FeOCl ($E0_5$) Structure: ABC_oP6_59_a_b_a-001

This structure originally had the label `ABC_oP6_59_a_b_a`. Calls to that address will be redirected here.

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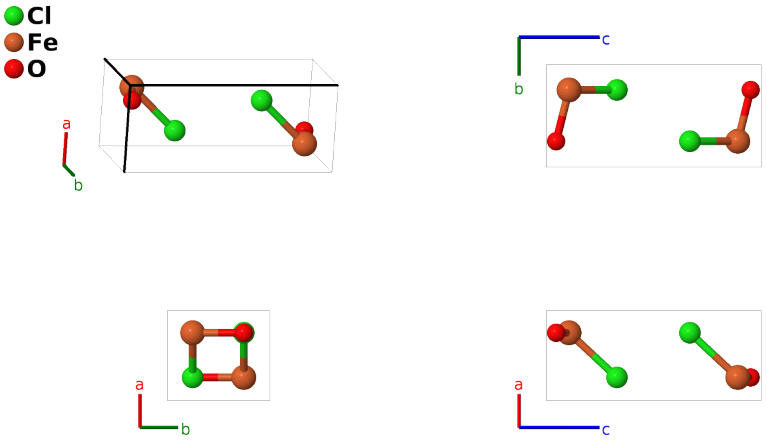
https://aflow.org/p/DN69

https://aflow.org/p/ABC_oP6_59_a_b_a-001



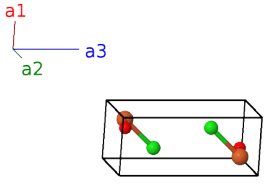
Prototype	ClFeO
AFLOW prototype label	ABC_oP6_59_a_b_a-001
***Strukturbericht* designation**	$E0_5$
ICSD	40963
Pearson symbol	oP6
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=ABC_oP6_59_a_b_a-001 --params=`$a, b/a, c/a, z_1, z_2, z_3$

Other compounds with this structure

AlOCl, CrOCl, CrOF, CrSBr, HfNBr, HfNCl, HfNI, IOBr, IOCl, TiNBr, TiNCl, TiNI, TiOCl, VOCl, ZrNBr, ZrNCl, ZrNI

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Cl I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	Cl I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	Fe I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2b)	Fe I

References

[1] S. M. Kauzlarich, J. L. Stanton, J. Faber, and B. A. Averill, *Neutron profile refinement of the structure of FeOCl and FeOCl(TTF)1/8.5*, J. Am. Chem. Soc. **108**, 7946–7951 (1986), doi:10.1021/ja00285a011.