

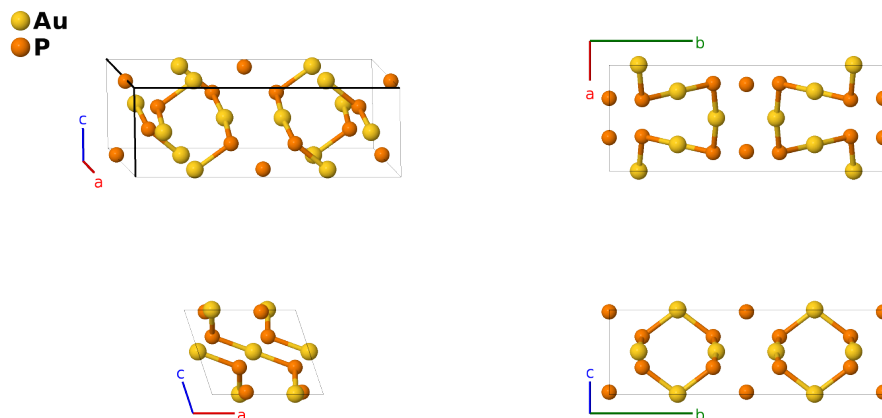
Au₂P₃ Structure:

A2B3_mC20_12_eh_ij-001

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

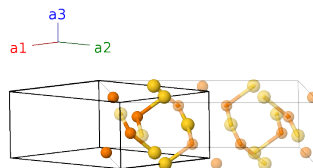
https://aflow.org/p/A2B3_mC20_12_eh_ij-001



Prototype	Au ₂ P ₃
AFLOW prototype label	A2B3_mC20_12_eh_ij-001
ICSD	8058
Pearson symbol	mC20
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A2B3_mC20_12_eh_ij-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>y</i> ₂ , <i>x</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}b\hat{y}$	(4e) Au I
\mathbf{B}_2	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{x} - \frac{1}{4}b\hat{y}$	(4e) Au I

$$\begin{aligned}
\mathbf{B}_3 &= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}} &(4h) & \text{Au II} \\
\mathbf{B}_4 &= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= \frac{1}{2} c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}} &(4h) & \text{Au II} \\
\mathbf{B}_5 &= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3 &= (ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}} &(4i) & \text{P I} \\
\mathbf{B}_6 &= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}} &(4i) & \text{P I} \\
\mathbf{B}_7 &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= (ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}} &(8j) & \text{P II} \\
\mathbf{B}_8 &= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}} &(8j) & \text{P II} \\
\mathbf{B}_9 &= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}} &(8j) & \text{P II} \\
\mathbf{B}_{10} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= (ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}} &(8j) & \text{P II}
\end{aligned}$$

References

- [1] W. Jeitschko and M. H. Möller, *The crystal structures of Au₂P₃ and Au₇P₁₀I, polyphosphides with weak Au-Au interactions*, Acta Crystallogr. Sect. B **35**, 573–579 (1979), doi:10.1107/S0567740879004180.