

CaO₂(H₂O)₈ Structure: AB8C2_tP22_124_a_n_h-001

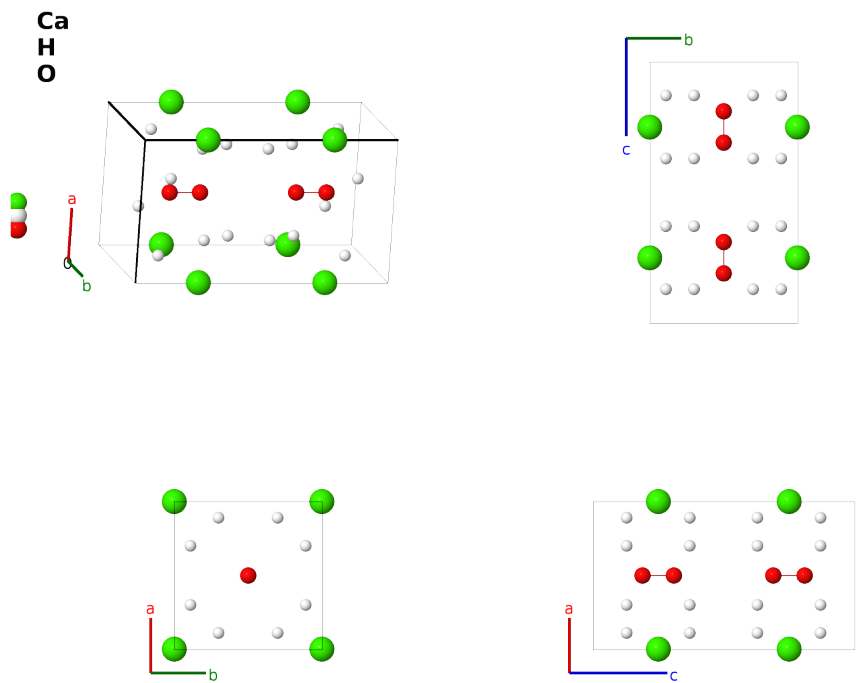
This structure previously used the label(s) **AB8C2.tP22.124.a.n.h**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB8C2_tP22_124_a_n_h-001



Prototype	Ca(H ₂ O) ₈ O ₂
AFLOW prototype label	AB8C2_tP22_124_a_n_h-001
ICSD	38168
CCDC	1608877
Pearson symbol	tP22
Space group number	124
Space group symbol	<i>P</i> 4/ <i>mcc</i>
AFLOW prototype command	<code>aflow --proto=AB8C2_tP22_124_a_n_h-001</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>z</i>₂, <i>x</i>₃, <i>y</i>₃, <i>z</i>₃</code>

Other compounds with this structure

$\text{BrO}_2(\text{H}_2\text{O})_8$, $\text{SrO}_2(\text{H}_2\text{O})_8$

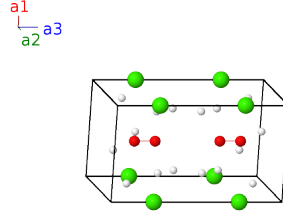
- This structure was proposed by (Shineman, 1951) to replace the $E6_2$ $\text{SrO}_2(\text{H}_2\text{O})_8$ structure. The unit cell is doubled in the (001) direction, and the oxygens are now molecular.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_9$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{10}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{13}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{14}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{16}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{17}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{18}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{19}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{20}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{21}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I
$\mathbf{B}_{22}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16n)	H I

References

- [1] R. S. Shineman and A. J. King, *The space group of calcium peroxide octahydrate*, Acta Cryst. **4**, 67–68 (1951), doi:10.1107/S0365110X5100012X.

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