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

This structure originally had the label `ABC2_tP8_100_b_a_c`. Calls to that address will be redirected here.

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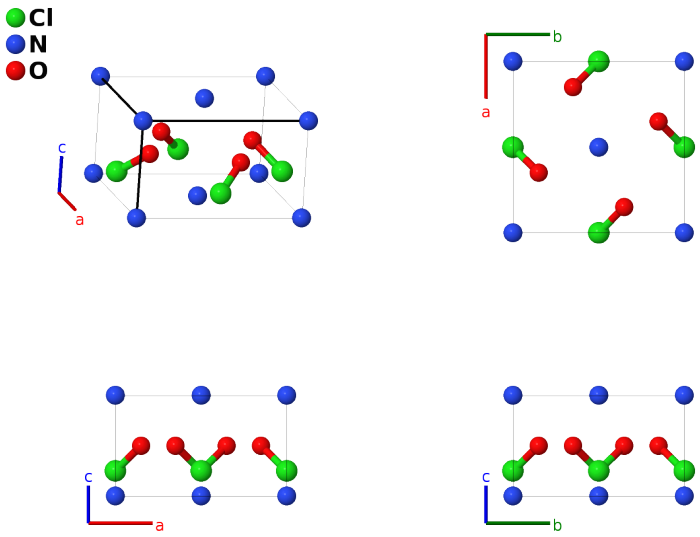
https://aflow.org/p/YZB2

https://aflow.org/p/ABC2_tP8_100_b_a_c-001

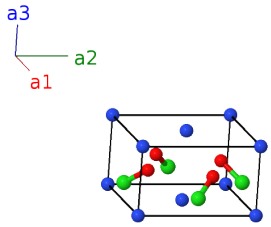


Prototype	$Cl(NH_4)O_2$
AFLOW prototype label	ABC2_tP8_100_b_a_c-001
***Strukturbericht* designation**	$F5_4$
ICSD	36179
Pearson symbol	tP8
Space group number	100
Space group symbol	$P4bm$
AFLOW prototype command	`aflow --proto=ABC2_tP8_100_b_a_c-001 --params=`$a, c/a, z_1, z_2, x_3, z_3$

- (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 γ-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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(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).