$CaSi_2$ ($C12$) Structure: AB2_hR6_166_c_2c-002

This structure originally had the label `AB2_hR6_166_c_2c`. Calls to that address will be redirected here.

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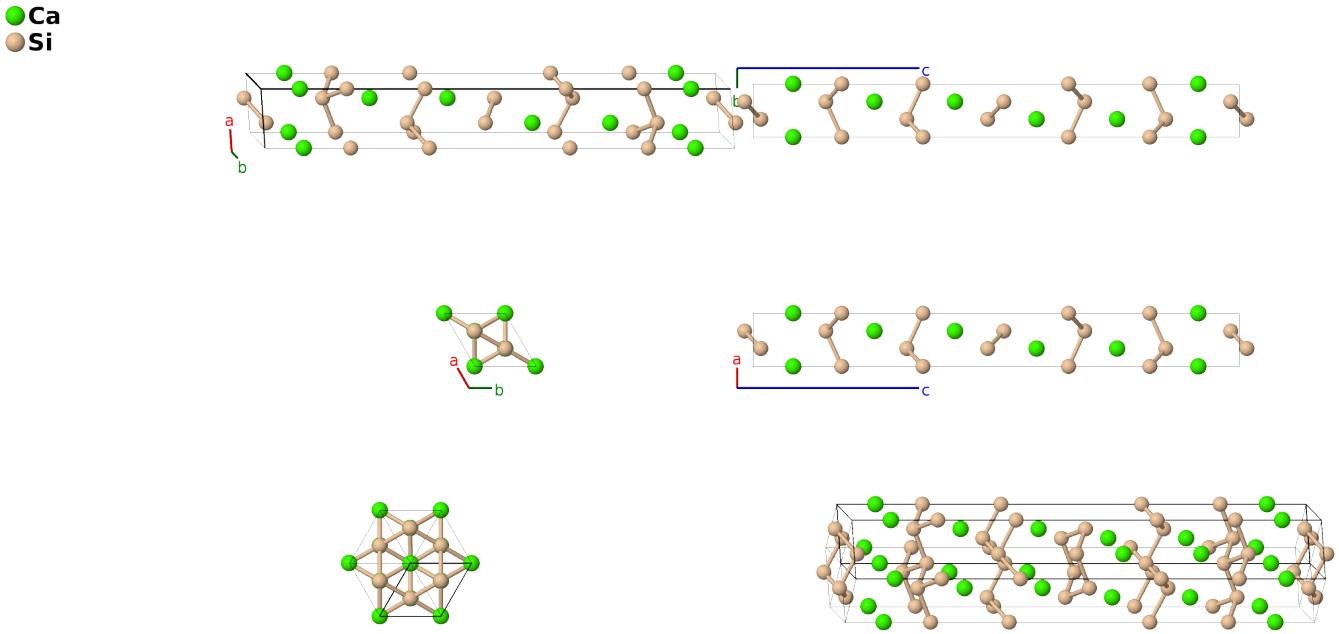
https://aflow.org/p/85MW

https://aflow.org/p/AB2_hR6_166_c_2c-002



Prototype	$CaSi_2$
AFLOW prototype label	AB2_hR6_166_c_2c-002
***Strukturbericht* designation**	$C12$
ICSD	32006
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB2_hR6_166_c_2c-002 --params=`$a, c/a, x_1, x_2, x_3$

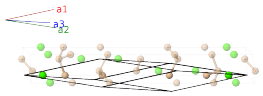
Other compounds with this structure
$CaGe_2$

- Although this has the same crystallographic structure as SmSI, the layering is substantially different.
- There is no ICSD or CCDC entry for (Castillo, 2016). We use the ICSD entry from (Evers, 1979).

- Hexagonal settings of this structure can be obtained with the option `-hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Si II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Si II

References

[1] S. M. Castillo, Z. Tang, A. P. Litvinchuk, and A. M. Guloy, *Lattice Dynamics of the Rhombohedral Polymorphs of $CaSi_2$*, Inorg. Chem. **55**, 10203–10207 (2016), doi:10.1021/acs.inorgchem.6b01399.

[2] J. Evers, *Transformation of Three-Centered Silicon Nets in $CaSi_2$*, J. Solid State Chem. **28**, 369–377 (1979), doi:10.1016/0022-4596(79)90087-2.