

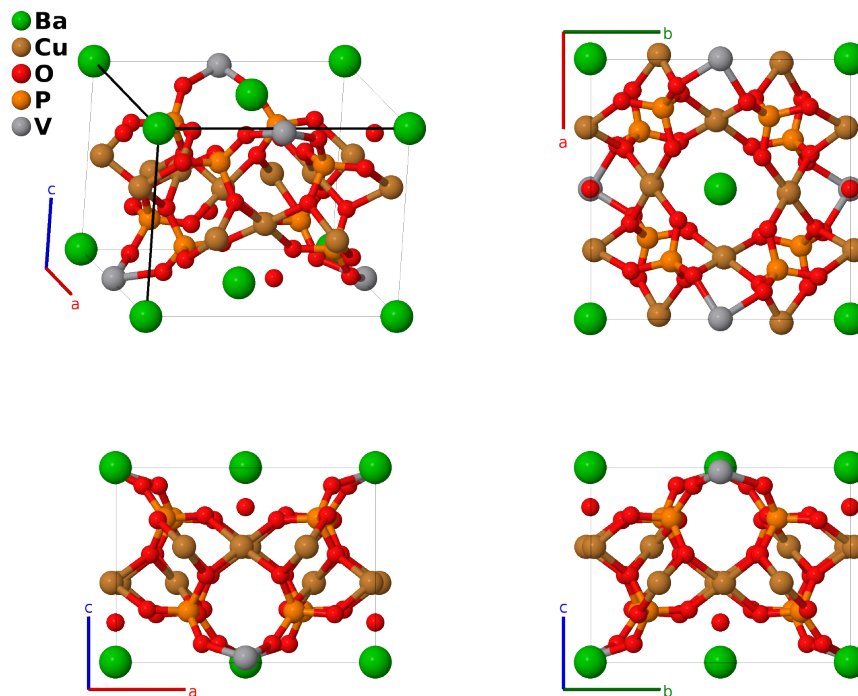
BaCu₄[VO][PO₄]₄ Structure: AB4C17D4E_tP54_90_a_g_c4g_g_c-001

This structure originally had the label AB4C17D4E_tP54_90_a_g_c4g_g_c. Calls to that address will be redirected here.

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<https://aflow.org/p/61ZR>

https://aflow.org/p/AB4C17D4E_tP54_90_a_g_c4g_g_c-001



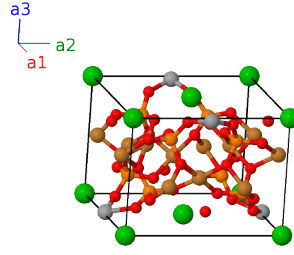
Prototype	BaCu ₄ O ₁₇ P ₄ V
AFLOW prototype label	AB4C17D4E_tP54_90_a_g_c4g_g_c-001
ICSD	406667
Pearson symbol	tP54
Space group number	90
Space group symbol	<i>P</i> 4 ₂ 1 ₂
AFLOW prototype command	<code>aflow --proto=AB4C17D4E_tP54_90_a_g_c4g_g_c-001 --params=a, c/a, z₂, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉</code>

Other compounds with this structure

BaCu₄[TiO][PO₄]₄

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Ba I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2a)	Ba I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	V I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(2c)	V I
\mathbf{B}_7	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_8	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_9	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{10}	$(y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{11}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{12}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{13}	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{14}	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	Cu I
\mathbf{B}_{15}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{16}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{17}	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{18}	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{19}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{20}	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{21}	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{22}	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{23}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{24}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{25}	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{26}	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O III

$$\begin{aligned}
\mathbf{B}_{27} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 = -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8g) & \text{O III} \\
\mathbf{B}_{28} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 = a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8g) & \text{O III} \\
\mathbf{B}_{29} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8g) & \text{O III} \\
\mathbf{B}_{30} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8g) & \text{O III} \\
\mathbf{B}_{31} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{32} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{33} &= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 = -a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{34} &= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 = a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{35} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 = -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{36} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 = a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{37} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{38} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = -ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8g) & \text{O IV} \\
\mathbf{B}_{39} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{40} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{41} &= -\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 = -a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{42} &= \left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 = a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{43} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{44} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{45} &= y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{46} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = -ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8g) & \text{O V} \\
\mathbf{B}_{47} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{48} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{49} &= -\left(y_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 = -a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{50} &= \left(y_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 = a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{51} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 = -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{52} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{53} &= y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B}_{54} &= -y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = -ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8g) & \text{P I}
\end{aligned}$$

References

- [1] S. Meyer and H. Müller-Buschbaum, *Cu₄O₁₂-Baugruppen aus planaren CuO₄-Polygonen im Barium-Vanadyl-Oxocuprat(II)-phosphat Ba(VO)Cu₄(PO₄)₄*, *Z. Anorganische und Allgemeine Chemie* **623**, 1693–1698 (1997), doi:10.1002/zaac.19976231103.

Found in

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