β-CaC_2O_4 Structure: A2BC4_mP28_10_ijmn_mn_2m2n2o-001

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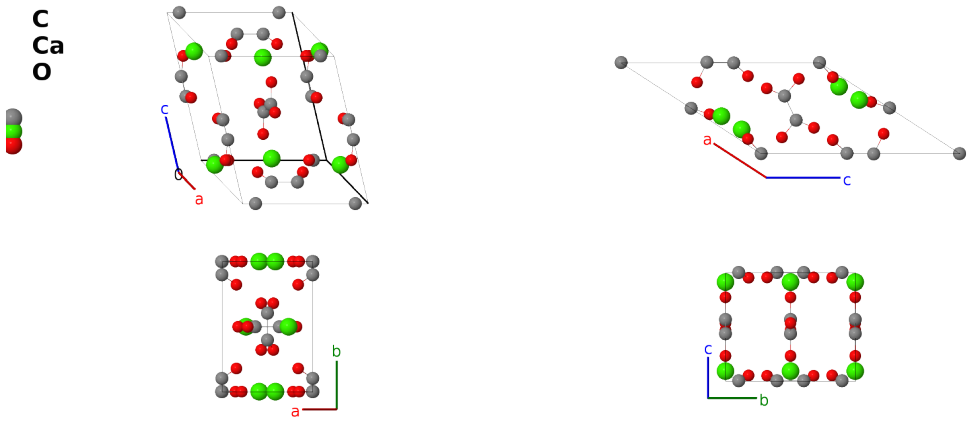
https://aflow.org/prototype-encyclopedia/CLFS

https://aflow.org/prototype-encyclopedia/A2BC4_mP28_10_ijmn_mn_2m2n2o-001

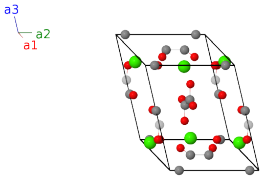


Prototype	C_2CaO_4
AFLOW prototype label	A2BC4_mP28_10_ijmn_mn_2m2n2o-001
ICSD	246005
CCDC	1712673
Pearson symbol	mP28
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=A2BC4_mP28_10_ijmn_mn_2m2n2o-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- Anhydrous CaC_2O_4 is found in three forms, but the β form is the only one with a known structure.
- Below 250°C it transforms into αCaC_2O_4, and above 410°C it transforms into γCaC_2O_4.
- The data for this structure was obtained at 25°C.
- The AFLOW label ordering protocol rewrites the axes for this monoclinic structure, moving the C I and C II sites from Wyckoff positions (2j) and (2l) to positions (2i) and (2j).

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(2i)	C I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_2$	=	$-by_1\,\hat{\mathbf{y}}$	(2i)	C I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}}$	(2j)	C II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}}$	(2j)	C II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	C III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	C III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2m)	Ca I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2m)	Ca I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2m)	O I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2m)	O I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2m)	O II
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2m)	O II
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2n)	C IV
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2n)	C IV
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2n)	Ca II
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2n)	Ca II
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2n)	O III
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2n)	O III
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O IV
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2n)	O IV
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O V
$\mathbf{B_{22}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O V
$\mathbf{B_{23}}$	=	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O V
$\mathbf{B_{24}}$	=	$x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O V
$\mathbf{B_{25}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O VI
$\mathbf{B_{26}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O VI
$\mathbf{B_{27}}$	=	$-x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O VI
$\mathbf{B_{28}}$	=	$x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4o)	O VI

References

[1] O. Hochrein, A. Thomas, and R. Kniep, *Revealing the Crystal Structure of Anhydrous Calcium Oxalate, $Ca[C_2O_4]$, by a Combination of Atomistic Simulation and Rietveld Refinement*, Z. Anorganische und Allgemeine Chemie **634**, 1826–1829 (2008), doi:10.1002/zaac.200800207.

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