Trigonal $Au_7P_{10}I$ Structure: A7BC10_hP18_162_ceg_a_hk-001

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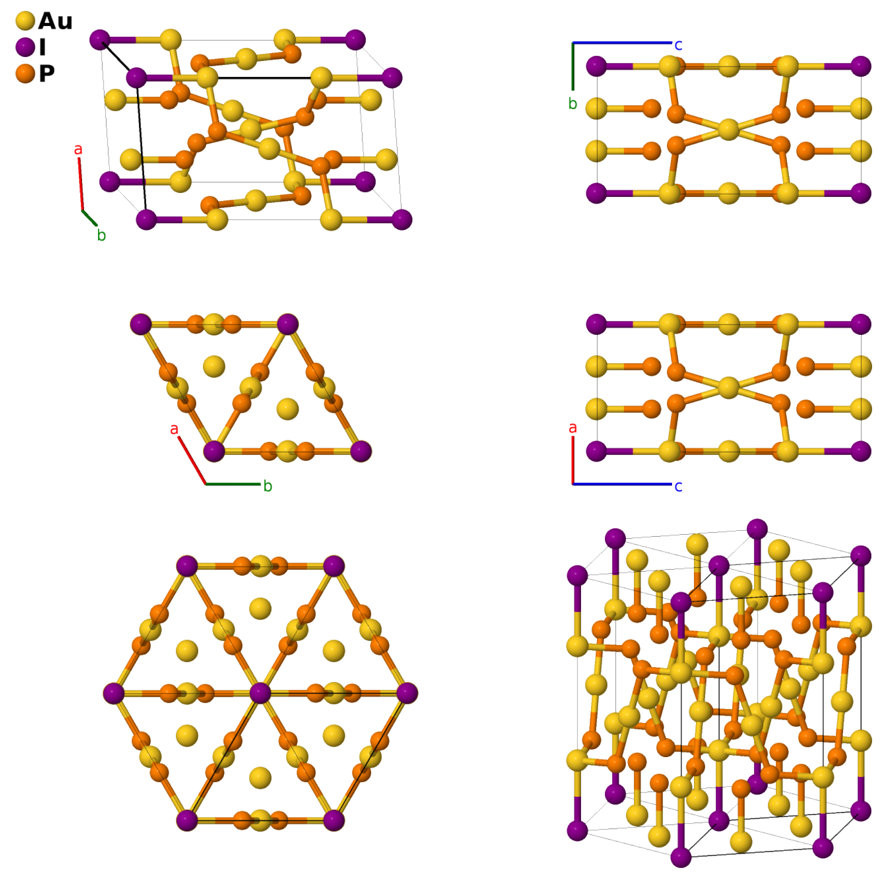
https://aflow.org/p/RQ68

https://aflow.org/p/A7BC10_hP18_162_ceg_a_hk-001



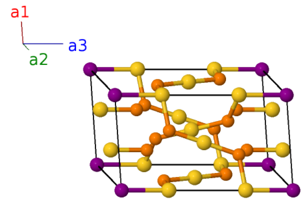
Prototype	Au_7IP_{10}
AFLOW prototype label	A7BC10_hP18_162_ceg_a_hk-001
ICSD	8059
Pearson symbol	hP18
Space group number	162
Space group symbol	$P\bar{3}1m$
AFLOW prototype command	`aflow --proto=A7BC10_hP18_162_ceg_a_hk-001` `--params=`$a, c/a, z_3, z_5, x_6, z_6$

- There is some controversy about the structure of $Au_7P_{10}I$. (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.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Au III
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Au III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6k)	P II
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6k)	P II
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(6k)	P II
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6k)	P II
$\mathbf{B_{17}}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6k)	P II
$\mathbf{B_{18}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(6k)	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.

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