

H₃P Structure:

A3B_cP16_208_i_c-001

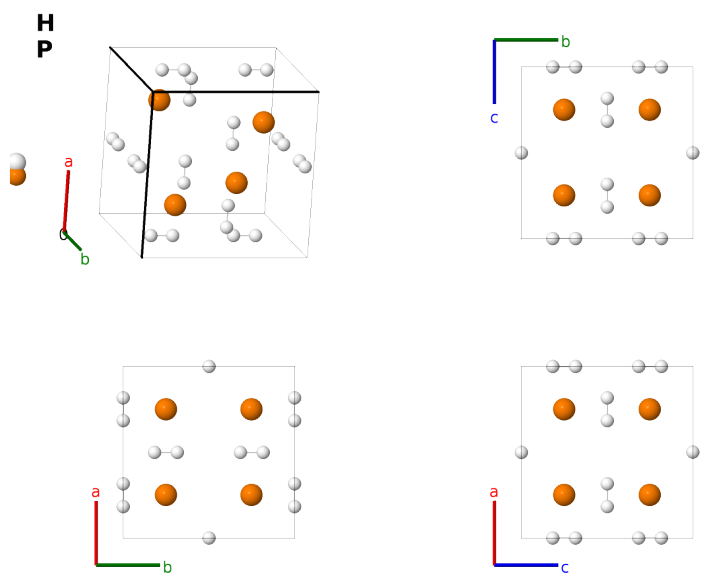
This structure previously used the label(s) **A3B_cP16_208_j_b**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A3B_cP16_208_i_c-001



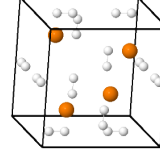
Prototype	H ₃ P
AFLOW prototype label	A3B_cP16_208_i_c-001
ICSD	24498
CCDC	1600524
Pearson symbol	cP16
Space group number	208
Space group symbol	$P4_232$
AFLOW prototype command	<code>aflow --proto=A3B_cP16_208_i_c-001</code> <code>--params=a, x_2</code>

Other compounds with this structure

H₃As

Simple Cubic primitive vectors

a1
a2
a3



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(12i)	H I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(12i)	H I
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(12i)	H I
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(12i)	H I
$\mathbf{B}_{13}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_{14}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_{15}$	$= \frac{1}{2} \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	H I
$\mathbf{B}_{16}$	$= \frac{1}{2} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12i)	H I

References

- [1] G. Natta and E. Casazza, *La struttura dell'idrogeno fosforato ($P H_3$) e dell'idrogeno arsenicale ($As H_3$)*, Gazzetta Chimica Italiana **60**, 851–859 (1930).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043