

$E3_2$ (CaB₂O₄ I) Structure: A2BC4_oP28_60_d_c_2d-001

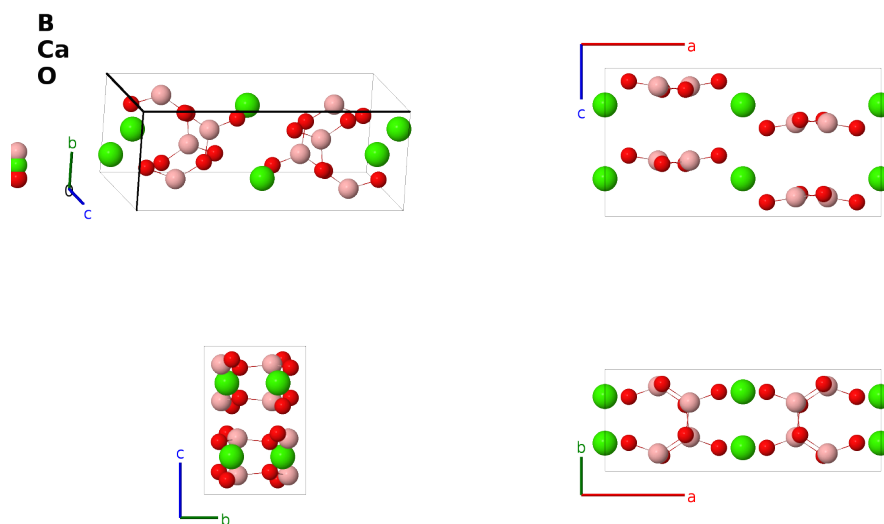
This structure previously used the label(s) **A2BC4_oP28_60_d_c_2d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/44A7>

https://aflow.org/prototype-encyclopedia/A2BC4_oP28_60_d_c_2d-001



Prototype	B ₂ CaO ₄
AFLOW prototype label	A2BC4_oP28_60_d_c_2d-001
<i>Strukturbericht</i> designation	$E3_2$
ICSD	34641
CCDC	1607016
Pearson symbol	oP28
Space group number	60
Space group symbol	$Pbcn$
AFLOW prototype command	<pre>aflow --proto=A2BC4_oP28_60_d_c_2d-001 --params=a, b/a, c/a, y₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</pre>

Other compounds with this structure

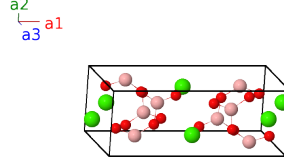
EuB₂O₄, SrB₂O₄

- CaB₂O₄ exists in at least four phase (Marezio, 1969):

- The ground state, stable below 1.2 GPa, *Strukturbericht E3₂* (this structure)
- Orthorhombic high pressure structure, stable between 1.2 and 1.5 GPa, presumably Calciborite
- Orthorhombic high pressure structure, stable between 1.5 and 2.5 GPa
- Cubic high pressure structure, stable between 2.5 and 4.0 GPa
- (Marezio, 1963) gives the crystal structure in the Pnca setting of space group #60. We have used FINDSYM to transform this to the standard Pbcn setting.
- CaB₂O₄ I and α -Li₃PO₄ have the same AFLOW prototype label, A2BC4_oP28_60_d_c_2d. They are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	$y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_1 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - b (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B}_3$	$-y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_1 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + b (y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_6$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_8$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_9$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_{10}$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_{11}$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_{12}$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b (y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	B I
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{14}$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{15}$	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{16}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{17}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{18}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_{19}$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O I

$$\begin{aligned}
\mathbf{B}_{20} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 = -a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (8d) & \text{O I} \\
\mathbf{B}_{21} &= 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) & \text{O II} \\
\mathbf{B}_{22} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 = -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{23} &= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{24} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 = a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{25} &= -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) & \text{O II} \\
\mathbf{B}_{26} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{27} &= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{28} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8d) & \text{O II}
\end{aligned}$$

References

- [1] M. Marezio, H. A. Plettinger, and W. H. Zachariasen, *Refinement of the calcium metaborate structure*, Acta Cryst. **16**, 390–392 (1963), doi:10.1107/S0365110X63001031.

Found in

- [1] M. Marezio, J. P. Remeika, and P. D. Dernier, *The crystal structure of the high-pressure phase $\text{CaB}_2\text{O}_4(\text{IV})$, and polymorphism in CaB_2O_4* , Acta Crystallogr. Sect. B **25**, 965–970 (1969), doi:10.1107/S0567740869003256.

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