

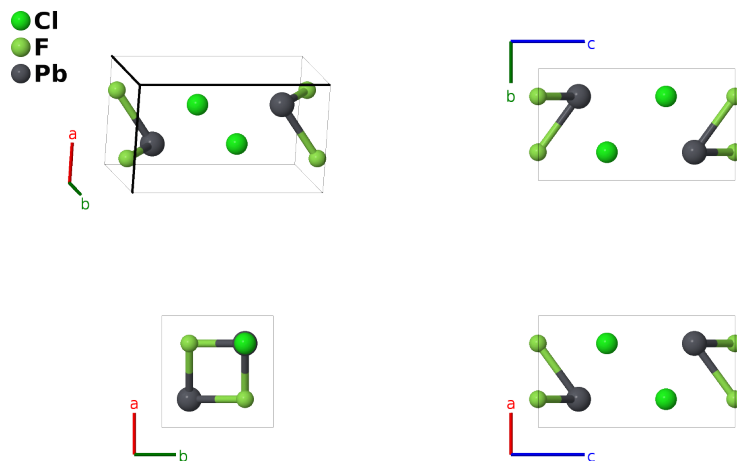
Matlockite ($E0_1$, PbFCl) Structure: ABC_tP6_129_c_a_c-001

This structure originally had the label ABC_tP6_129_c_a_c. Calls to that address will be redirected here.

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<https://aflow.org/p/0VRY>

https://aflow.org/p/ABC_tP6_129_c_a_c-001



Prototype	CIFPb
AFLOW prototype label	ABC_tP6_129_c_a_c-001
<i>Strukturbericht</i> designation	$E0_1$
Mineral name	matlockite
ICSD	82884
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<code>aflow --proto=ABC_tP6_129_c_a_c-001 --params=a, c/a, z₂, z₃</code>

Other compounds with this structure

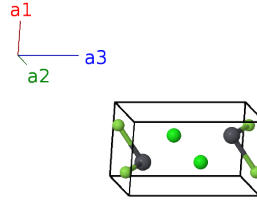
AcOBr, AlGeMn, AmOCl, BaHCl, BiOBr, BiOI, CaHBr, CeCoSi, CeFeSi, CeOCl, CuFeAs, CuFeSb, DyOCl, GeSZr, GeSeZr, GeTeZr, LaOI, LiFeAs, NaFeAs, NdOCl, NpOS, PbFBr, PrOCl, SSiZr, SeSiZr, SiTeZr, SmOI, SrHI, ThOTe, UOS, UTe₂, YbOI

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	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	F I
\mathbf{B}_2	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	F I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Cl I
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Cl I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	Pb I
\mathbf{B}_6	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	Pb I

References

- [1] N. Pasero and N. Perchiazzi, *Crystal structure refinement of matlockite*, Mineral. Mag. **60**, 833–836 (1996), doi:10.1180/minmag.1996.060.402.15.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).