

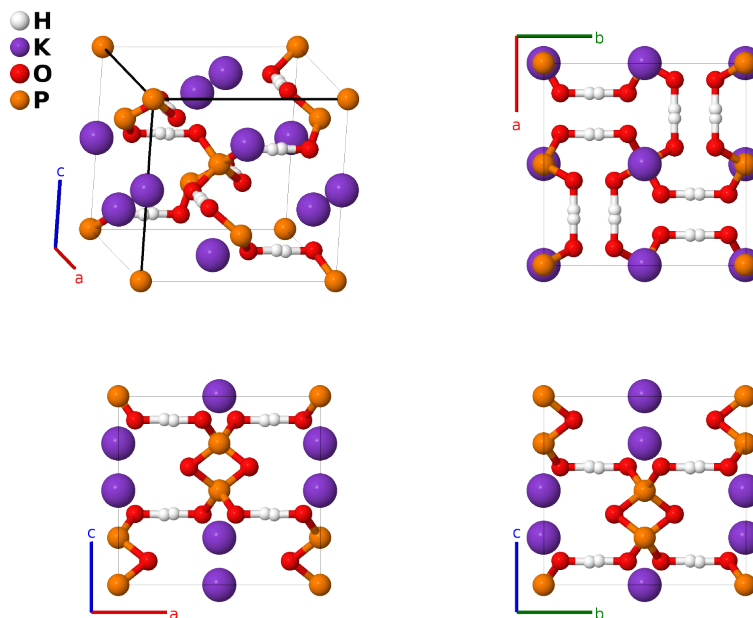
# $\text{KH}_2\text{PO}_4$ ( $H2_2$ ) Structure: A4BC4D\_tI40\_122\_e\_b\_e\_a-001

This structure originally had the label A4BC4D\_tI40\_122\_e\_b\_e\_a. Calls to that address will be redirected here.

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<https://afLOW.org/p/TLFW>

[https://afLOW.org/p/A4BC4D\\_tI40\\_122\\_e\\_b\\_e\\_a-001](https://afLOW.org/p/A4BC4D_tI40_122_e_b_e_a-001)



Prototype	$\text{KH}_2\text{PO}_4$
AFLOW prototype label	A4BC4D_tI40_122_e_b_e_a-001
<i>Strukturbericht</i> designation	$H2_2$
ICSD	201370
Pearson symbol	tI40
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	<pre>aflow --proto=A4BC4D_tI40_122_e_b_e_a-001       --params=a, c/a, x3, y3, z3, x4, y4, z4</pre>

## Other compounds with this structure

$\text{RbH}_2\text{PO}_4$ ,  $\text{KH}_2\text{AsO}_4$ ,  $\text{RbH}_2\text{AsO}_4$ ,  $\text{CsH}_2\text{AsO}_4$ ,  $\text{NH}_4\text{H}_2\text{PO}_4$ ,  $\text{NH}_4\text{H}_2\text{AsO}_4$

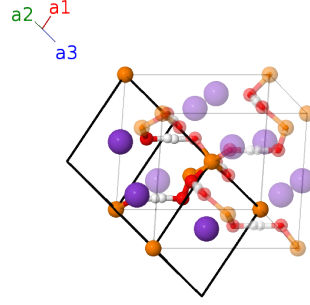
- The hydrogen (16e) sites are half-occupied. Given the closeness of pairs of hydrogen positions presumably only one site in each pair is ever occupied. This partial occupancy gives a structure that differs slightly from the  $H2_2$  structure described by (Ewald, 1928). There the hydrogen atoms are at their averaged positions, Wyckoff position (8d).

- The x position of the oxygen atom was inadvertently listed as 0.1933. We have changed this to the correct value, 0.14933

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### Body-centered Tetragonal primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(4a)	P I
$\mathbf{B}_2$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_4$	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_5$	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_6$	$-(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_7$	$-(x_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_8$	$(x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_9$	$(y_3 - z_3 + \frac{3}{4}) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{4}) \mathbf{a}_2 + (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_{10}$	$-(y_3 + z_3 - \frac{3}{4}) \mathbf{a}_1 + (x_3 - z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_{11}$	$(-x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + (-y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_{12}$	$(x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + (y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B}_{13}$	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B}_{14}$	$-(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B}_{15}$	$-(x_4 + z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B}_{16}$	$(x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16e)	O I

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{pmatrix} (y_4 - z_4 + \frac{3}{4}) \mathbf{a}_1 - \\ (x_4 + z_4 - \frac{1}{4}) \mathbf{a}_2 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{O I} \\
\mathbf{B}_{18} &= \begin{pmatrix} -(y_4 + z_4 - \frac{3}{4}) \mathbf{a}_1 + \\ (x_4 - z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{O I} \\
\mathbf{B}_{19} &= \begin{pmatrix} (-x_4 + z_4 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 - \\ (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{O I} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_4 + z_4 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{O I}
\end{aligned}$$

## References

- [1] R. J. Nelmes, G. M. Meyer, and J. E. Tibballs, *The crystal structure of tetragonal  $KH_2PO_4$  and  $KD_2PO_4$  as a function of temperature*, J. Phys. C: Solid State Phys. **15**, 59–75 (1982), doi:10.1088/0022-3719/15/1/005. Corrigendum: R. J. Nelmes and G. M. Meyer and J. E. Tibballs, J. Phys. C 15, 3040 (1982).
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).