$PNCl_2$ ($E1_4$) Structure: A2BC_tP32_86_2g_g_g-001

This structure previously used the label(s) `A2BC_tP32_86_2g_g_g`. Calls to these addresses will be redirected here.

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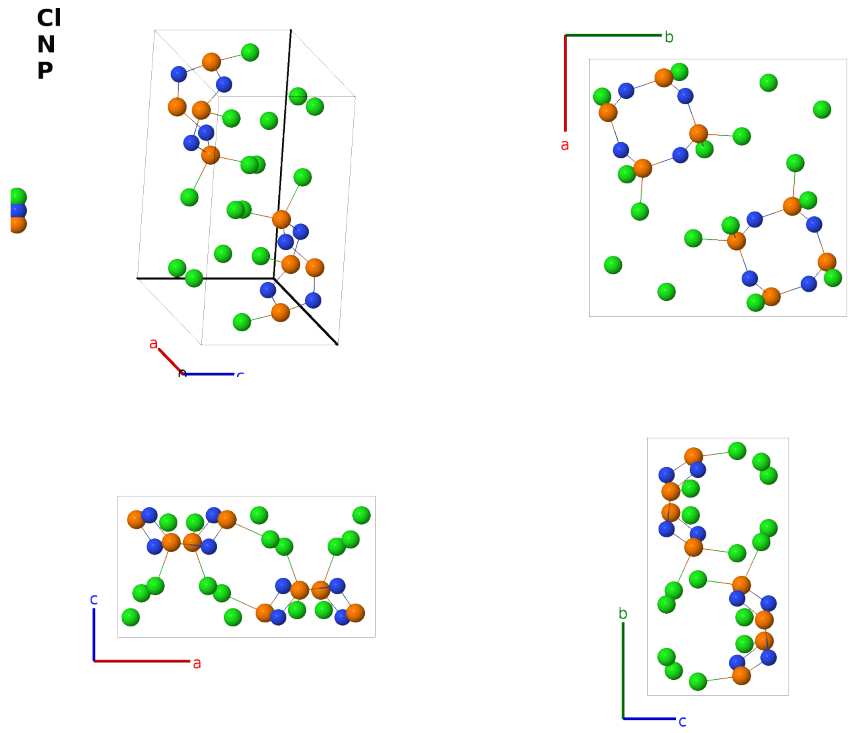
https://aflow.org/prototype-encyclopedia/QLZ6

https://aflow.org/prototype-encyclopedia/A2BC_tP32_86_2g_g_g-001

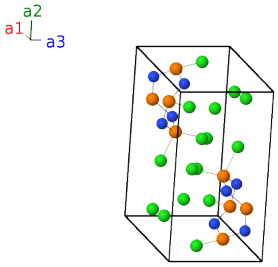


Prototype	Cl_2NP
AFLOW prototype label	A2BC_tP32_86_2g_g_g-001
***Strukturbericht* designation**	$E1_4$
ICSD	33711
CCDC	1606453
Pearson symbol	tP32
Space group number	86
Space group symbol	$P4_2/n$
AFLOW prototype command	`aflow --proto=A2BC_tP32_86_2g_g_g-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- (Ketellar, 1939) gave the atomic positions in setting 1 of space group $P4_2/n$ #86. We have shifted the origin to the inversion site for this lattice and present the atomic positions in setting 2.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_1 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} + a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_4}$	=	$\left(y_1+\frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ay_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_6}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_7}$	=	$y_1\,\mathbf{a}_1 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} - a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_8}$	=	$-\left(y_1-\frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{10}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{11}}$	=	$-y_2\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{12}}$	=	$\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{14}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{15}}$	=	$y_2\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{16}}$	=	$-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	Cl II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_{18}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_{19}}$	=	$-y_3\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	N I

$$
\begin{array}{lcccccc}
\mathbf{B_{20}} & = & \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{N I} \\
\mathbf{B_{21}} & = & -x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3 & = & -ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}} & (8g) & \text{N I} \\
\mathbf{B_{22}} & = & \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2-z_3\,\mathbf{a}_3 & = & a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}} & (8g) & \text{N I} \\
\mathbf{B_{23}} & = & y_3\,\mathbf{a}_1-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_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}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{N I} \\
\mathbf{B_{24}} & = & -\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_1+x_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{N I} \\
\mathbf{B_{25}} & = & x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3 & = & ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{26}} & = & -\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2+z_4\,\mathbf{a}_3 & = & -a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{27}} & = & -y_4\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_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}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{28}} & = & \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{29}} & = & -x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3 & = & -ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{30}} & = & \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3 & = & a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{31}} & = & y_4\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_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}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{P I} \\
\mathbf{B_{32}} & = & -\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}} & (8g) & \text{P I}
\end{array}
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References

[1] J. A. A. Ketelaar and T. A. de Vries, *The crystal structure of tetra phosphonitrile chloride, $P_4N_4Cl_8$*, Recueil Trav. Chimiq. des Pays-Bas **58**, 1081–1099 (1939), doi:10.1002/recl.19390581205.

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