

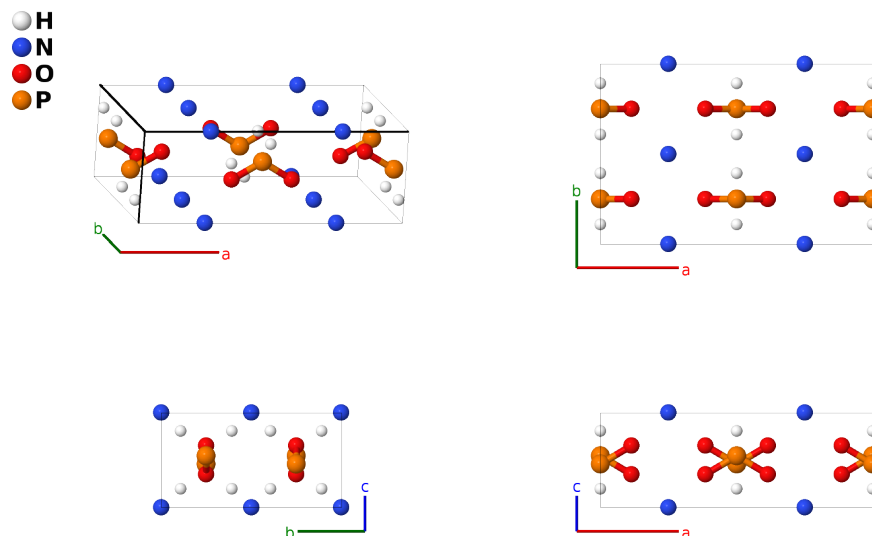
# NH<sub>4</sub>H<sub>2</sub>PO<sub>2</sub> (*F*5<sub>7</sub>) Structure: A2BC2D\_oC24\_67\_m\_a\_n\_g-001

This structure originally had the label `A2BC2D_oC24_67_m_a_n_g`. Calls to that address will be redirected here.

Cite this page as: 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.

<https://afLOW.org/p/ZLA7>

[https://afLOW.org/p/A2BC2D\\_oC24\\_67\\_m\\_a\\_n\\_g-001](https://afLOW.org/p/A2BC2D_oC24_67_m_a_n_g-001)

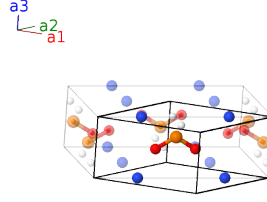


<b>Prototype</b>	H <sub>2</sub> (NH <sub>4</sub> )O <sub>2</sub> P
<b>AFLOW prototype label</b>	A2BC2D_oC24_67_m_a_n_g-001
<b>Strukturbericht designation</b>	<i>F</i> 5 <sub>7</sub>
<b>ICSD</b>	26929
<b>Pearson symbol</b>	oC24
<b>Space group number</b>	67
<b>Space group symbol</b>	<i>Cmme</i>
<b>AFLOW prototype command</b>	<code>afLOW --proto=A2BC2D_oC24_67_m_a_n_g-001 --params=a, b/a, c/a, z<sub>2</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub></code>

- (Zachariasen, 1934) state that the H atoms in the ammonium ion must be along the lines between the nitrogen and oxygen atoms, but give no further information, so we only provide the position of the nitrogen atoms (labeled as NH<sub>4</sub>).
- The data for this structure was presented in the *Acmm* setting of space group #67. We transformed this to the standard *Cmma* setting using FINDSYM.

## Base-centered Orthorhombic primitive vectors

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}}$	(4a)	N I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}}$	(4a)	N I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4g)	P I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4g)	P I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8m)	H I
$\mathbf{B}_6$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8m)	H I
$\mathbf{B}_7$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8m)	H I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8m)	H I
$\mathbf{B}_9$	$= (x_4 + \frac{3}{4}) \mathbf{a}_1 + (x_4 + \frac{1}{4}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8n)	O I
$\mathbf{B}_{10}$	$= -(x_4 - \frac{3}{4}) \mathbf{a}_1 - (x_4 - \frac{1}{4}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8n)	O I
$\mathbf{B}_{11}$	$= -(x_4 - \frac{1}{4}) \mathbf{a}_1 - (x_4 - \frac{3}{4}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8n)	O I
$\mathbf{B}_{12}$	$= (x_4 + \frac{1}{4}) \mathbf{a}_1 + (x_4 + \frac{3}{4}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8n)	O I

## References

- [1] W. H. Zachariasen and R. C. L. Mooney, *The Structure of the Hypophosphite Group as Determined from the Crystal Lattice of Ammonium Hypophosphite*, J. Chem. Phys. **2**, 34–37 (1934), doi:10.1063/1.1749354.

## Found in

- [1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).