Ca I}$$

$$\mathbf{B_{19}} = x_4\,\mathbf{a}_1 - \left(y_4-\tfrac{1}{2}\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - b\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{Ca I}$$

$$\mathbf{B_{20}} = -\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_4+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{Ca I}$$

$$\mathbf{B_{21}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{22}} = -\left(x_5-\tfrac{1}{2}\right)\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{23}} = -x_5\,\mathbf{a}_1 + \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + b\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{24}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{25}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{26}} = \left(x_5+\tfrac{1}{2}\right)\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{27}} = x_5\,\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - b\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{28}} = -\left(x_5-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_5+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O II}$$

$$\mathbf{B_{29}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{30}} = -\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{31}} = -x_6\,\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{32}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{33}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{34}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{35}} = x_6\,\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

$$\mathbf{B_{36}} = -\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

References

[1] A. L. Shaula, Y. V. Pivak, J. C. Waerenborgh, P. G. nski, A. A. Yaremchenko, and V. V. Kharton, *Ionic conductivity of brownmillerite-type calcium ferrite under oxidizing conditions*, Solid State Ion. **177**, 2923–2930 (2006), doi:10.1016/j.ssi.2006.08.030.

[2] G. J. Redhammer, G. Tippelt, G. Roth, and G. Amthauer, *Structural variations in the brownmillerite series Ca2(Fe$_{2-x}$Al$_x$)O$_5$: Single-crystal X-ray diffraction at 25 °C and high-temperature X-ray powder diffraction (25 °C T 1000 °C)*, Am. Mineral. **89**, 405–420 (2004).

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).