

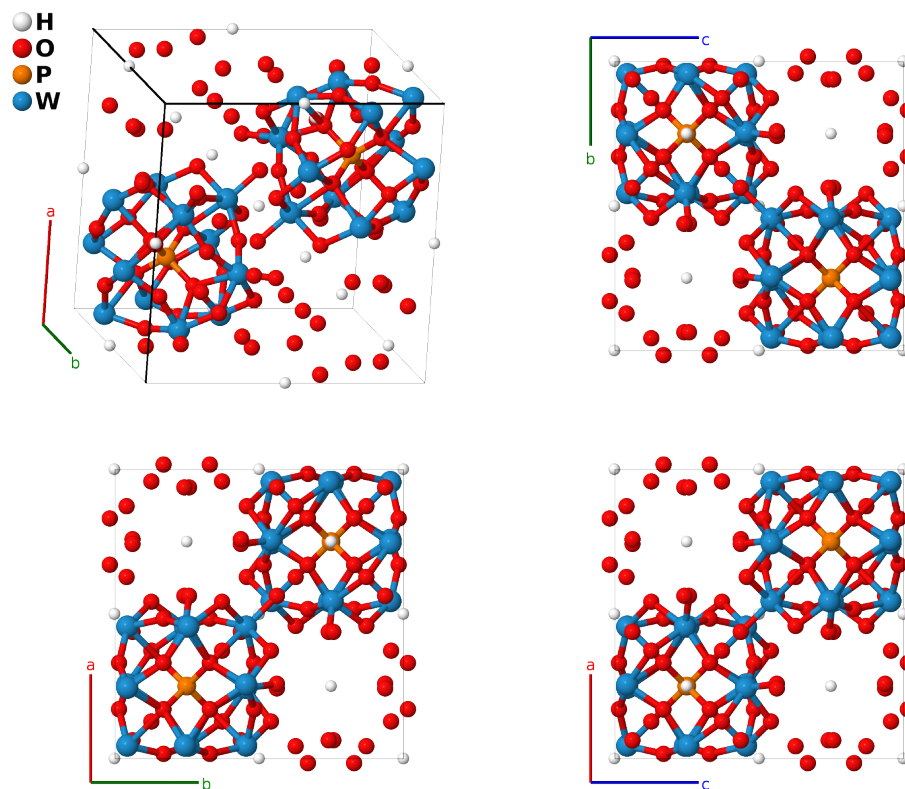
12-phosphotungstic acid $[H_3PW_{12}O_{40} \cdot 5H_2O]$ ($H4_{16}$) Structure: A5B40CD12_cP116_224_bd_e3k_a_k-001

This structure originally had the label A5B40CD12_cP116_224_cd_e3k_a_k. Calls to that address will be redirected here.

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<https://aflow.org/p/E8XB>

https://aflow.org/p/A5B40CD12_cP116_224_bd_e3k_a_k-001

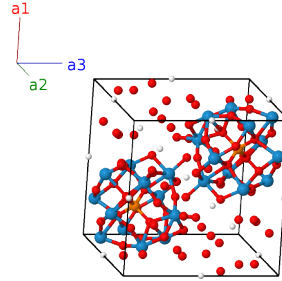


Prototype	$(H_2O)_5O_{40}PW_{12}$
AFLOW prototype label	A5B40CD12_cP116_224_bd_e3k_a_k-001
<i>Strukturbericht</i> designation	$H4_{16}$
Mineral name	12-phosphotungstic acid
ICSD	31897
Pearson symbol	cP116
Space group number	224
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	<pre>aflow --proto=A5B40CD12_cP116_224_bd_e3k_a_k-001 --params=a, x4, x5, z5, x6, z6, x7, z7, x8, z8</pre>

- This structure is a bit problematic. (Brown, 1977) offers evidence that the true structure of the hydrated phosphotungstic acid is $\text{H}_3\text{PW}_{12}\text{O}_{40} \cdot 6\text{H}_2\text{O}$, rather than $5\text{H}_2\text{O}$ as deduced by (Keggin, 1934). The presence of the extra water molecule does change the structure somewhat, and Keggin does not give the positions of the hydrogen atoms not attached to water molecules. Ordinarily we would mark this structure obsolete, but it is possible to remove water molecules from this structure and still have a molecule that is recognizably related to the acid, as in $\text{H}_3\text{PW}_{12}\text{O}_{40} \cdot 3\text{H}_2\text{O}$. In addition, the lattice constant reported by Keggin is 12.141\AA compared to Brown's 12.506\AA , a change consistent with the loss of a water molecule. Given this, we will not depreciate this five Water molecule structure.
- (Gottfried, 1937) does not give the positions of the water molecules, and they reverse the x and z coordinates for O-IV and W.
- This structure is a partially dehydrated form of $\text{H}_3\text{PW}_{12}\text{O}_{40} \cdot 29\text{H}_2\text{O}$ ($H4_{21}$). Further dehydration produces the $\text{H}_3\text{PW}_{12}\text{O}_{40} \cdot 3\text{H}_2\text{O}$ structure.
- The positions of the three hydrogen atoms are unknown. If we follow (Marosi, 2000), then the 'free' hydrogens are likely to be bound to some of the water molecules, giving the unusual stoichiometry in the prototype.
- The ICSD entry for (Keggin, 1934) does not list the positions of the water molecules.

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	$= 0$	$=$	0	(4b)	H I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4b)	H I
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	H I
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	H I
\mathbf{B}_7	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_8	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_9	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_{10}	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_{11}	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_{12}	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	H II
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{15}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I

$$\mathbf{B}_{112} = (x_8 + \frac{1}{2}) \mathbf{a}_1 - z_8 \mathbf{a}_2 + (x_8 + \frac{1}{2}) \mathbf{a}_3 = a (x_8 + \frac{1}{2}) \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{z}} \quad (24k) \quad \text{W I}$$

$$\mathbf{B}_{113} = (z_8 + \frac{1}{2}) \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 - x_8 \mathbf{a}_3 = a (z_8 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} \quad (24k) \quad \text{W I}$$

$$\mathbf{B}_{114} = (z_8 + \frac{1}{2}) \mathbf{a}_1 - x_8 \mathbf{a}_2 + (x_8 + \frac{1}{2}) \mathbf{a}_3 = a (z_8 + \frac{1}{2}) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{z}} \quad (24k) \quad \text{W I}$$

$$\mathbf{B}_{115} = -z_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + (x_8 + \frac{1}{2}) \mathbf{a}_3 = -az_8 \hat{\mathbf{x}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{y}} + a (x_8 + \frac{1}{2}) \hat{\mathbf{z}} \quad (24k) \quad \text{W I}$$

$$\mathbf{B}_{116} = -z_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - x_8 \mathbf{a}_3 = -az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} \quad (24k) \quad \text{W I}$$

References

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- [3] L. Marosi, E. E. Platero, J. Cifre, and C. O. Areána, *Thermal dehydration of $H_{3+x}PV_xM_{12}O_{40} \cdot yH_2O$ Keggin type heteropolyacids; formation, thermal stability and structure of the anhydrous acids $H_3PM_{12}O_{40}$, of the corresponding anhydrides $PM_{12}O_{38.5}$ and of a novel trihydrate $H_3PW_{12}O_{40} \cdot 3H_2O$* , Journal of Materials Chemistry **10**, 1949–1955 (2000), doi:10.1039/b001476l.

Found in

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