

InPS₄ Structure:

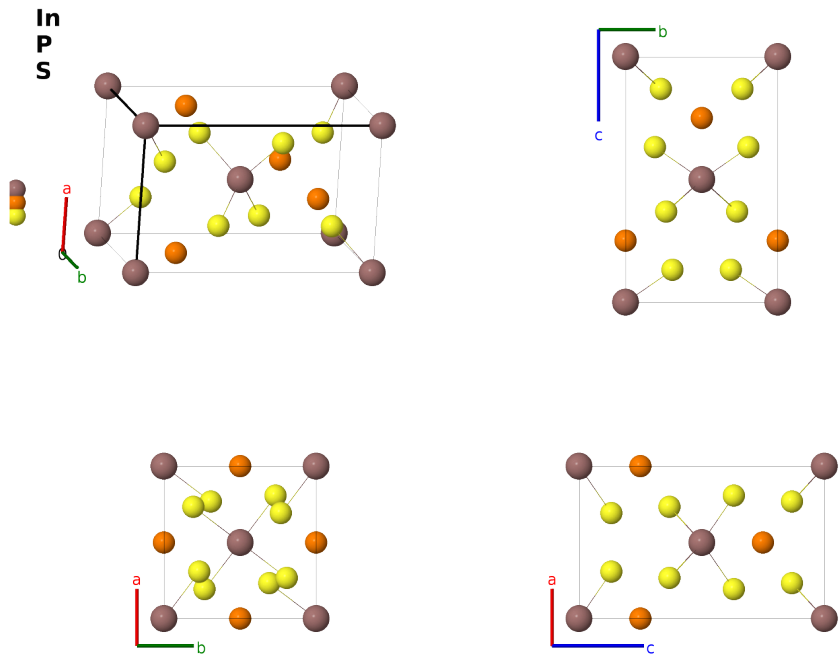
ABC4_tI12_82_a_c_g-001

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

https://aflow.org/prototype-encyclopedia/ABC4_tI12_82_a_c_g-001



Prototype	InPS ₄
AFLOW prototype label	ABC4_tI12_82_a_c_g-001
ICSD	23612
CCDC	1599712
Pearson symbol	tI12
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	<code>aflow --proto=ABC4_tI12_82_a_c_g-001</code> <code>--params=a, c/a, x₃, y₃, z₃</code>

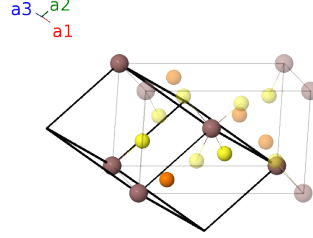
Other compounds with this structure

AlPO₄

- 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

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



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, CrPS₄*, *Acta Crystallogr. Sect. B* **33**, 1399–1404 (1977), doi:10.1107/S0567740877006165.

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