

CaB₂O₄ (III) Structure: A2BC4_oP84_33_6a_3a_12a-001

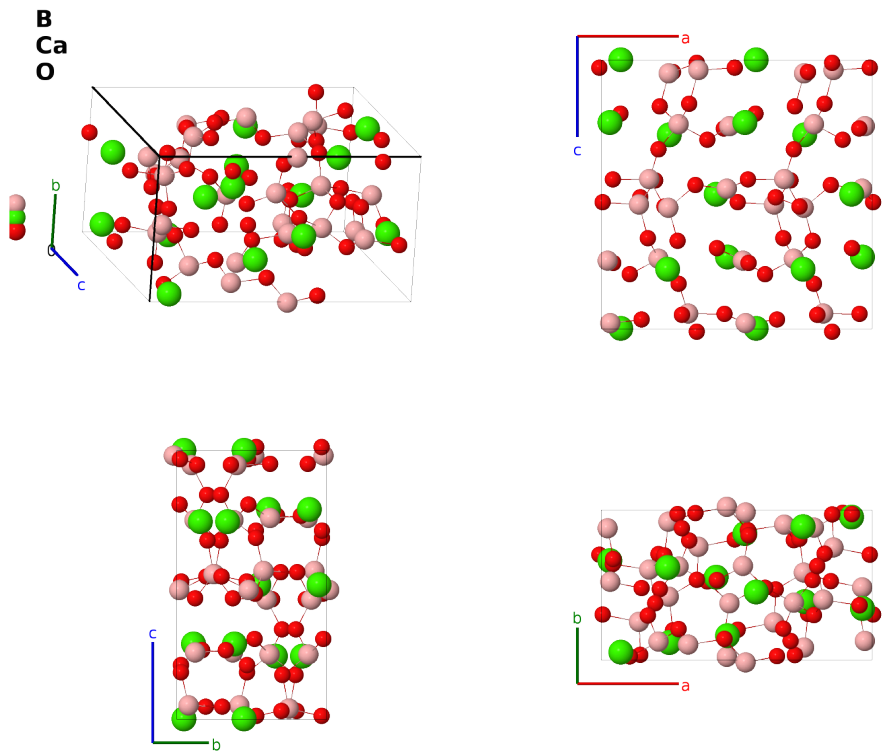
This structure previously used the label(s) **A2BC4_oP84_33_6a_3a_12a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/S26L>

https://aflow.org/prototype-encyclopedia/A2BC4_oP84_33_6a_3a_12a-001



Prototype	B ₂ CaO ₄
AFLOW prototype label	A2BC4_oP84_33_6a_3a_12a-001
ICSD	23240
CCDC	1599372
Pearson symbol	oP84
Space group number	33
Space group symbol	<i>Pna</i> 2 ₁
AFLOW prototype command	<pre>aflow --proto=A2BC4_oP84_33_6a_3a_12a-001 --params=a,b/a,c/a,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅, y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉,x₂₀,y₂₀,z₂₀,x₂₁,y₂₁,z₂₁</pre>

- CaB_2O_4 exists in at least four phases (Marezio, 1969):

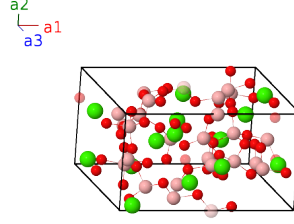
- The ground state, stable below 1.2 GPa, *Strukturbericht E3₂*
- Orthorhombic high pressure structure, stable between 1.2 and 1.5 GPa, presumably Calciborite
- Orthorhombic high pressure structure, stable between 1.5 and 2.5 GPa (this structure)
- Cubic high pressure structure, stable between 2.5 and 4.0 GPa

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(4a)$		B I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B I
$\mathbf{B}_3$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(4a)$		B I
$\mathbf{B}_4$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(4a)$		B II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B II
$\mathbf{B}_7$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(4a)$		B II
$\mathbf{B}_8$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(4a)$		B III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B III
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(4a)$		B III
$\mathbf{B}_{12}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	$(4a)$		B IV
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B IV
$\mathbf{B}_{15}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	$(4a)$		B IV
$\mathbf{B}_{16}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B IV
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	$(4a)$		B V
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		B V
$\mathbf{B}_{19}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	$(4a)$		B V

$$\mathbf{B}_{82} = -x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + \left(z_{21} + \frac{1}{2}\right) \mathbf{a}_3 = -ax_{21} \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + c\left(z_{21} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{O XII}$$

$$\mathbf{B}_{83} = \left(x_{21} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{21} - \frac{1}{2}\right) \mathbf{a}_2 + z_{21} \mathbf{a}_3 = a\left(x_{21} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{21} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}} \quad (4a) \quad \text{O XII}$$

$$\mathbf{B}_{84} = -\left(x_{21} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{21} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{21} + \frac{1}{2}\right) \mathbf{a}_3 = -a\left(x_{21} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{21} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{21} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{O XII}$$

References

- [1] M. Marezio, J. P. Remeika, and P. D. Dernier, *The crystal structure of the high-pressure phase $\text{CaB}_2\text{O}_4(\text{III})$* , Acta Crystallogr. Sect. B **25**, 955–964 (1969), doi:10.1107/S0567740869003244.

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