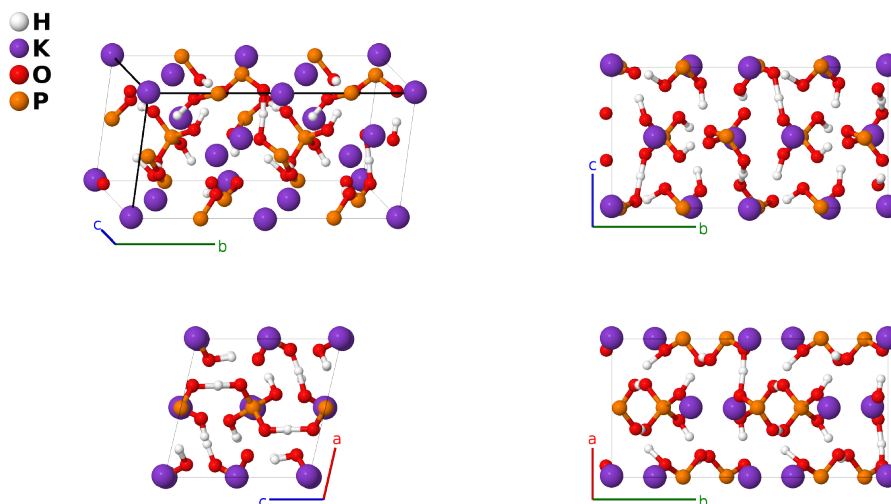


# Monoclinic $\text{KH}_2\text{PO}_4$ Structure: A5B2C8D2\_mP68\_4\_10a\_4a\_16a\_4a-001

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<https://aflow.org/p/MD4G>

[https://aflow.org/p/A5B2C8D2\\_mP68\\_4\\_10a\\_4a\\_16a\\_4a-001](https://aflow.org/p/A5B2C8D2_mP68_4_10a_4a_16a_4a-001)



Prototype	$\text{H}_5\text{K}_2\text{O}_8\text{P}_2$
AFLOW prototype label	A5B2C8D2_mP68_4_10a_4a_16a_4a-001
ICSD	155806
Pearson symbol	mP68
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	<pre>aflow --proto=A5B2C8D2_mP68_4_10a_4a_16a_4a-001       --params=a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7, y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15, y15,z15,x16,y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22, z22,x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,z26,x27,y27,z27,x28,y28,z28,x29,y29,z29, x30,y30,z30,x31,y31,z31,x32,y32,z32,x33,y33,z33,x34,y34,z34</pre>

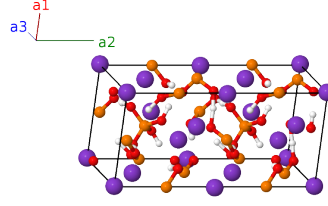
- This structure was grown from slow evaporation from an aqueous solution of  $\text{KH}_2\text{PO}_4$  and  $\text{K}_4\text{P}_2\text{O}_7$  at room temperature, and is metastable. The ground state of  $\text{KH}_2\text{PO}_4$  is the ferroelectric mineral archerite, stable below 121K, and above that temperature the stable phase is the paraelectric  $H2_2$  structure.
- Although (Fukami, 2006) give the chemical formula for this structure as  $\text{KH}_2\text{PO}_4$ , they list 10 hydrogen Wyckoff positions, making the actual formula  $\text{K}_2\text{H}_5\text{P}_2\text{O}_8$ . These hydrogens form O-H-O bonds between the oxygen atoms on neighboring  $\text{PO}_4$  tetrahedra, but are not centered between the oxygens.
- Space group  $P2_1$  #4 does not specify an origin for the  $y$ -axis. Here we set it by taking  $y_{11} = 0$  for the K-I Wyckoff position.

- The ICSD entry claims to be from (Fukami, 2006), but it only includes the first five oxygen sites from Table II of that paper, with no information about the hydrogen atoms.

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### Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	H III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	H III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	H IV
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	H IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	H V
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	H V
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	H VI
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	H VI
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	H VII
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	H VII
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	H VIII
$\mathbf{B}_{16}$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	H VIII
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	H IX
$\mathbf{B}_{18}$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	H IX
$\mathbf{B}_{19}$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	H X
$\mathbf{B}_{20}$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	=	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	H X
$\mathbf{B}_{21}$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2a)	K I



$$\begin{aligned}
\mathbf{B}_{52} &= -x_{26} \mathbf{a}_1 + \left(y_{26} + \frac{1}{2}\right) \mathbf{a}_2 - z_{26} \mathbf{a}_3 = -\left(ax_{26} + cz_{26} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{26} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{26} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XII} \\
\mathbf{B}_{53} &= x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 = \left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XIII} \\
\mathbf{B}_{54} &= -x_{27} \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 - z_{27} \mathbf{a}_3 = -\left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{27} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XIII} \\
\mathbf{B}_{55} &= x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3 = \left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XIV} \\
\mathbf{B}_{56} &= -x_{28} \mathbf{a}_1 + \left(y_{28} + \frac{1}{2}\right) \mathbf{a}_2 - z_{28} \mathbf{a}_3 = -\left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XIV} \\
\mathbf{B}_{57} &= x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + z_{29} \mathbf{a}_3 = \left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XV} \\
\mathbf{B}_{58} &= -x_{29} \mathbf{a}_1 + \left(y_{29} + \frac{1}{2}\right) \mathbf{a}_2 - z_{29} \mathbf{a}_3 = -\left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{29} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XV} \\
\mathbf{B}_{59} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 = \left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XVI} \\
\mathbf{B}_{60} &= -x_{30} \mathbf{a}_1 + \left(y_{30} + \frac{1}{2}\right) \mathbf{a}_2 - z_{30} \mathbf{a}_3 = -\left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{30} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XVI} \\
\mathbf{B}_{61} &= x_{31} \mathbf{a}_1 + y_{31} \mathbf{a}_2 + z_{31} \mathbf{a}_3 = \left(ax_{31} + cz_{31} \cos \beta\right) \hat{\mathbf{x}} + by_{31} \hat{\mathbf{y}} + cz_{31} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P I} \\
\mathbf{B}_{62} &= -x_{31} \mathbf{a}_1 + \left(y_{31} + \frac{1}{2}\right) \mathbf{a}_2 - z_{31} \mathbf{a}_3 = -\left(ax_{31} + cz_{31} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{31} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{31} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P I} \\
\mathbf{B}_{63} &= x_{32} \mathbf{a}_1 + y_{32} \mathbf{a}_2 + z_{32} \mathbf{a}_3 = \left(ax_{32} + cz_{32} \cos \beta\right) \hat{\mathbf{x}} + by_{32} \hat{\mathbf{y}} + cz_{32} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P II} \\
\mathbf{B}_{64} &= -x_{32} \mathbf{a}_1 + \left(y_{32} + \frac{1}{2}\right) \mathbf{a}_2 - z_{32} \mathbf{a}_3 = -\left(ax_{32} + cz_{32} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{32} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{32} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P II} \\
\mathbf{B}_{65} &= x_{33} \mathbf{a}_1 + y_{33} \mathbf{a}_2 + z_{33} \mathbf{a}_3 = \left(ax_{33} + cz_{33} \cos \beta\right) \hat{\mathbf{x}} + by_{33} \hat{\mathbf{y}} + cz_{33} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P III} \\
\mathbf{B}_{66} &= -x_{33} \mathbf{a}_1 + \left(y_{33} + \frac{1}{2}\right) \mathbf{a}_2 - z_{33} \mathbf{a}_3 = -\left(ax_{33} + cz_{33} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{33} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{33} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P III} \\
\mathbf{B}_{67} &= x_{34} \mathbf{a}_1 + y_{34} \mathbf{a}_2 + z_{34} \mathbf{a}_3 = \left(ax_{34} + cz_{34} \cos \beta\right) \hat{\mathbf{x}} + by_{34} \hat{\mathbf{y}} + cz_{34} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P IV} \\
\mathbf{B}_{68} &= -x_{34} \mathbf{a}_1 + \left(y_{34} + \frac{1}{2}\right) \mathbf{a}_2 - z_{34} \mathbf{a}_3 = -\left(ax_{34} + cz_{34} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{34} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{34} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P IV}
\end{aligned}$$

## References

- [1] T. Fukami and R.-H. Chen, *Crystal Structure and Transitions for Monoclinic  $KH_2PO_4$  Crystal*, J. Phys. Soc. Jpn. **75**, 074602 (2006), doi:10.1143/JPSJ.75.074602.