PNCl$_2$ ($E1_4$) Structure: A2BC_tP32_86_2g_g_g-001
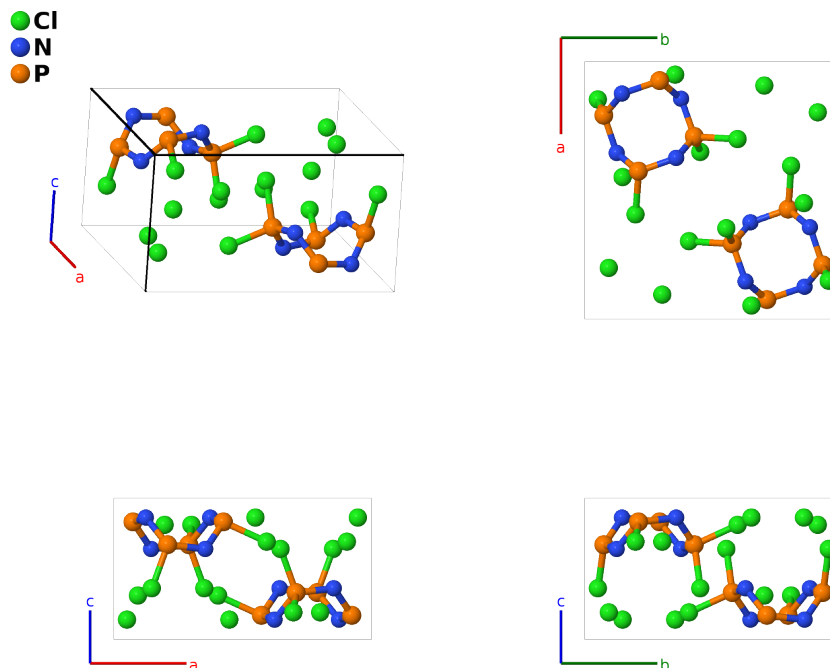
This structure originally had the label `A2BC_tP32_86_2g_g_g`. Calls to that address will be redirected here.

https://aflow.org/p/QLZ6

https://aflow.org/p/A2BC_tP32_86_2g_g_g-001

Prototype	Cl$_2$NP
AFLOW prototype label	A2BC_tP32_86_2g_g_g-001
***Strukturbericht* designation**	$E1_4$
ICSD	33711
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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
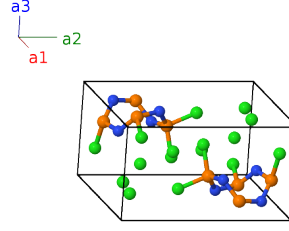
Basis vectors

		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
$\mathbf{B_{20}}$	$=$	$\left(y_3 + \frac{1}{2}\right)\mathbf{a_1} - x_3\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	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)	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)	N I

$$\mathbf{B_{23}} = y_3\,\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a}_3 = ay_3\,\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{N I}$$

$$\mathbf{B_{24}} = -\left(y_3 - \tfrac{1}{2}\right)\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{N I}$$

$$\mathbf{B_{25}} = x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{26}} = -\left(x_4 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3 = -a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{27}} = -y_4\,\mathbf{a}_1 + \left(x_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ay_4\,\hat{\mathbf{x}} + a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{28}} = \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{29}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{30}} = \left(x_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_4\,\mathbf{a}_3 = a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{31}} = y_4\,\mathbf{a}_1 - \left(x_4 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3 = ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

$$\mathbf{B_{32}} = -\left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8g) \qquad \text{P I}$$

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.