

Kotoite ($\text{Mg}_3(\text{BO}_3)_2$) Structure: A2B3C6_oP22_58_g_af_gh-001

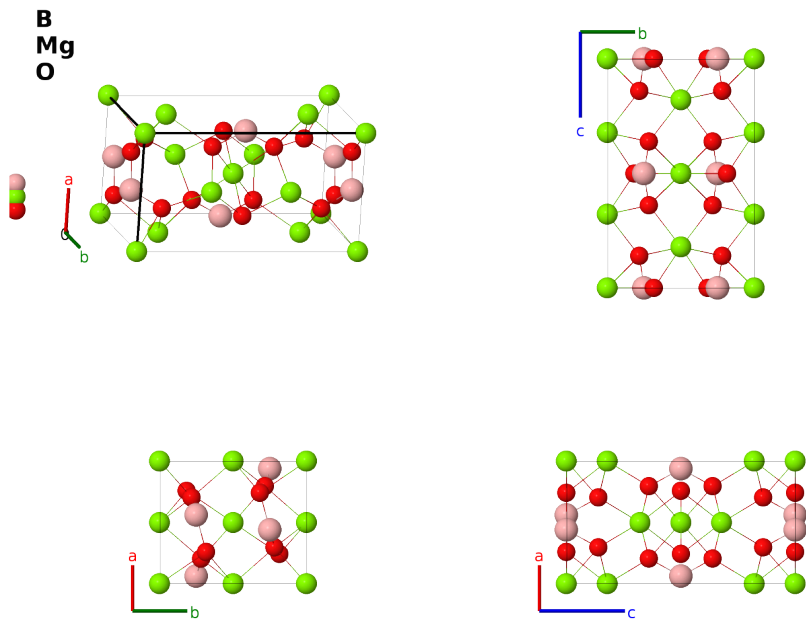
This structure previously used the label(s) **A2B3C6_oP22_58_g_af_gh**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/59YW>

https://aflow.org/prototype-encyclopedia/A2B3C6_oP22_58_g_af_gh-001



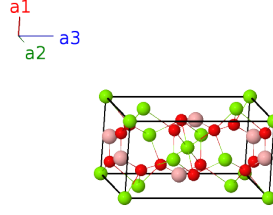
Prototype	$\text{B}_2\text{Mg}_3\text{O}_6$
AFLOW prototype label	A2B3C6_oP22_58_g_af_gh-001
Mineral name	kotoite
ICSD	24036
CCDC	1600092
Pearson symbol	oP22
Space group number	58
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A2B3C6_oP22_58_g_af_gh-001</code> <code>--params=a, b/a, c/a, z₂, x₃, y₃, x₄, y₄, x₅, y₅, z₅</code>

Other compounds with this structure

$\text{Co}_3(\text{BO}_3)_2$, $\text{Ni}_3(\text{BO}_3)_2$, $\text{Mn}_3(\text{BO}_3)_2$ (jimboite), $\text{CoNi}_2(\text{BO}_3)_2$, $\text{KNa}_2(\text{BO}_3)_2$, $\text{Eu}_3(\text{BO}_3)_2$

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Mg I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B}_9$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	B I
$\mathbf{B}_{10}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	B I
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_{13}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_{14}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4g)	O I
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{17}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{18}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{21}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	O II
$\mathbf{B}_{22}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	O II

References

- [1] S. V. Berger, *The Crystal Structure of the Isomorphous Orthoborates of Cobalt and Magnesium*, Acta Chem. Scand. **3**, 660–675 (1949), doi:10.3891/acta.chem.scand.03-0660.

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