Ca_3PI_3 Structure: A3B3C_cI56_214_g_h_a-001

This structure previously used the label(s) `A3B3C_cI56_214_g_h_a`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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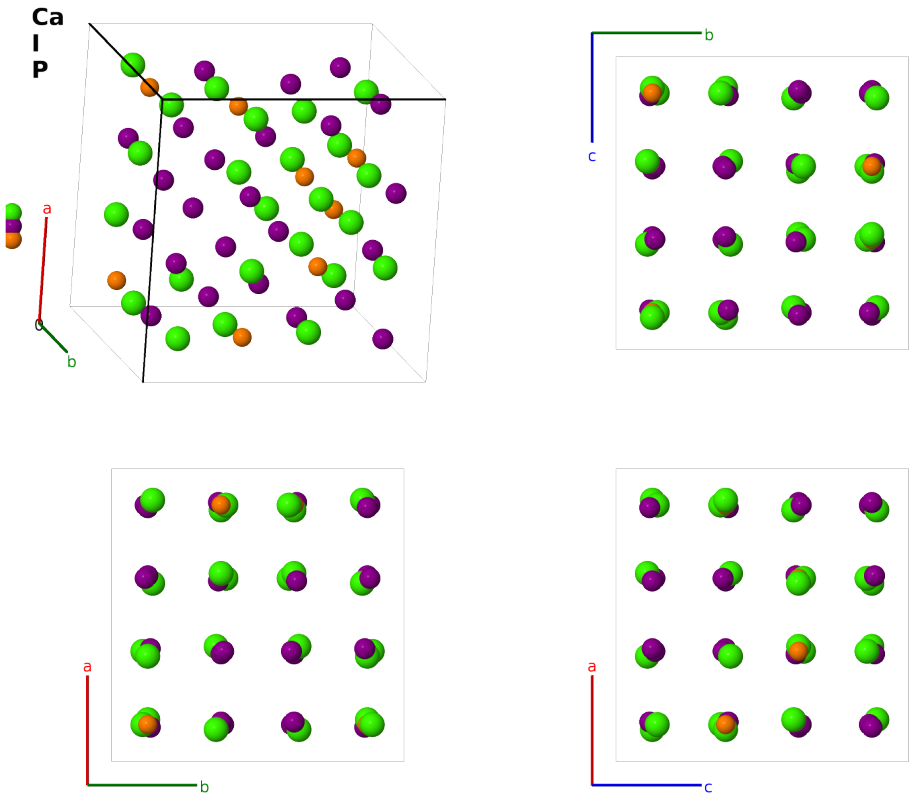
https://aflow.org/prototype-encyclopedia/4XVN

https://aflow.org/prototype-encyclopedia/A3B3C_cI56_214_g_h_a-001

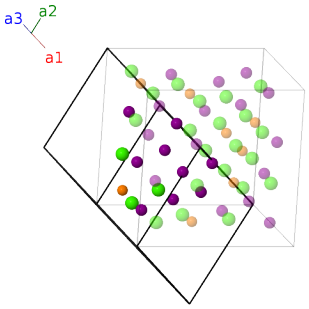


Prototype	Ca_3I_3P
AFLOW prototype label	A3B3C_cI56_214_g_h_a-001
ICSD	9026
CCDC	1594096
Pearson symbol	cI56
Space group number	214
Space group symbol	$I4_132$
AFLOW prototype command	`aflow --proto=A3B3C_cI56_214_g_h_a-001 --params=`a, y_2, y_3

Other compounds with this structure
Gd_3CCl_3

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_5}$	=	$\left(2y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_8}$	=	$-\left(2y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_9}$	=	$\left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_1 + \left(2y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{10}}$	=	$-\left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{11}}$	=	$\left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{8}a\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{12}}$	=	$-\left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_1 - \left(2y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{13}}$	=	$\left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(2y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{14}}$	=	$\left(y_2 + \frac{1}{8}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{15}}$	=	$-\left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{16}}$	=	$-\left(y_2 - \frac{3}{8}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(2y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{17}}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \frac{3}{8}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{8}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I
$\mathbf{B_{18}}$	=	$-\left(2y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{8}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I

$$\mathbf{B_{19}} = \left(2y_3+\tfrac{3}{4}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{8}\right)\mathbf{a}_2+\left(y_3+\tfrac{3}{8}\right)\mathbf{a}_3 = -\tfrac{1}{8}a\,\hat{\mathbf{x}}+a\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{20}} = \tfrac{1}{4}\mathbf{a}_1+\left(y_3+\tfrac{3}{8}\right)\mathbf{a}_2-\left(y_3-\tfrac{1}{8}\right)\mathbf{a}_3 = \tfrac{1}{8}a\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}+a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{21}} = \left(y_3+\tfrac{1}{8}\right)\mathbf{a}_1+\tfrac{1}{4}\mathbf{a}_2-\left(y_3-\tfrac{3}{8}\right)\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{8}a\,\hat{\mathbf{y}}+ay_3\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{22}} = -\left(y_3-\tfrac{3}{8}\right)\mathbf{a}_1-\left(2y_3-\tfrac{3}{4}\right)\mathbf{a}_2-\left(y_3-\tfrac{1}{8}\right)\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{8}a\,\hat{\mathbf{y}}-a\left(y_3-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{23}} = \left(y_3+\tfrac{3}{8}\right)\mathbf{a}_1+\left(2y_3+\tfrac{3}{4}\right)\mathbf{a}_2+\left(y_3+\tfrac{1}{8}\right)\mathbf{a}_3 = a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{8}a\,\hat{\mathbf{y}}+a\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{24}} = -\left(y_3-\tfrac{1}{8}\right)\mathbf{a}_1+\tfrac{1}{4}\mathbf{a}_2+\left(y_3+\tfrac{3}{8}\right)\mathbf{a}_3 = a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{8}a\,\hat{\mathbf{y}}-ay_3\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{25}} = -\left(y_3-\tfrac{3}{8}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{8}\right)\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3 = ay_3\,\hat{\mathbf{x}}-a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{y}}+\tfrac{1}{8}a\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{26}} = -\left(y_3-\tfrac{1}{8}\right)\mathbf{a}_1-\left(y_3-\tfrac{3}{8}\right)\mathbf{a}_2-\left(2y_3-\tfrac{3}{4}\right)\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{y}}-\tfrac{1}{8}a\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{27}} = \left(y_3+\tfrac{1}{8}\right)\mathbf{a}_1+\left(y_3+\tfrac{3}{8}\right)\mathbf{a}_2+\left(2y_3+\tfrac{3}{4}\right)\mathbf{a}_3 = a\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{y}}-\tfrac{1}{8}a\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

$$\mathbf{B_{28}} = \left(y_3+\tfrac{3}{8}\right)\mathbf{a}_1-\left(y_3-\tfrac{1}{8}\right)\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3 = -ay_3\,\hat{\mathbf{x}}+a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{y}}+\tfrac{1}{8}a\,\hat{\mathbf{z}} \quad \text{(24h)} \quad \text{I I}$$

References

[1] C. Hamon, R. Marchand, Y. Laurent, and J. Lang, *Étude d'halogénopnictures. III. Structure de Ca_2PI et Ca_3PI_3. Surstructures de type NaCl*, Bull. Soc. fr. Minéral. Cristallogr. **97**, 6–12 (1974), doi:10.3406/bulmi.1974.6909.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043