

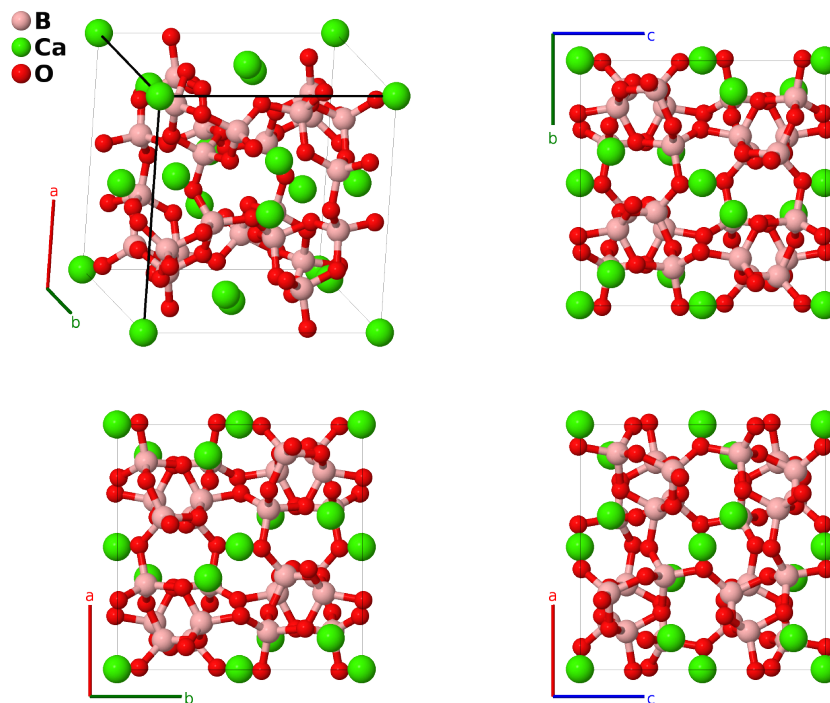
# CaB<sub>2</sub>O<sub>4</sub> (IV) Structure: A2BC4\_cP84\_205\_d\_ac\_2d-001

This structure originally had the label A2BC4\_cP84\_205\_d\_ac\_2d. Calls to that address will be redirected here.

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<https://aflow.org/p/TZRB>

[https://aflow.org/p/A2BC4\\_cP84\\_205\\_d\\_ac\\_2d-001](https://aflow.org/p/A2BC4_cP84_205_d_ac_2d-001)



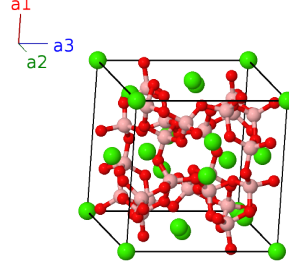
Prototype	B <sub>2</sub> CaO <sub>4</sub>
AFLOW prototype label	A2BC4_cP84_205_d_ac_2d-001
ICSD	23241
Pearson symbol	cP84
Space group number	205
Space group symbol	$P\bar{a}3$
AFLOW prototype command	<code>aflow --proto=A2BC4_cP84_205_d_ac_2d-001 --params=a, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></code>

- CaB<sub>2</sub>O<sub>4</sub> exists in at least four phase (Marezio, 1969):
  - The ground state, stable below 1.2 GPa, *Strukturbericht E3<sub>2</sub>*
  - 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 (this structure)

### Simple Cubic primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	$0$	(4a)	Ca I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a)	Ca I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{10}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{16}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{17}$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{18}$	$= (z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{19}$	$= -(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{20}$	$= -z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{21}$	$= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(24d)	B I





## References

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