

$F5_4$ (NH_4ClO_2) (*Obsolete*) Structure: ABC2_tP8_100_b_a_c-001

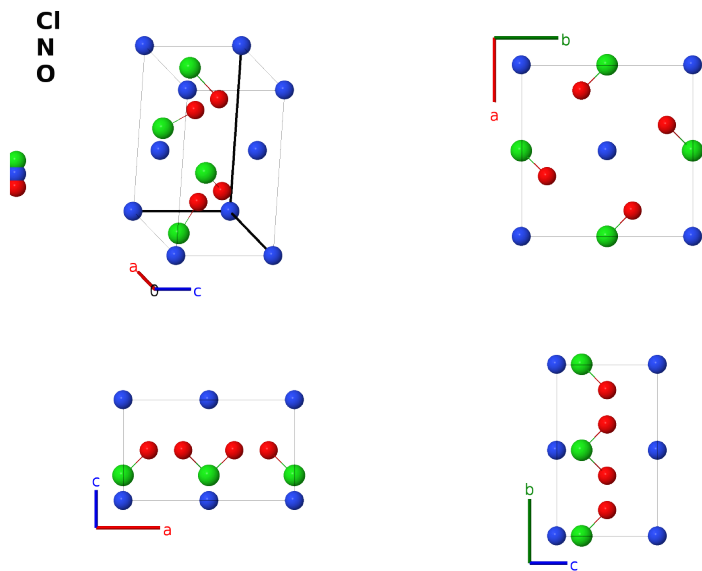
This structure previously used the label(s) `ABC2_tP8_100_b_a_c`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/YZB2>

https://aflow.org/prototype-encyclopedia/ABC2_tP8_100_b_a_c-001

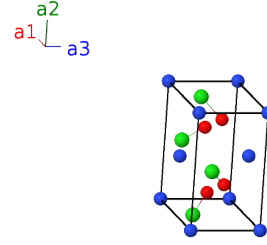


Prototype	$\text{Cl}(\text{NH}_4)\text{O}_2$
AFLOW prototype label	ABC2_tP8_100_b_a_c-001
<i>Strukturbericht</i> designation	$F5_4$
ICSD	36179
CCDC	1607953
Pearson symbol	tP8
Space group number	100
Space group symbol	$P4bm$
AFLOW prototype command	<code>aflow --proto=ABC2_tP8_100_b_a_c-001</code> <code>--params=$a, c/a, z_1, z_2, x_3, z_3$</code>

- (Levi, 1931) first determined this structure, but they were actually looking at a combination of ammonium chlorite, NH_4ClO_2 and ammonium chlorate, NH_4ClO_3 , which takes on the $\gamma\text{-KNO}_3$ structure. In addition, they were unable to determine the positions of the hydrogen atoms, and it appears that space group $P4bm$ #100 is incompatible with having four hydrogen atoms in a tetrahedral arrangement about the nitrogen atom. (Smolentsev, 2005) determined the positions of the hydrogen atoms, and placed this structure in space group $P\bar{4}2_1m$ #113, making the structure of (Levi, 1931) obsolete. We present it here for historical interest.
- Since the position of the hydrogen atoms in the NH_4 ions were not determined, we only provide the nitrogen atom positions (labeled as NH_4).

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	NH I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	NH I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(2b)	Cl I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	Cl I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_7$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_8$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I

References

- [1] G. R. Levi and A. Scherillo, *Ricerche cristallografiche sui sali dell'acido cloroso*, Z. Kristallogr. **76**, 431–452 (1931), doi:10.1524/zkri.1931.76.1.431.
- [2] A. I. Smolentsev and D. Y. Naumov, *Ammonium chlorite, NH_4ClO_2 , at 150 K*, Acta Crystallogr. Sect. E **61**, i38–i40 (2005), doi:10.1107/S1600536805005088.

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.