

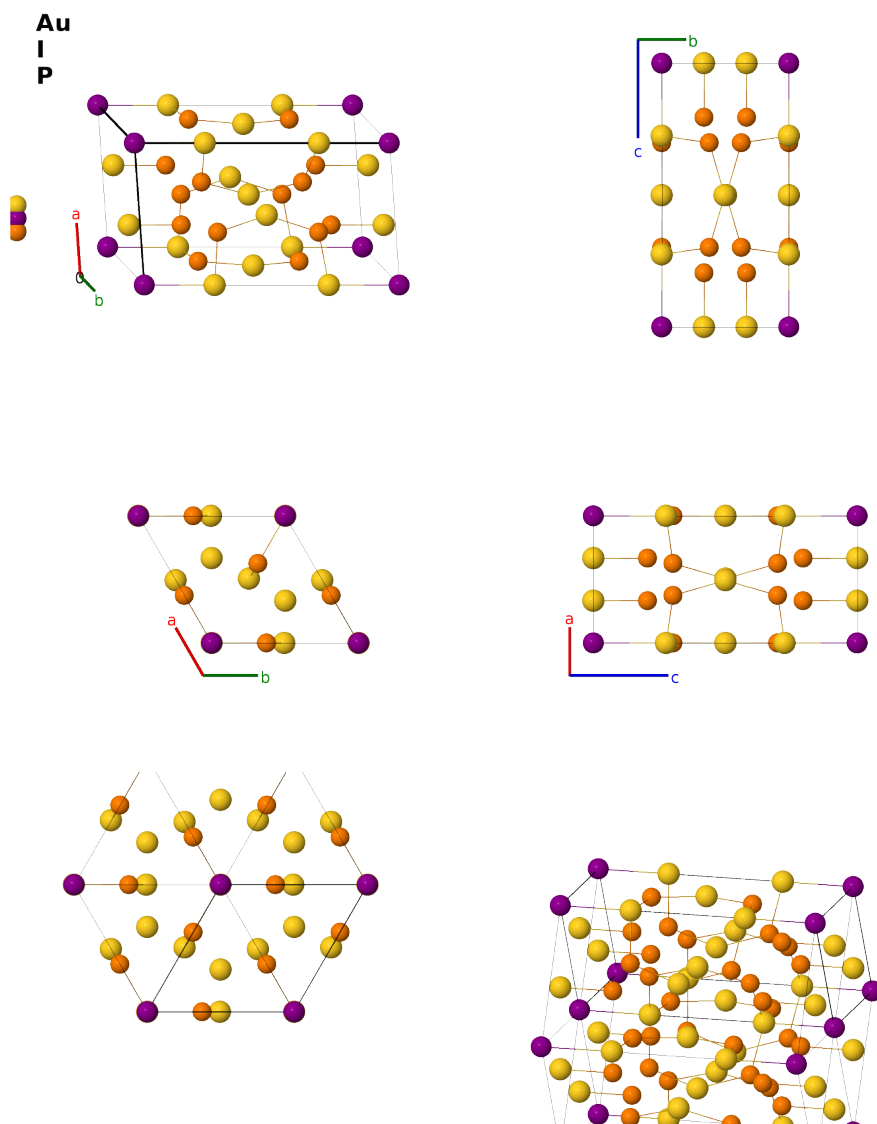
Hexagonal $\text{Au}_7\text{P}_{10}\text{I}$ Structure: A7BC10_hP18_189_ceg_a_hi-001

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<https://aflow.org/prototype-encyclopedia/16HD>

https://aflow.org/prototype-encyclopedia/A7BC10_hP18_189_ceg_a_hi-001



Prototype

$\text{Au}_7\text{IP}_{10}$

AFLOW prototype label

A7BC10_hP18_189_ceg_a_hi-001

ICSD

12162

CCDC

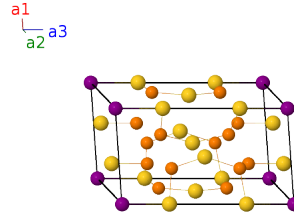
1595406

Pearson symbol	hP18
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	aflow --proto=A7BC10_hP18_189_ceg_a_hi-001 --params= $a, c/a, z_3, x_4, z_5, x_6, z_6$

- There is some controversy about the structure of $\text{Au}_7\text{P}_{10}\text{I}$. (Binnewies, 1978) put it in the hexagonal $P\bar{6}2m$ #189 space group, but (Jeitschko, 1979) place it in the trigonal $P\bar{3}1m$ #162 space group. The structures are distinct, and to our knowledge the dispute has not been resolved, so we present both structures.
- We have shifted the origin, moving the iodine atoms from the (1b) to (1a) Wyckoff positions.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	I I
$\mathbf{B}_2$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Au I
$\mathbf{B}_3$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Au I
$\mathbf{B}_4$	$z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(2e)	Au II
$\mathbf{B}_5$	$-z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(2e)	Au II
$\mathbf{B}_6$	$x_4 \mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Au III
$\mathbf{B}_7$	$x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Au III
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3g)	Au III
$\mathbf{B}_9$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4h)	P I
$\mathbf{B}_{10}$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4h)	P I
$\mathbf{B}_{11}$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4h)	P I
$\mathbf{B}_{12}$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4h)	P I
$\mathbf{B}_{13}$	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6i)	P II
$\mathbf{B}_{14}$	$x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6i)	P II
$\mathbf{B}_{15}$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(6i)	P II
$\mathbf{B}_{16}$	$x_6 \mathbf{a}_1 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6i)	P II
$\mathbf{B}_{17}$	$x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6i)	P II

$$\mathbf{B}_{18} = -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}} \quad (6i) \quad \text{P II}$$

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- [1] M. Binnewies, *Darstellung, Kristallstruktur und Eigenschaften von $Au_7P_{10}I$* , Z. Naturforsch. B **33**, 570–571 (1978), doi:10.1515/znb-1978-0521.

Found in

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