

Au₂P₃ Structure:

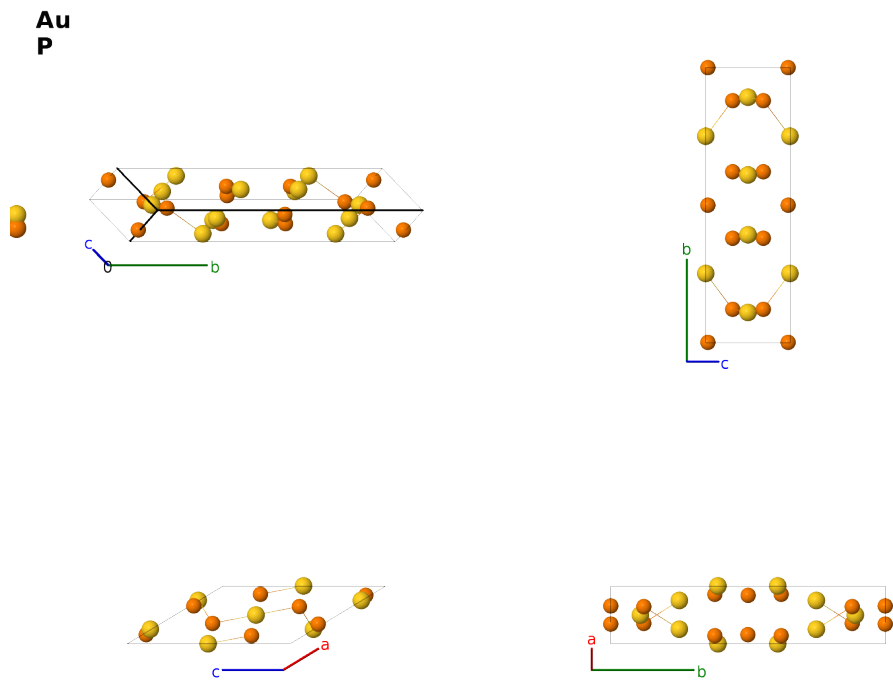
A2B3_mC20_12_eh_ij-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/PQQZ>

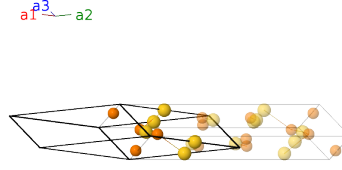
https://aflow.org/prototype-encyclopedia/A2B3_mC20_12_eh_ij-001



Prototype	Au ₂ P ₃
AFLOW prototype label	A2B3_mC20_12_eh_ij-001
ICSD	8058
CCDC	1593860
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A2B3_mC20_12_eh_ij-001</code> <code>--params=a, b/a, c/a, β, y_2, x_3, z_3, x_4, y_4, z_4</code>

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
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Au I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Au I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	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)	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)	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)	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)	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)	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)	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)	P II

References

- [1] W. Jeitschko and M. H. Möller, *The crystal structures of Au_2P_3 and $Au_7P_{10}I$, polyphosphides with weak Au-Au interactions*, Acta Crystallogr. Sect. B **35**, 573–579 (1979), doi:10.1107/S0567740879004180.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.