

CaCu₄P₂ Structure:

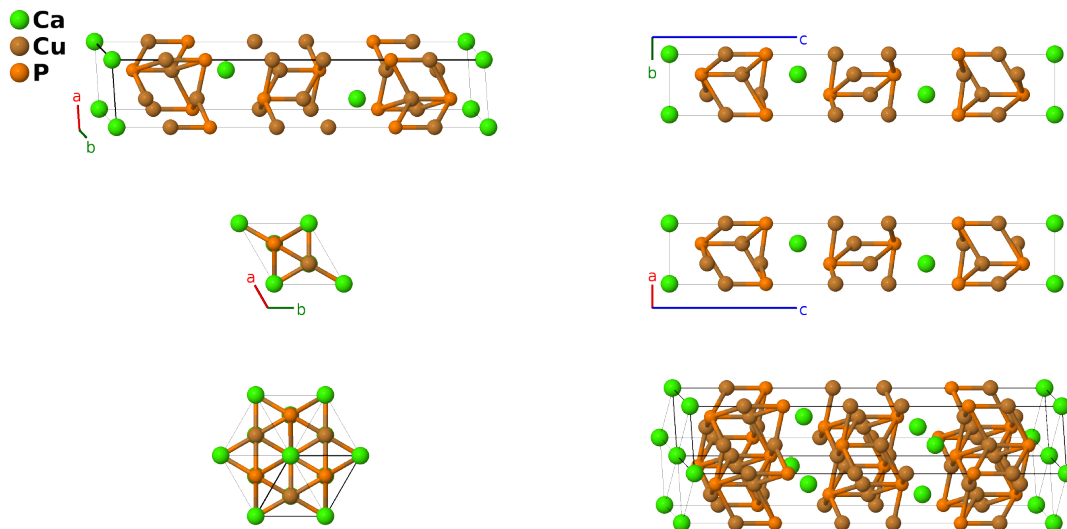
AB4C2_hR7_166_a_2c_c-001

This structure originally had the label AB4C2_hR7_166_a_2c_c. Calls to that address will be redirected here.

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<https://aflow.org/p/SFS1>

https://aflow.org/p/AB4C2_hR7_166_a_2c_c-001



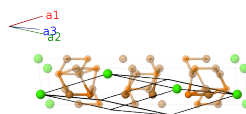
Prototype	CaCu ₄ P ₂
AFLOW prototype label	AB4C2_hR7_166_a_2c_c-001
ICSD	23251
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	aflow --proto=AB4C2_hR7_166_a_2c_c-001 --params=a, c/a, x ₂ , x ₃ , x ₄

Other compounds with this structure

BaAg₄As₂, CaAg₄As₂, EuAg₄As₂, EuAg₄Sb₂, SrAg₄As₂, SrAg₄Sb₂, ZrLi₄Ge₂

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(1a) Ca I
\mathbf{B}_2	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$cx_2 \hat{\mathbf{z}}$	(2c) Cu 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) Cu I
\mathbf{B}_4	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c) Cu II
\mathbf{B}_5	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c) Cu II
\mathbf{B}_6	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(2c) P I
\mathbf{B}_7	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-cx_4 \hat{\mathbf{z}}$	(2c) P I

References

- [1] A. Mewis, *Darstellung und Struktur der Verbindung CaCu_4P_2* , Z. Naturforsch. B **35**, 942–945 (1980), doi:10.1515/znb-1980-0802.