

CaC₂-I (*C*11_a) Structure: A2B_tI6_139_e_a-001

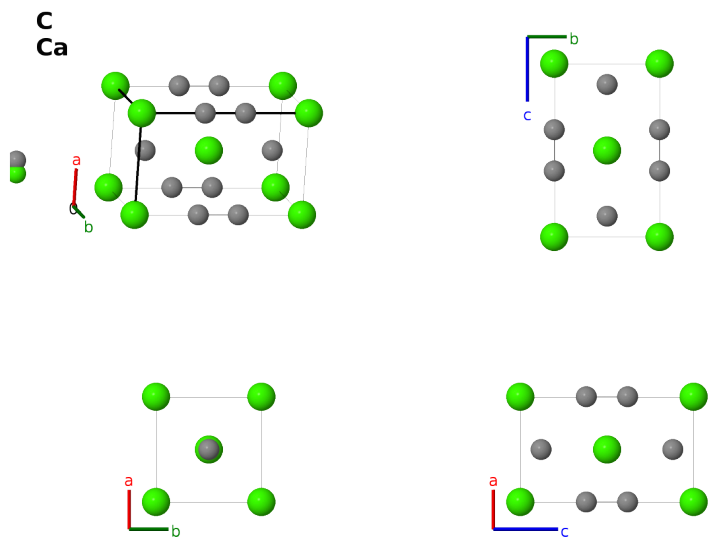
This structure previously used the label(s) **A2B_tI6_139_e_a**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B_tI6_139_e_a-001



Prototype	C ₂ Ca
AFLOW prototype label	A2B_tI6_139_e_a-001
<i>Strukturbericht</i> designation	<i>C</i> 11 _a
ICSD	56164
CCDC	1620435
Pearson symbol	tI6
Space group number	139
Space group symbol	<i>I</i> 4/ <i>mmm</i>
AFLOW prototype command	<code>aflow --proto=A2B_tI6_139_e_a-001 --params=a,c/a,z₂</code>

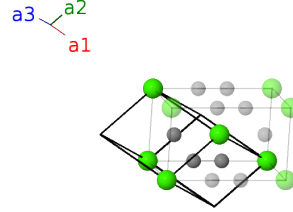
Other compounds with this structure

BaC₂, BaO₂, CeC₂, CsO₂, DyC₂, ErC₂, EuC₂, GdC₂, HoC₂, KO₂, LaC₂, LuC₂, NdC₂, PrC₂, PuC₂, RbO₂, SmC₂, SrC₂, SrO₂, TbC₂, TmC₂, UC₂, YC₂, YbC₂

- (Ewald, 1931) designated both CaC_2 and MoSi_2 as *Strukturbericht* C11. (Smithells, 1955) separated them into $C11_a$ (CaC_2) and $C11_b$ (MoSi_2 , AB2.tI6_139_a.e).
- This is the stable room-temperature structure for CaC_2 . At low temperatures it transforms into the ThC_2 (C_g) structure. There is also a meta-stable room temperature structure CaC_2 -III (A2B.mC12_12_2i.i).
- (v. Stackelberg, 1930) describes this structure in a face-centered-tetragonal setting. We follow (Smithells, 1955) and place it in the equivalent body-centered tetragonal setting. (Stackelberg, 1930) gives $a = 5.84\text{\AA}$ for the face-centered lattice. If we divide this by $\sqrt{2}$ we get $a = 3.87\text{\AA}$ for the body-centered lattice. The ICSD entry gives $a = 3.83$, which we attribute to an arithmetic error.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	$(2a)$ Ca I
$\mathbf{B}_2$	$=$	$z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$cz_2 \hat{\mathbf{z}}$	$(4e)$ C I
$\mathbf{B}_3$	$=$	$-z_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	$=$	$-cz_2 \hat{\mathbf{z}}$	$(4e)$ C I

References

- [1] M. von Stackelberg, *Die Krystallstruktur des CaC_2* , *Naturwissenschaften* **18**, 305–306 (1930), doi:10.1007/BF01.
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [3] C. J. Smithells, *Metals Reference Book* (Butterworths Scientific, London, 1955), second edn.

Found in

- [1] N.-G. Vannerberg, *The Crystal Structure of Calcium Carbide III*, *Acta Chem. Scand.* **15**, 769–774 (1961), doi:10.3891/acta.chem.scand.15-0769.

First cited in

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