

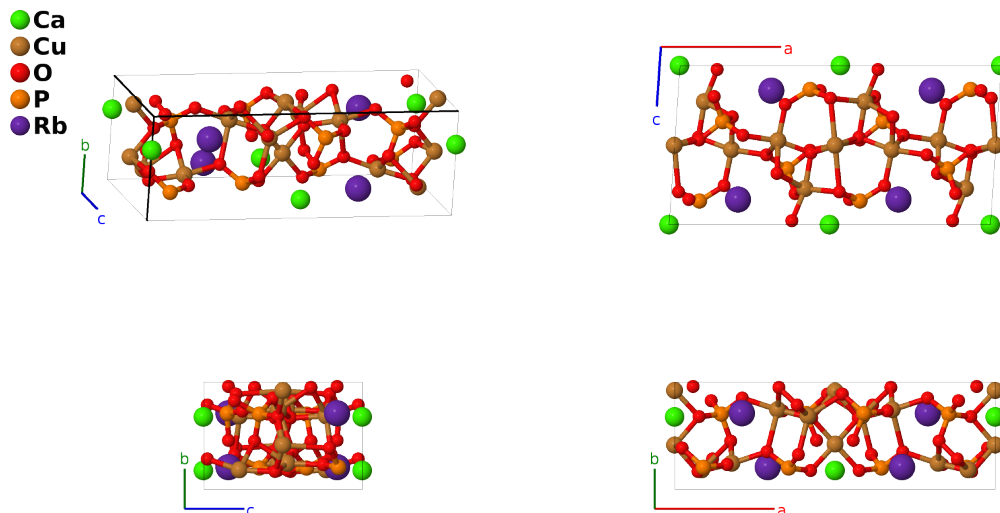
Rb₂CaCu₆(PO₄)₄O₂ Structure: AB6C18D4E2_mC62_5_b_2a2c_9c_2c_c-001

This structure originally had the label AB6C18D4E2_mC62_5_a_2b2c_9c_2c_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/74YK>

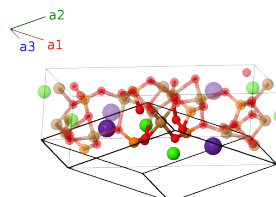
https://afLOW.org/p/AB6C18D4E2_mC62_5_b_2a2c_9c_2c_c-001



Prototype	CaCu ₆ O ₁₈ P ₄ Rb ₂
AFLOW prototype label	AB6C18D4E2_mC62_5_b_2a2c_9c_2c_c-001
ICSD	403504
Pearson symbol	mC62
Space group number	5
Space group symbol	C2
AFLOW prototype command	afLOW --proto=AB6C18D4E2_mC62_5_b_2a2c_9c_2c_c-001 --params=a, b/a, c/a, β, y ₁ , y ₂ , y ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁ , x ₁₂ , y ₁₂ , z ₁₂ , x ₁₃ , y ₁₃ , z ₁₃ , x ₁₄ , y ₁₄ , z ₁₄ , x ₁₅ , y ₁₅ , z ₁₅ , x ₁₆ , y ₁₆ , z ₁₆ , x ₁₇ , y ₁₇ , z ₁₇

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(2a)	Cu I
\mathbf{B}_2	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(2a)	Cu II
\mathbf{B}_3	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2b)	Ca I
\mathbf{B}_4	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Cu III
\mathbf{B}_5	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	Cu III
\mathbf{B}_6	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Cu IV
\mathbf{B}_7	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	Cu IV
\mathbf{B}_8	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_9	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{10}	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{11}	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{12}	$= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{13}	$= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	O III
\mathbf{B}_{14}	$= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{15}	$= -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	O IV
\mathbf{B}_{16}	$= (x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{17}	$= -(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	O V
\mathbf{B}_{18}	$= (x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{19}	$= -(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
\mathbf{B}_{20}	$= (x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
\mathbf{B}_{21}	$= -(x_{12} + y_{12}) \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
\mathbf{B}_{22}	$= (x_{13} - y_{13}) \mathbf{a}_1 + (x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII
\mathbf{B}_{23}	$= -(x_{13} + y_{13}) \mathbf{a}_1 - (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII

$$\begin{aligned}
\mathbf{B}_{24} &= \begin{pmatrix} (x_{14} - y_{14}) \mathbf{a}_1 + \\ (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3 \end{pmatrix} = (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} & (4c) & \text{O IX} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(x_{14} + y_{14}) \mathbf{a}_1 - \\ (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - \\ cz_{14} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4c) & \text{O IX} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_{15} - y_{15}) \mathbf{a}_1 + \\ (x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 \end{pmatrix} = (ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}} & (4c) & \text{P I} \\
\mathbf{B}_{27} &= \begin{pmatrix} -(x_{15} + y_{15}) \mathbf{a}_1 - \\ (x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - \\ cz_{15} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4c) & \text{P I} \\
\mathbf{B}_{28} &= \begin{pmatrix} (x_{16} - y_{16}) \mathbf{a}_1 + \\ (x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3 \end{pmatrix} = (ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}} & (4c) & \text{P II} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(x_{16} + y_{16}) \mathbf{a}_1 - \\ (x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - \\ cz_{16} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4c) & \text{P II} \\
\mathbf{B}_{30} &= \begin{pmatrix} (x_{17} - y_{17}) \mathbf{a}_1 + \\ (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 \end{pmatrix} = (ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} & (4c) & \text{Rb I} \\
\mathbf{B}_{31} &= \begin{pmatrix} -(x_{17} + y_{17}) \mathbf{a}_1 - \\ (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - \\ cz_{17} \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4c) & \text{Rb I}
\end{aligned}$$

References

- [1] S. M. Aksenov, E. Y. Borovikova, V. S. Mironov, N. A. Yamnova, A. S. Volkov, D. A. Ksenofontov, O. A. Gurbanova, O. V. Dimitrova, D. V. Deyneko, E. A. Zvereva, O. V. Maximova, S. V. Krivovichev, P. C. Burns, and A. N. Vasiliev, *Rb₂CaCu₆(PO₄)₄O₂, a novel oxophosphate with a shchurovskiyite-type topology: synthesis, structure, magnetic properties and crystal chemistry of rubidium copper phosphates*, Acta Crystallogr. Sect. B **75**, 903–913 (2019), doi:10.1107/S2052520619008527.