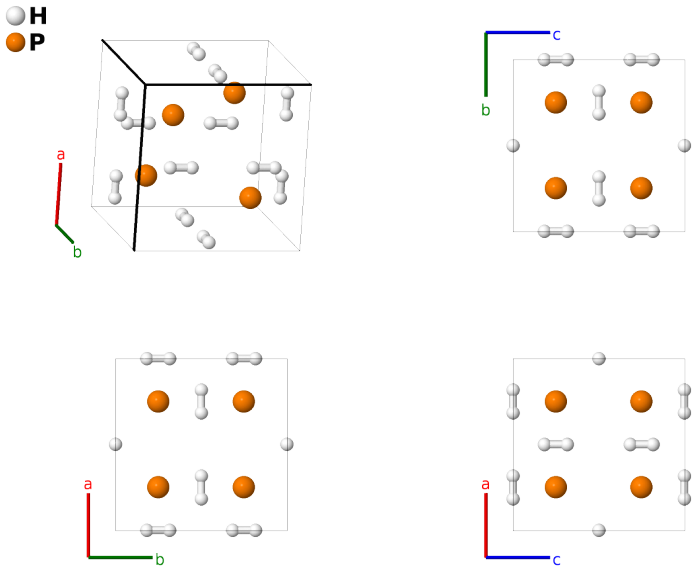
# $H_3P$ Structure: A3B_cP16_208_i_c-001

This structure originally had the label `A3B_cP16_208_j_b`. Calls to that address will be redirected here.

Cite this page as: 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

https://aflow.org/p/CCPW

https://aflow.org/p/A3B_cP16_208_i_c-001



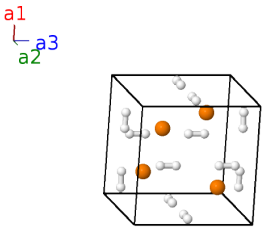

| | |
|---|---|
| **Prototype** | $H_3P$ |
| **AFLOW prototype label** | A3B_cP16_208_i_c-001 |
| **ICSD** | 24498 |
| **Pearson symbol** | cP16 |
| **Space group number** | 208 |
| **Space group symbol** | $P4_232$ |
| **AFLOW prototype command** | `aflow --proto=A3B_cP16_208_i_c-001 --params=`$a, x_2$ |

**Other compounds with this structure**

$H_3As$

**Simple Cubic primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$

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**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 |
| $\mathbf{B_{11}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$ | (12i) | H I |
| $\mathbf{B_{12}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$ | (12i) | H I |
| $\mathbf{B_{13}}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (12i) | H I |
| $\mathbf{B_{14}}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (12i) | H I |
| $\mathbf{B_{15}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12i) | H I |
| $\mathbf{B_{16}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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).