Ca_3PI_3 Structure: A3B3C_cI56_214_g_h_a-001

This structure originally had the label `A3B3C_cI56_214_g_h_a`. Calls to that address will be redirected here.

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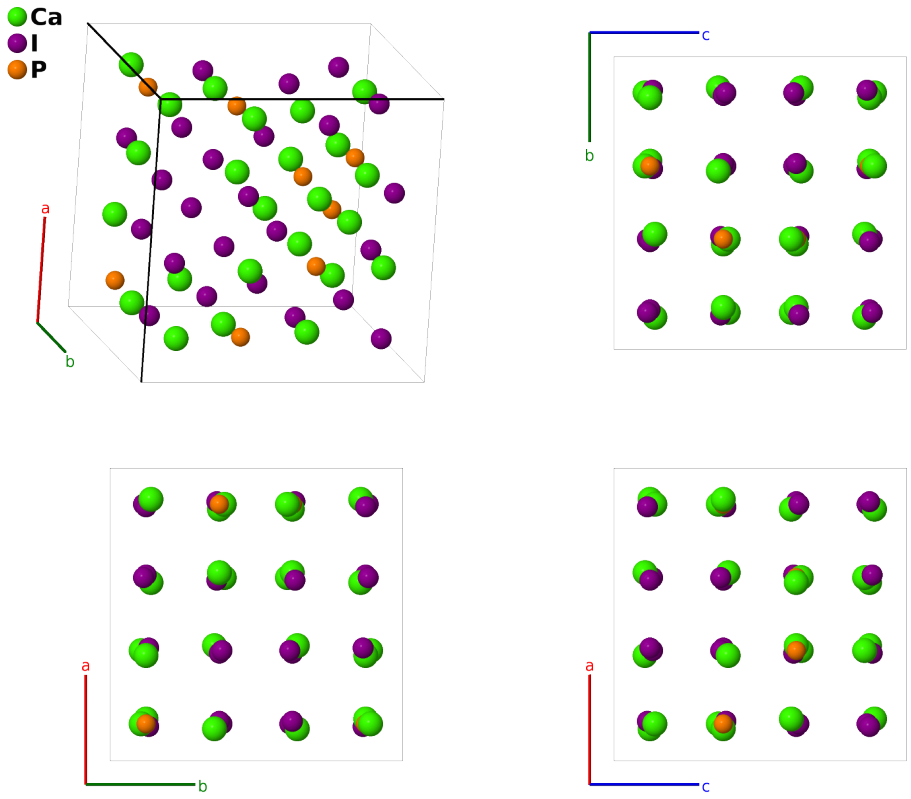
https://aflow.org/p/4XVN

https://aflow.org/p/A3B3C_cI56_214_g_h_a-001

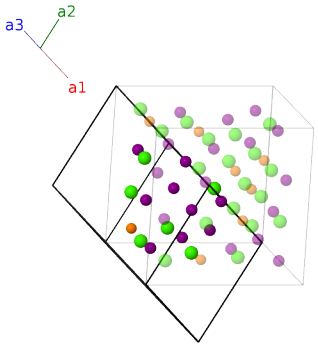


Prototype	Ca_3I_3P
AFLOW prototype label	A3B3C_cI56_214_g_h_a-001
ICSD	9026
Pearson symbol	cI56
Space group number	214
Space group symbol	$I4_132$
AFLOW prototype command	`aflow --proto=A3B3C_cI56_214_g_h_a-001 --params=`a, y_2, y_3

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
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_2}$	=	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_3$	=	$-\tfrac{1}{8}a\,\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_3}$	=	$\tfrac{1}{4}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{3}{8}a\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} - \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_4}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} - \tfrac{1}{8}a\,\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_5}$	=	$\left(2y_2 + \tfrac{1}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_2 + \left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_6}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_2 - \left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-\tfrac{1}{8}a\,\hat{\mathbf{x}} - a\left(y_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_7}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_2 + \left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-\tfrac{1}{8}a\,\hat{\mathbf{x}} + a\left(y_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_8}$	=	$-\left(2y_2 - \tfrac{1}{4}\right)\,\mathbf{a}_1 - \left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_2 - \left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_9}$	=	$\left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_1 + \left(2y_2 + \tfrac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{10}}$	=	$-\left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 + \left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - \tfrac{1}{8}a\,\hat{\mathbf{y}} - a\left(y_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{11}}$	=	$\left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - \left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} - \tfrac{1}{8}a\,\hat{\mathbf{y}} + a\left(y_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{12}}$	=	$-\left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_1 - \left(2y_2 - \tfrac{1}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{13}}$	=	$\left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_1 + \left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_2 + \left(2y_2 + \tfrac{1}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{14}}$	=	$\left(y_2 + \tfrac{1}{8}\right)\,\mathbf{a}_1 - \left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	=	$-a\left(y_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2 + \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{15}}$	=	$-\left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_1 + \left(y_2 + \tfrac{3}{8}\right)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	=	$a\left(y_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} - \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{16}}$	=	$-\left(y_2 - \tfrac{3}{8}\right)\,\mathbf{a}_1 - \left(y_2 - \tfrac{1}{8}\right)\,\mathbf{a}_2 - \left(2y_2 - \tfrac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - a\left(y_2 - \tfrac{1}{4}\right)\,\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}}$	(24g)	Ca I
$\mathbf{B_{17}}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \tfrac{3}{8}\right)\,\mathbf{a}_2 + \left(y_3 + \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I
$\mathbf{B_{18}}$	=	$-\left(2y_3 - \tfrac{3}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \tfrac{1}{8}\right)\,\mathbf{a}_2 - \left(y_3 - \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-\tfrac{1}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I
$\mathbf{B_{19}}$	=	$\left(2y_3 + \tfrac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \tfrac{1}{8}\right)\,\mathbf{a}_2 + \left(y_3 + \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-\tfrac{1}{8}a\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I
$\mathbf{B_{20}}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(y_3 + \tfrac{3}{8}\right)\,\mathbf{a}_2 - \left(y_3 - \tfrac{1}{8}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{8}a\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\,\hat{\mathbf{z}}$	(24h)	I I
$\mathbf{B_{21}}$	=	$\left(y_3 + \tfrac{1}{8}\right)\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 - \left(y_3 - \tfrac{3}{8}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \tfrac{1}{4}\right)\,\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	I I

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

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

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

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

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

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

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

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.

Found in

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