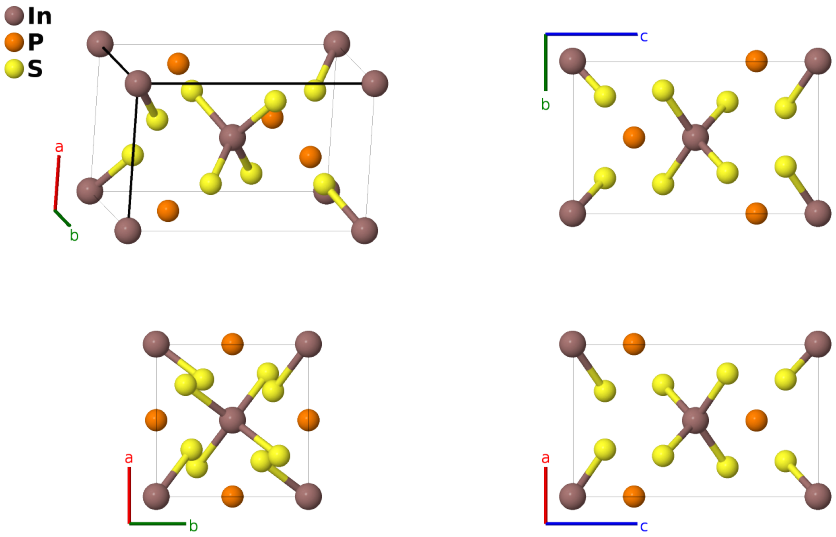
$InPS_4$ Structure: ABC4_tI12_82_a_c_g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/SUXC

https://aflow.org/p/ABC4_tI12_82_a_c_g-001



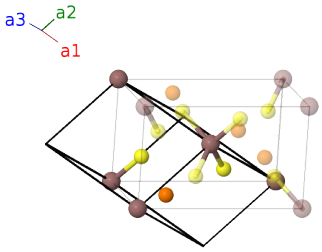
Prototype	$InPS_4$
AFLOW prototype label	ABC4_tI12_82_a_c_g-001
ICSD	23612
Pearson symbol	tI12
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=ABC4_tI12_82_a_c_g-001 --params=`$a, c/a, x_3, y_3, z_3$

Other compounds with this structure
$AlPO_4$

- Some references give $AlPO_4$ as the prototype for this structure, however this is not related to any $AlPO_4$ phase we have found in the literature, so we use $InPS_4$ as the prototype.
- The ICSD entry references another article on the same page, but gives the correct structural information.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	In I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_3}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_4}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_5}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_6}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8g)	S I

References

[1] C. D. Carpentier, R. Diehl, and R. Nitsche, *Die Kristallstruktur des InPS*, Naturwissenschaften **57**, 393 (1970), doi:10.1007/BF00599980.

Found in

[1] R. Diehl and C.-D. Carpentier, *The crystal structure of chromium thiophosphate, $CrPS_4$*, Acta Crystallogr. Sect. B **33**, 1399–1404 (1977), doi:10.1107/S0567740877006165.