$NH_4H_2PO_4$ Structure: A8BC4D_tI56_122_2e_b_e_a-001

This structure originally had the label `A8BC4D_tI56_122_2e_b_e_a`. Calls to that address will be redirected here.

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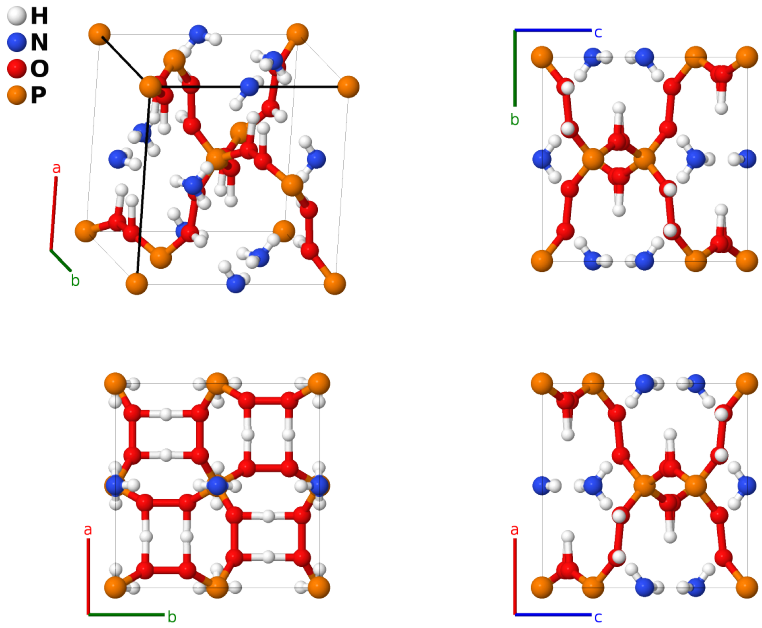
https://aflow.org/p/PGWH

https://aflow.org/p/A8BC4D_tI56_122_2e_b_e_a-001



Prototype	H_6NO_4P
AFLOW prototype label	A8BC4D_tI56_122_2e_b_e_a-001
ICSD	28154
Pearson symbol	tI56
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	`aflow --proto=A8BC4D_tI56_122_2e_b_e_a-001 --params=`$a, c/a, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

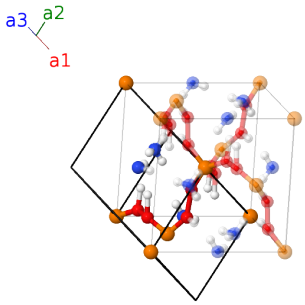
Other compounds with this structure
$NH_4H_2AsO_4$

- $NH_4H_2PO_4$ and $NH_4H_2AsO_4$ are usually considered to be isomorphous with the KH_2PO_4 ($H2_2$) structure, but (Khan, 1973) and (Fukami, 1987) were able to locate the hydrogen atoms in the NH_4 radical so we include this as a new structure.
- As in KH_2PO_4 the H-I site, associated with the PO_4 ion, is 50% occupied.
- Below 148K the H-I atoms become locked in place, and $NH_4H_2PO_4$ distorts in to a orthorhombic ferroelectric phase.

- The ICSD entry for this structure reverses the x and y coordinates of the H I atoms, placing them on an (8d) site which would be fully occupied. This makes minimal changes to the crystal structure, but we are investigating it further.

Body-centered Tetragonal primitive vectors

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



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)	N 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)	N 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
$\mathbf{B_9}$	=	$\left(y_3-z_3+\frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_3+z_3-\frac{1}{4}\right)\,\mathbf{a}_2 + \left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B_{10}}$	=	$-\left(y_3+z_3-\frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3-z_3+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B_{11}}$	=	$\left(-x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(-y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	H I
$\mathbf{B_{12}}$	=	$\left(x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(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)	H II
$\mathbf{B_{14}}$	=	$-(y_4-z_4)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{15}}$	=	$-(x_4+z_4)\,\mathbf{a}_1 + (y_4-z_4)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16e)	H II

$\mathbf{B_{16}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{17}}$	=	$\left(y_4 - z_4 + \frac{3}{4}\right)\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{4}\right)\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{18}}$	=	$-\left(y_4 + z_4 - \frac{3}{4}\right)\mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_4 - y_4 + \frac{1}{2}\right)\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{19}}$	=	$\left(-x_4 + z_4 + \frac{3}{4}\right)\mathbf{a}_1 + \left(-y_4 + z_4 + \frac{1}{4}\right)\mathbf{a}_2 - \left(x_4 + y_4 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{20}}$	=	$\left(x_4 + z_4 + \frac{3}{4}\right)\mathbf{a}_1 + \left(y_4 + z_4 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_4 + y_4 + \frac{1}{2}\right)\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	H II
$\mathbf{B_{21}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{22}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{23}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{24}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{25}}$	=	$\left(y_5 - z_5 + \frac{3}{4}\right)\mathbf{a}_1 - \left(x_5 + z_5 - \frac{1}{4}\right)\mathbf{a}_2 + \left(-x_5 + y_5 + \frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{26}}$	=	$-\left(y_5 + z_5 - \frac{3}{4}\right)\mathbf{a}_1 + \left(x_5 - z_5 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{27}}$	=	$\left(-x_5 + z_5 + \frac{3}{4}\right)\mathbf{a}_1 + \left(-y_5 + z_5 + \frac{1}{4}\right)\mathbf{a}_2 - \left(x_5 + y_5 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	O I
$\mathbf{B_{28}}$	=	$\left(x_5 + z_5 + \frac{3}{4}\right)\mathbf{a}_1 + \left(y_5 + z_5 + \frac{1}{4}\right)\mathbf{a}_2 + \left(x_5 + y_5 + \frac{1}{2}\right)\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16e)	O I

References

[1] A. A. Khan and W. H. Baur, *Refinement of the crystal structures of ammonium dihydrogen phosphate and ammonium dihydrogen arsenate*, Acta Crystallogr. Sect. B **29**, 2721–2726 (1973), doi:10.1107/S0567740873007442.

Found in

[1] T. Fukami, S. Akahoshi, K. Hukuda, and T. Yagi, *Refinement of the Crystal Structure of $NH_4H_2PO_4$ above and below Antiferroelectric Phase Transition Temperature*, J. Phys. Soc. of Japan **56**, 2223–2224 (1987), doi:10.1143/JPSJ.56.2223.