

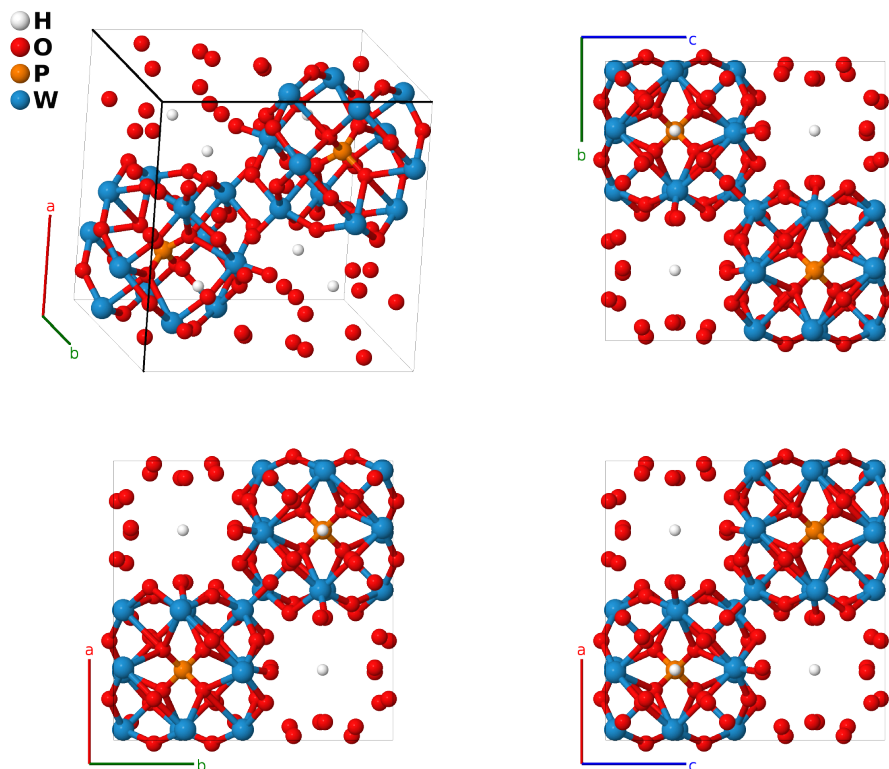
PW₁₂O₄₀·3H₃O Structure: A3B40CD12_cP112_224_d_e3k_a_k-001

This structure originally had the label A3B40CD12_cP112_224_d_e3k_a_k. Calls to that address will be redirected here.

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<https://aflow.org/p/R1HF>

https://aflow.org/p/A3B40CD12_cP112_224_d_e3k_a_k-001



Prototype	(H ₃ O) ₃ O ₄₀ PW ₁₂
AFLOW prototype label	A3B40CD12_cP112_224_d_e3k_a_k-001
ICSD	90637
Pearson symbol	cP112
Space group number	224
Space group symbol	<i>Pn</i> $\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B40CD12_cP112_224_d_e3k_a_k-001 --params=a, x3, x4, z4, x5, z5, x6, z6, x7, z7</code>

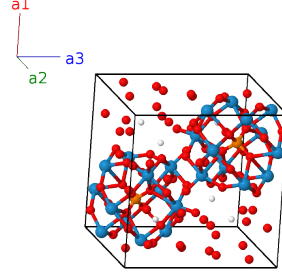
- This is a partially dehydrated version of H₃PW₁₂O₄₀ · 29H₂O (*H4*₂₁) and H₃PW₁₂O₄₀ · 5H₂O (*H4*₁₆) or H₃PW₁₂O₄₀ · 6H₂O. The six H₅O₂⁺ ions of the later structure have been replaced by three H₃O⁺ ions.
- The ICSD entry classifies the H₃O⁺ ions as oxygen atoms, labeling them “O5.”

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



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	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{11}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{12}	$= x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{13}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{14}	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{15}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{16}	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + a z_4 \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{18}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a z_4 \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{19}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{20}	$= x_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{21}	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$a z_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + a x_4 \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{22}	$= z_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a z_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24k)	O II
\mathbf{B}_{23}	$= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a x_4 \hat{\mathbf{z}}$	(24k)	O II

$$\begin{aligned}
\mathbf{B}_{88} &= -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) & \text{O IV} \\
\mathbf{B}_{89} &= 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) & \text{W I} \\
\mathbf{B}_{90} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + &= & -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad z_7 \mathbf{a}_3 \\
\mathbf{B}_{91} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + x_7 \mathbf{a}_2 - &= & -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{92} &= x_7 \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & ax_7 \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{93} &= 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) & \text{W I} \\
\mathbf{B}_{94} &= z_7 \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & az_7 \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{95} &= -\left(z_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + &= & -a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad x_7 \mathbf{a}_3 \\
\mathbf{B}_{96} &= -\left(z_7 - \frac{1}{2}\right) \mathbf{a}_1 + x_7 \mathbf{a}_2 - &= & -a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(x_7 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{97} &= 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) & \text{W I} \\
\mathbf{B}_{98} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + z_7 \mathbf{a}_2 - &= & -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(x_7 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{99} &= x_7 \mathbf{a}_1 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & ax_7 \hat{\mathbf{x}} - a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{100} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_2 + &= & -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad x_7 \mathbf{a}_3 \\
\mathbf{B}_{101} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{102} &= -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) & \text{W I} \\
\mathbf{B}_{103} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{104} &= -x_7 \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + &= & -ax_7 \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{105} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_2 - x_7 \mathbf{a}_3 &= & a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{106} &= -x_7 \mathbf{a}_1 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_2 + &= & -ax_7 \hat{\mathbf{x}} + a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(x_7 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{107} &= -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) & \text{W I} \\
\mathbf{B}_{108} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - z_7 \mathbf{a}_2 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{109} &= \left(z_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 - x_7 \mathbf{a}_3 &= & a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{110} &= \left(z_7 + \frac{1}{2}\right) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & a \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
\mathbf{B}_{111} &= -z_7 \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + &= & -az_7 \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24k) & \text{W I} \\
&\quad \left(x_7 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{112} &= -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) & \text{W I}
\end{aligned}$$

References

- [1] L. Marosi, E. E. Platero, J. Cifre, and C. O. Areána, *Thermal dehydration of $H_{3+x}PV_xM_{12x}O_{40} \cdot yH_2O$ 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 $H_3PW_{12}O_{40} \cdot 3H_2O$* , J. Mater. Chem. **10**, 1949–1955 (2000), doi:10.1039/b001476l.

Found in

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