

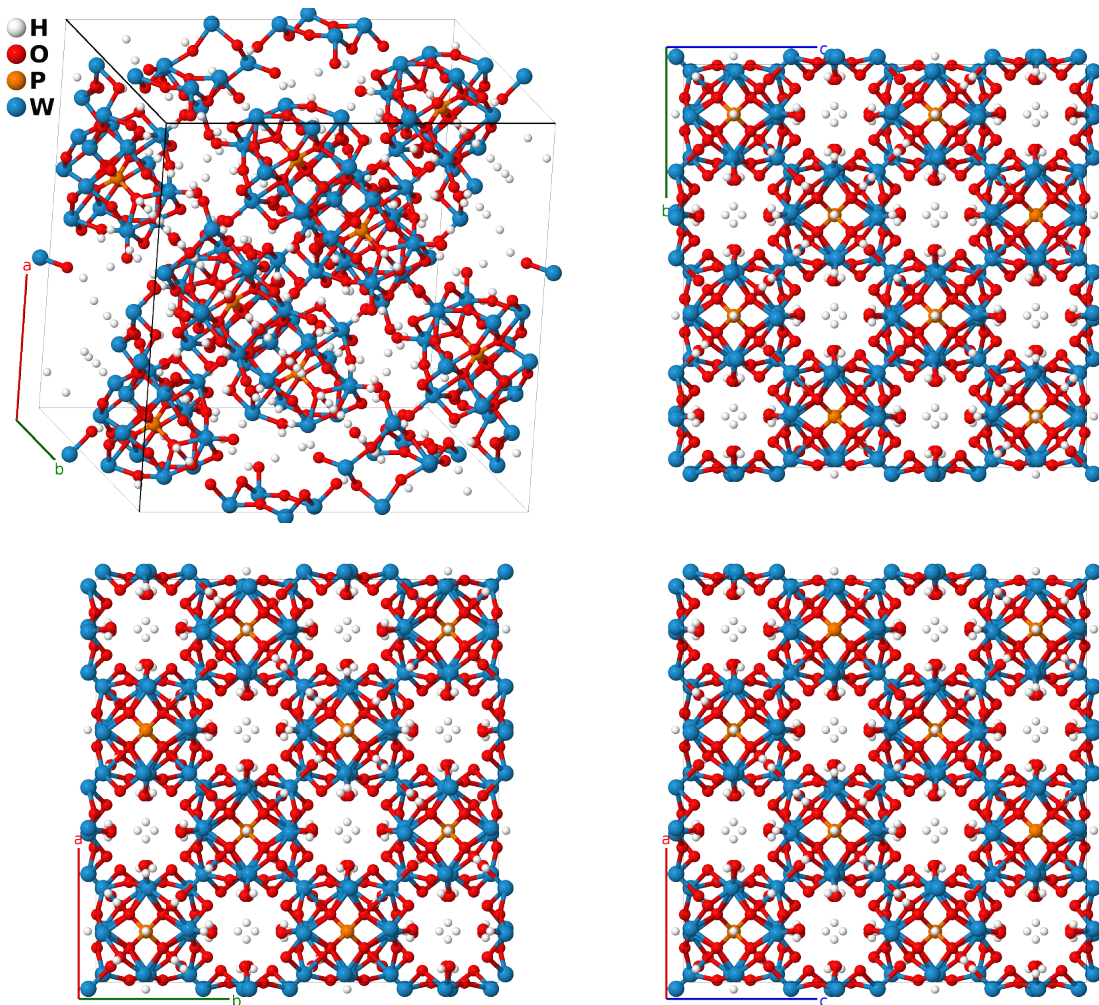
$H_3PW_{12}O_{40} \cdot 29H_2O$ ($H4_{21}$) Structure: A29B40CD12_cF656_227_ae2fg_e3g_b_g-001

This structure originally had the label A29B40CD12_cF656_227_ae2fg_e3g_b_g. Calls to that address will be redirected here.

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<https://aflow.org/p/3VYY>

https://aflow.org/p/A29B40CD12_cF656_227_ae2fg_e3g_b_g-001



Prototype	$H_3(H_2O)_{29}O_{40}PW_{12}$
AFLOW prototype label	A29B40CD12_cF656_227_ae2fg_e3g_b_g-001
<i>Strukturbericht</i> designation	$H4_{21}$
Mineral name	29-phosphotungstic acid (PWA-29)
ICSD	36274
Pearson symbol	cF656
Space group number	227

Space group symbol

$Fd\bar{3}m$

AFLOW prototype command

aflow --proto=A29B40CD12_cF656_227_ae2fg_e3g_b_g-001
 --params= $a, x_3, x_4, x_5, x_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}$

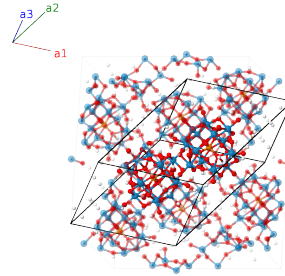
Other compounds with this structure

$H_3PMo_{12}O_{40} \cdot 30H_2O$

- This compound is often colloquially called “PWA-29.” On heating some water molecules will disassociate, leaving $H_3PW_{12}O_{40} \cdot 6H_2O$, $H_3PW_{12}O_{40} \cdot 5H_2O$ (H_{416}), or $H_3PW_{12}O_{40} \cdot 3H_2O$.
- The three hydrogen atoms not formally associated with the water molecules are not located. Presumably they join with some water molecules to form form H_3O^+ ions.
- Even the exact number and position of the water molecules is uncertain. (Clark, 1976), studying the related compound $H_3PMo_{12}O_{40} \cdot 30H_2O$, states that the composition is approximately $30H_2O$ and that “only six of the water molecules occupy ordered sites.”

Face-centered Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{y} + \frac{1}{2}a \hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B_1	$= \frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{8}a \hat{x} + \frac{1}{8}a \hat{y} + \frac{1}{8}a \hat{z}$	(8a)	H I
B_2	$= \frac{7}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{7}{8}a \hat{x} + \frac{7}{8}a \hat{y} + \frac{7}{8}a \hat{z}$	(8a)	H I
B_3	$= \frac{3}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$\frac{3}{8}a \hat{x} + \frac{3}{8}a \hat{y} + \frac{3}{8}a \hat{z}$	(8b)	P I
B_4	$= \frac{5}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{5}{8}a \hat{x} + \frac{5}{8}a \hat{y} + \frac{5}{8}a \hat{z}$	(8b)	P I
B_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$	(32e)	H II
B_6	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (3x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4}) \hat{x} - a(x_3 - \frac{1}{4}) \hat{y} + ax_3 \hat{z}$	(32e)	H II
B_7	$= x_3 \mathbf{a}_1 - (3x_3 - \frac{1}{2}) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4}) \hat{x} + ax_3 \hat{y} - a(x_3 - \frac{1}{4}) \hat{z}$	(32e)	H II
B_8	$= -(3x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} - a(x_3 - \frac{1}{4}) \hat{y} - a(x_3 - \frac{1}{4}) \hat{z}$	(32e)	H II
B_9	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (3x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4}) \hat{x} + a(x_3 + \frac{1}{4}) \hat{y} - ax_3 \hat{z}$	(32e)	H II
B_{10}	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$	(32e)	H II
B_{11}	$= -x_3 \mathbf{a}_1 + (3x_3 + \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4}) \hat{x} - ax_3 \hat{y} + a(x_3 + \frac{1}{4}) \hat{z}$	(32e)	H II
B_{12}	$= (3x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} + a(x_3 + \frac{1}{4}) \hat{y} + a(x_3 + \frac{1}{4}) \hat{z}$	(32e)	H II
B_{13}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} + ax_4 \hat{y} + ax_4 \hat{z}$	(32e)	O I
B_{14}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (3x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4}) \hat{x} - a(x_4 - \frac{1}{4}) \hat{y} + ax_4 \hat{z}$	(32e)	O I
B_{15}	$= x_4 \mathbf{a}_1 - (3x_4 - \frac{1}{2}) \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4}) \hat{x} + ax_4 \hat{y} - a(x_4 - \frac{1}{4}) \hat{z}$	(32e)	O I

$$\mathbf{B}_{161} = \begin{matrix} -z_{11} \mathbf{a}_1 - (2x_{11} - z_{11}) \mathbf{a}_2 + \\ (2x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a \left(z_{11} + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_{11} + \frac{1}{4} \right) \hat{\mathbf{y}} - ax_{11} \hat{\mathbf{z}} \quad (96g) \quad \text{W I}$$

$$\mathbf{B}_{162} = \begin{matrix} -z_{11} \mathbf{a}_1 + (2x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_2 - \\ (2x_{11} - z_{11}) \mathbf{a}_3 \end{matrix} = a \left(z_{11} + \frac{1}{4} \right) \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} + a \left(x_{11} + \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96g) \quad \text{W I}$$

$$\mathbf{B}_{163} = \begin{matrix} (2x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_1 - z_{11} \mathbf{a}_2 - \\ z_{11} \mathbf{a}_3 \end{matrix} = -az_{11} \hat{\mathbf{x}} + a \left(x_{11} + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_{11} + \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96g) \quad \text{W I}$$

$$\mathbf{B}_{164} = -(2x_{11} - z_{11}) \mathbf{a}_1 - z_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -az_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - ax_{11} \hat{\mathbf{z}} \quad (96g) \quad \text{W I}$$

References

- [1] A. J. Bradley and J. W. Illinworth, *The Crystal Structure of $H_3PW_{12}O_{40} \cdot 29H_2O$* , Proc. Roy. Soc. London A **157**, 113–131 (1936), doi:10.1098/rspa.1936.0183.
- [2] C. J. Clark and D. Hall, *Dodecamolybdophosphoric acid circa 30-hydrate*, Acta Crystallogr. Sect. B **32**, 1545–1547 (1976), doi:10.1107/S0567740876005748.

Found in

- [1] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).