

CaC₂-III Structure:

A2B_mC12_12_2i_i-004

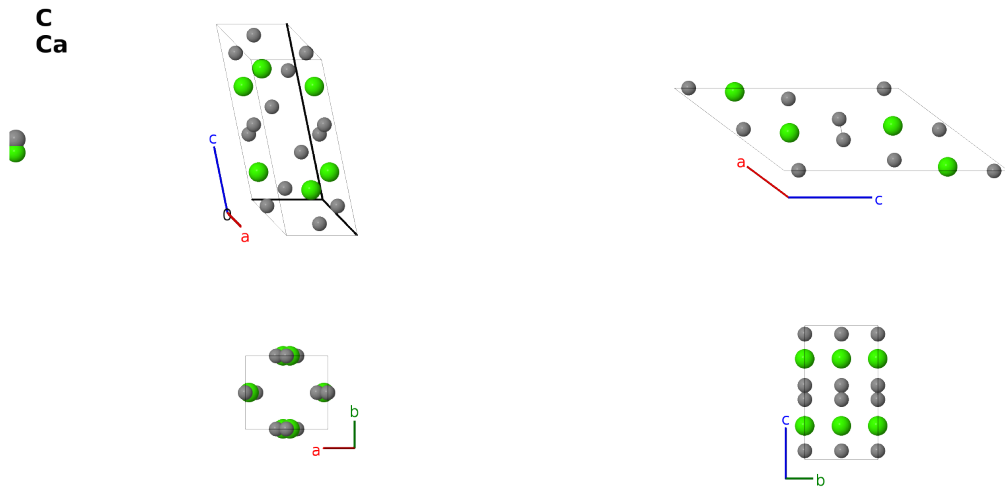
This structure previously used the label(s) **A2B_mC12_12_2i_i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/2JVM>

https://aflow.org/prototype-encyclopedia/A2B_mC12_12_2i_i-004

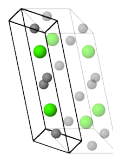


Prototype	C ₂ Ca
AFLOW prototype label	A2B_mC12_12_2i_i-004
ICSD	54188
CCDC	1773608
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A2B_mC12_12_2i_i-004</code> <code>--params=a, b/a, c/a, β, x_1, z_1, x_2, z_2, x_3, z_3</code>

- This is a metastable room temperature structure.
- The stable room temperature configuration has the CaC₂-I ($C11_a$) structure.
- At low temperatures CaC₂ transforms into the ThC₂ (C_g) structure.
- CaC₂-III shares the same AFLOW label, A2B_mC12_12_2i_i, with α -Bi₂Pd and OsGe₂. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Ca I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Ca I

References

- [1] M. Knapp and U. Ruschewitz, *Structural Phase Transitions in CaC_2* , Chemistry, A European Journal **7**, 874–880 (2001), doi:10.1002/1521-3765(20010216)7:4<874::AID-CHEM874>E3.0.CO;2-V.

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