CaGaN Structure: ABC_tP6_129_c_c_c-001

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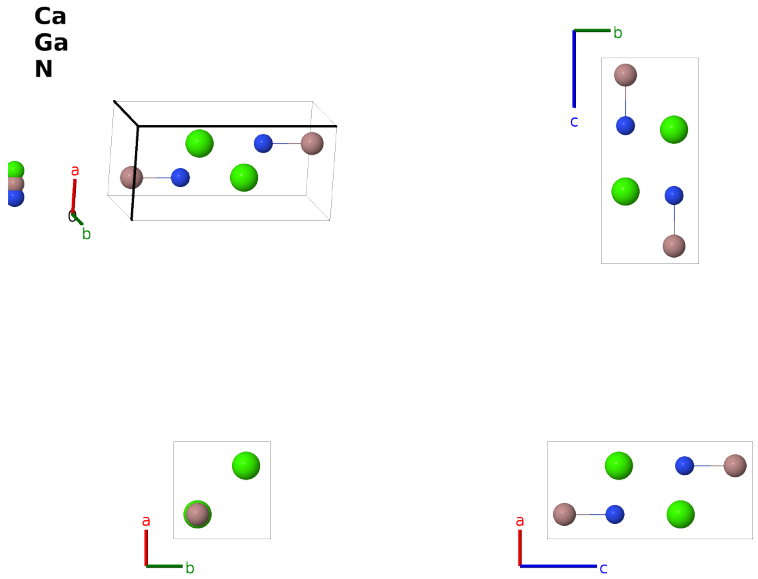
https://aflow.org/prototype-encyclopedia/QTMD

https://aflow.org/prototype-encyclopedia/ABC_tP6_129_c_c_c-001



Prototype	CaGaN
AFLOW prototype label	ABC_tP6_129_c_c_c-001
ICSD	2027
CCDC	1591978
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=ABC_tP6_129_c_c_c-001 --params=`$a, c/a, z_1, z_2, z_3$

Other compounds with this structure
EuSnP, SrSnP

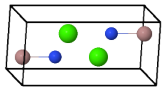
- There are two prototypes with the AFLOW label ABC_tP6_129_c_c_c:

  - CaGaN (this structure), with c/a $\approx$ 2.1, and
  - TaMoN, with c/a $\approx$ 2.5.

- (Verdier, 1974) give the atomic coordinates in setting 1 of space group $P4/nmm$ #129. We shifted the origin to place the system in our standard setting 2.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Ga I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	Ga I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	N I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	N I

References

[1] P. Verdier, P. L'Hardon, M. Maunaye, and R. Marchand, *Etude structurale de CaGaN*, Acta Crystallogr. Sect. B **30**, 226–228 (1974), doi:10.1107/S0567740874002500.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 2027 (CaGaN).

First cited in

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