

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

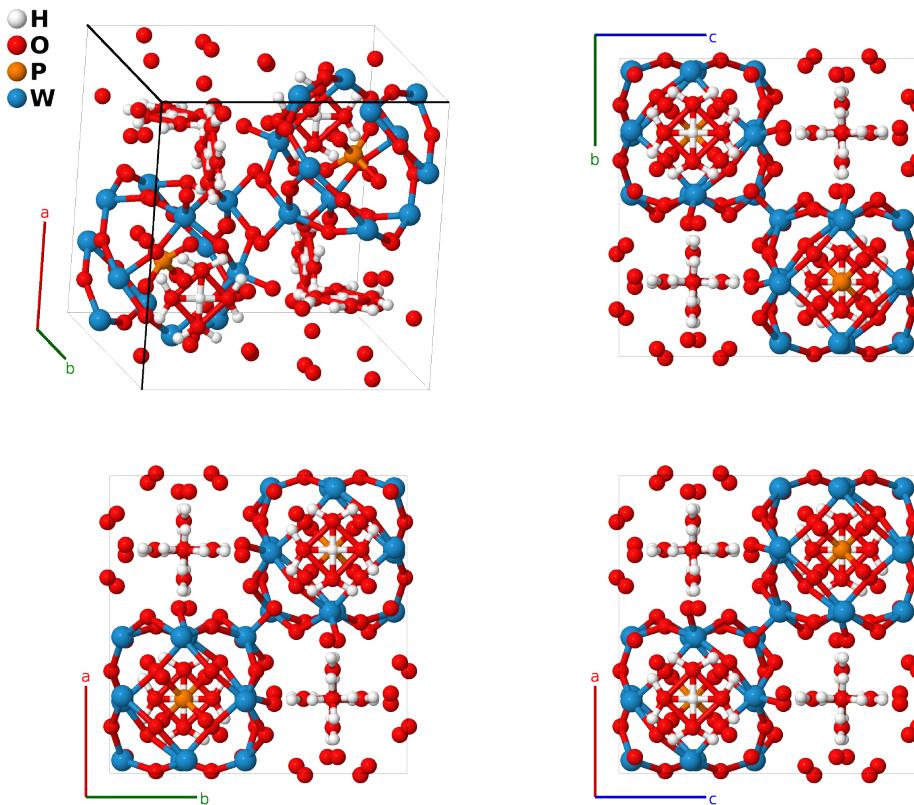
A27B52CD12_cP184_224_dl_eh3k_a_k-001

This structure originally had the label A27B52CD12_cP184_224_dl_eh3k_a_k. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

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

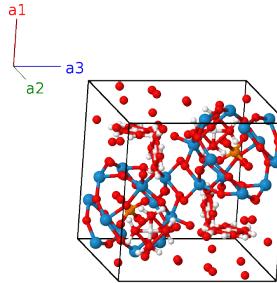


Prototype	$\text{H}_{15}\text{O}_{46}\text{PW}_{12}$
AFLOW prototype label	A27B52CD12_cP184_224_dl_eh3k_a_k-001
Mineral name	dodecatungstophosphoric acid hexahydrate
ICSD	904
Pearson symbol	cP184
Space group number	224
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	<pre>aflow --proto=A27B52CD12_cP184_224_dl_eh3k_a_k-001 --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}	$-(x_3 - \frac{1}{2})\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2})\hat{\mathbf{x}} - a(x_3 - \frac{1}{2})\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{11}	$-(x_3 - \frac{1}{2})\mathbf{a}_1 + x_3\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2})\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} - a(x_3 - \frac{1}{2})\hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{12}	$x_3\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}} - a(x_3 - \frac{1}{2})\hat{\mathbf{y}} - a(x_3 - \frac{1}{2})\hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{13}	$(x_3 + \frac{1}{2})\mathbf{a}_1 + (x_3 + \frac{1}{2})\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$a(x_3 + \frac{1}{2})\hat{\mathbf{x}} + a(x_3 + \frac{1}{2})\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(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}	$(x_3 + \frac{1}{2})\mathbf{a}_1 - x_3\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	=	$a(x_3 + \frac{1}{2})\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + a(x_3 + \frac{1}{2})\hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{16}	$-x_3\mathbf{a}_1 + (x_3 + \frac{1}{2})\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}} + a(x_3 + \frac{1}{2})\hat{\mathbf{y}} + a(x_3 + \frac{1}{2})\hat{\mathbf{z}}$	(8e)	O I

B₈₇	$-z_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (x_6 + \frac{1}{2}) \mathbf{a}_3$	=	$-az_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O IV
B₈₈	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$-az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(24k)	O IV
B₈₉	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24k)	O V
B₉₀	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24k)	O V
B₉₁	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₉₂	$x_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₉₃	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₉₄	$z_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$az_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₉₅	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-a(z_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₉₆	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(z_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₉₇	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₉₈	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + z_7 \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₉₉	$x_7 \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₀₀	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₀₁	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₀₂	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₀₃	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₀₄	$-x_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₀₅	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₀₆	$-x_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₀₇	$-x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₀₈	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - z_7 \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	=	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₀₉	$(z_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$a(z_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₁₀	$(z_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	=	$a(z_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₁₁	$-z_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-az_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	O V
B₁₁₂	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	=	$-az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(24k)	O V
B₁₁₃	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(24k)	W I
B₁₁₄	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(24k)	W I
B₁₁₅	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - a(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	W I
B₁₁₆	$x_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	W I
B₁₁₇	$z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	=	$az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(24k)	W I
B₁₁₈	$z_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 - (x_8 - \frac{1}{2}) \mathbf{a}_3$	=	$az_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	W I

$$\begin{aligned}
\mathbf{B}_{182} &= - \left(z_9 - \frac{1}{2} \right) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(x_9 - \frac{1}{2} \right) \mathbf{a}_3 & = & -a \left(z_9 - \frac{1}{2} \right) \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} - a \left(x_9 - \frac{1}{2} \right) \hat{\mathbf{z}} & (48l) & \text{H II} \\
\mathbf{B}_{183} &= z_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2} \right) \mathbf{a}_2 - \left(x_9 - \frac{1}{2} \right) \mathbf{a}_3 & = & az_9 \hat{\mathbf{x}} - a \left(y_9 - \frac{1}{2} \right) \hat{\mathbf{y}} - a \left(x_9 - \frac{1}{2} \right) \hat{\mathbf{z}} & (48l) & \text{H II} \\
\mathbf{B}_{184} &= z_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + x_9 \mathbf{a}_3 & = & az_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} & (48l) & \text{H II}
\end{aligned}$$

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.