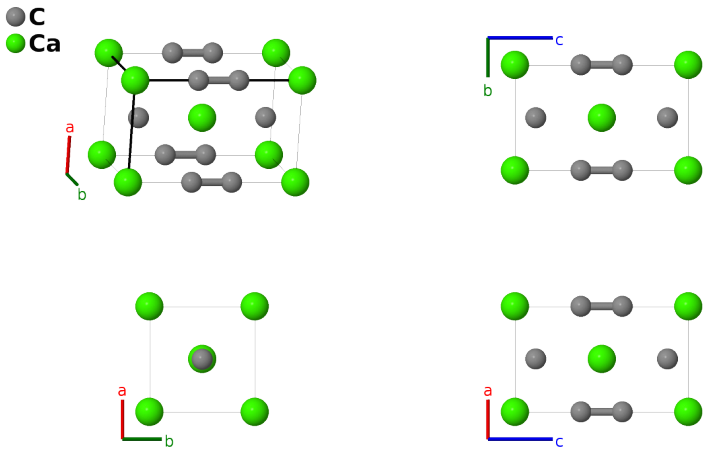
CaC_2-I ($C11_a$) Structure: A2B_tI6_139_e_a-001

This structure originally had the label `A2B_tI6_139_e_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/RDQF

https://aflow.org/p/A2B_tI6_139_e_a-001



Prototype	C_2Ca
AFLOW prototype label	A2B_tI6_139_e_a-001
***Strukturbericht* designation**	$C11_a$
ICSD	56164
Pearson symbol	tI6
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B_tI6_139_e_a-001 --params=`$a, c/a, z_2$

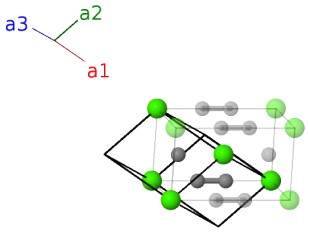
Other compounds with this structure

BaC_2, BaO_2, CeC_2, CsO_2, DyC_2, ErC_2, EuC_2, GdC_2, HoC_2, KO_2, LaC_2, LuC_2, NdC_2, PrC_2, PuC_2, RbO_2, SmC_2, SrC_2, SrO_2, TbC_2, TmC_2, UC_2, YC_2, YbC_2

- (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 $a = 5.84$Å for the face-centered lattice. If we divide this by $\sqrt{2}$ we get $a = 3.87$Å for the body-centered lattice. The ICSD entry gives $a = 3.83$, which we attribute to an arithmetic error.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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.