

Dodecatungstophosphoric Acid Hexahydrate ($\text{H}_3\text{PW}_{12}\text{O}_{40}\cdot 6\text{H}_2\text{O}$) Structure:

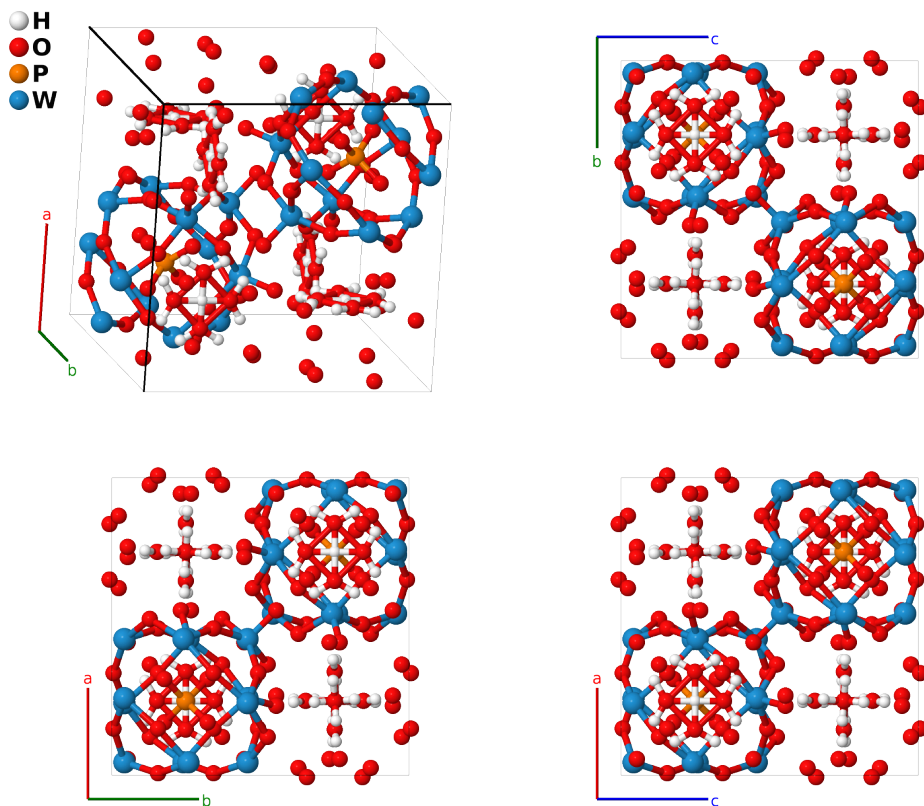
A27B52CD12_cP184_224_dl_eh3k_a_k-001

This structure originally had the label A27B52CD12_cP184_224_dl_eh3k_a.k. Calls to that address will be redirected here.

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<https://aflow.org/p/XBJQ>

https://aflow.org/p/A27B52CD12_cP184_224_dl_eh3k_a_k-001

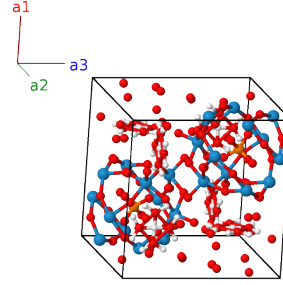


Prototype	$\text{H}_{15}\text{O}_{46}\text{PW}_{12}$
AFLOW prototype label	A27B52CD12_cP184_224_dl_eh3k_a_k-001
Mineral name	dodecatungstophosphoric acid hexahydrate
ICSD	904
Pearson symbol	cP184
Space group number	224
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	<pre>aflow --proto=A27B52CD12_cP184_224_dl_eh3k_a_k-001 --params=a, x3, x4, x5, z5, x6, z6, x7, z7, x8, z8, x9, y9, z9</pre>

- (Brown, 1977) presents this as an improvement on the $H4_{16}$ structure, $H_3PW_{12}O_{40} \cdot 5H_2O$. The primary difference is the addition of a sixth water molecule and the location of the hydrogen molecules not directly attached to a water molecule.
- The water molecules are formed by the H-II and O-II atoms, and the (24h) (O-II) and (48k) (H-II) Wyckoff sites are only occupied half of the time. Presumably this means that the nearly flat H-O molecular ions in this structure actually consist of one water molecule, the central hydrogen atom (H-I), and a water molecule on the other side of the central hydrogen, with the other water positions empty. Exactly which water molecules are occupied on around each H-I atom is completely up to chance. (Brown, 1977) state that the molecule has a positive charge, and write it as $H_5O_2^+$.
- We use the neutron data from (Brown, 1977) to locate the non-hydrogen atoms.
- This structure is a partially dehydrated form of $H_3PW_{12}O_{40} \cdot 29H_2O$ ($H4_{21}$). Further dehydration produces the $H_3PW_{12}O_{40} \cdot 3H_2O$ structure.

Simple Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(2a)	P I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(2a)	P I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_5	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_6	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_7	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_8	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{11}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{12}	$= x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{13}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{14}	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{15}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{16}	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I

$$\mathbf{B}_{182} = \begin{matrix} -(z_9 - \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \\ (x_9 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(z_9 - \frac{1}{2}) \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{z}} \quad (481) \quad \text{H II}$$

$$\mathbf{B}_{183} = z_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - (x_9 - \frac{1}{2}) \mathbf{a}_3 = az_9 \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{z}} \quad (481) \quad \text{H II}$$

$$\mathbf{B}_{184} = z_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + x_9 \mathbf{a}_3 = az_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} \quad (481) \quad \text{H II}$$

References

- [1] G. M. Brown, M.-R. Noe-Spirlet, W. R. Busing, and H. A. Levy, *Dodecatungstophosphoric acid hexahydrate, $(H_5O_2^+)_3(PW_{12}O_{40}^{3-})$. The true structure of Keggin's 'pentahydrate' from single-crystal X-ray and neutron diffraction data*, Acta Crystallogr. Sect. B **33**, 1038–1046 (1977), doi:10.1107/S0567740877005330.