Archerite (KH_2PO_4) Structure: A2BC4D_oF64_43_b_a_2b_a-001

This structure originally had the label `A2BC4D_oF64_43_b_a_2b_a`. Calls to that address will be redirected here.

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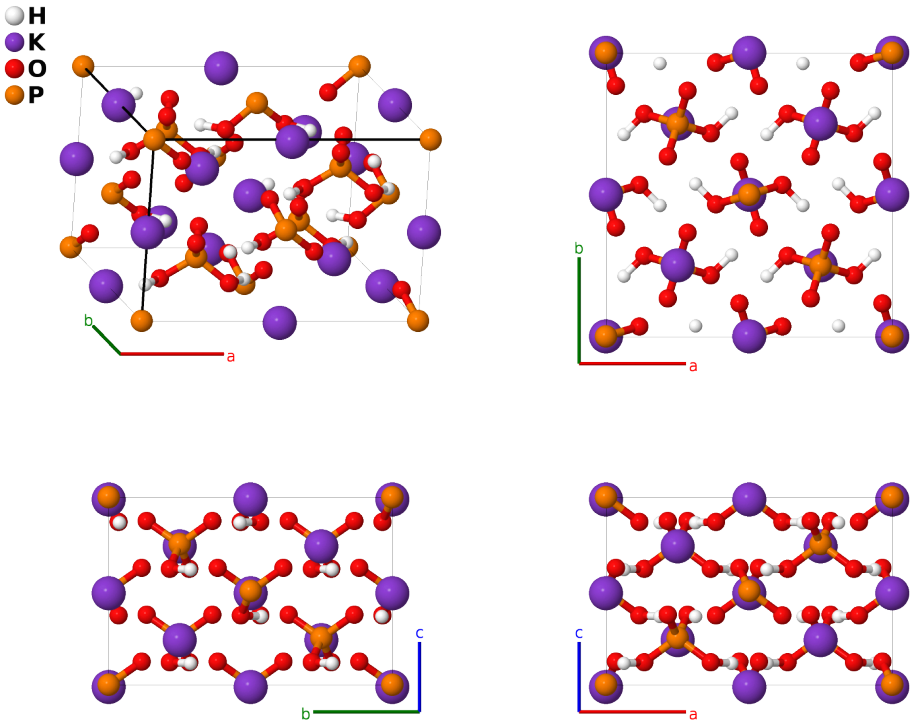
https://aflow.org/p/DS2R

https://aflow.org/p/A2BC4D_oF64_43_b_a_2b_a-001

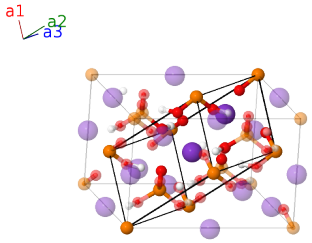


Prototype	H_2KO_4P
AFLOW prototype label	A2BC4D_oF64_43_b_a_2b_a-001
Mineral name	archerite
ICSD	31151
Pearson symbol	oF64
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A2BC4D_oF64_43_b_a_2b_a-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

- In our original determination of this structure (Hicks, 2019) we neglected to note that (Levy, 1954) used a non-standard representation of space group $Fdd2$ #43, effectively changing the direction of the screw axis and inaccurately describing the H_2PO_4 radicals. After viewing the ICSD entry and consulting the original work we realized our error and correct it here.
- This structure is stable below 121K, and the data was taken at 113K. The high temperature structure is tetragonal with disordered hydrogen. (Levy, 1954)
- The origin of the z-axis is not restricted in space group $Fdd2$ #43. Here it is fixed by putting the phosphorous atom at the origin.

Face-centered Orthorhombic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(8a)	K I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 - \left(z_1-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	K I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{4}\right)\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\mathbf{a}_2 - \left(z_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_5}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1 + (x_3-y_3+z_3)\,\mathbf{a}_2 + (x_3+y_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_6}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1 + (-x_3+y_3+z_3)\,\mathbf{a}_2 - (x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_7}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_1 + \left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_2 + \left(x_3-y_3-z_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_8}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_1 - \left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_3-y_3+z_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_9}$	=	$(-x_4+y_4+z_4)\,\mathbf{a}_1 + (x_4-y_4+z_4)\,\mathbf{a}_2 + (x_4+y_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16b)	O I
$\mathbf{B_{10}}$	=	$(x_4-y_4+z_4)\,\mathbf{a}_1 + (-x_4+y_4+z_4)\,\mathbf{a}_2 - (x_4+y_4+z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16b)	O I

$$\mathbf{B_{11}} = -\left(x_4+y_4-z_4-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_4+y_4+z_4+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_4-y_4-z_4+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_4+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_4-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{O I}$$

$$\mathbf{B_{12}} = \left(x_4+y_4+z_4+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_4+y_4-z_4-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_4-y_4+z_4-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_4-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_4+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{O I}$$

$$\mathbf{B_{13}} = (-x_5+y_5+z_5)\mathbf{a}_1+(x_5-y_5+z_5)\mathbf{a}_2+(x_5+y_5-z_5)\mathbf{a}_3 = ax_5\hat{\mathbf{x}}+by_5\hat{\mathbf{y}}+cz_5\hat{\mathbf{z}} \quad (16b) \quad \text{O II}$$

$$\mathbf{B_{14}} = (x_5-y_5+z_5)\mathbf{a}_1+(-x_5+y_5+z_5)\mathbf{a}_2-(x_5+y_5+z_5)\mathbf{a}_3 = -ax_5\hat{\mathbf{x}}-by_5\hat{\mathbf{y}}+cz_5\hat{\mathbf{z}} \quad (16b) \quad \text{O II}$$

$$\mathbf{B_{15}} = -\left(x_5+y_5-z_5-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_5+y_5+z_5+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_5-y_5-z_5+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_5-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{O II}$$

$$\mathbf{B_{16}} = \left(x_5+y_5+z_5+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_5+y_5-z_5-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_5-y_5+z_5-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_5+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{O II}$$

References

[1] H. A. Levy, S. W. Peterson, and S. H. Simonsen, *Neutron Diffraction Study of the Ferroelectric Modification of Potassium Dihydrogen Phosphate*, Phys. Rev. **93**, 1120–1121 (1954), doi:10.1103/PhysRev.93.1120.

[2] 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.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).