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

This structure previously used the label(s) `ABC_tP6_129_c_a_c`. Calls to these addresses will be redirected here.

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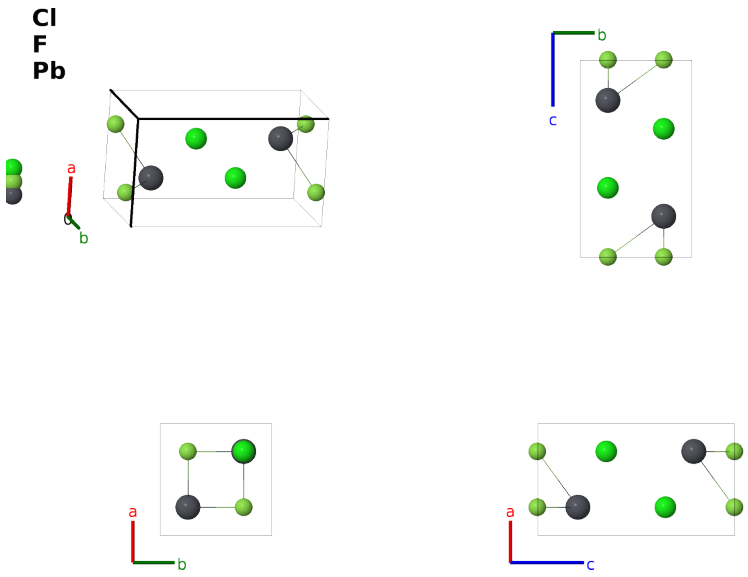
https://aflow.org/prototype-encyclopedia/0VRY

https://aflow.org/prototype-encyclopedia/ABC_tP6_129_c_a_c-001



Prototype	ClFPb
AFLOW prototype label	ABC_tP6_129_c_a_c-001
***Strukturbericht* designation**	$E0_1$
Mineral name	matlockite
ICSD	82884
CCDC	1642941
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=ABC_tP6_129_c_a_c-001 --params=`$a, c/a, z_2, z_3$

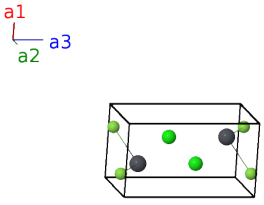
Other compounds with this structure

AlMnGe, AmOI, AmSbTe, AsBeLi, AsCoLi, AsCrLi, AsCuMn, AsFeLi, AsMgNa, AsMnNa, AsNiRh, AsSiSb, AsSiTa, AsVMn, AsZnNa, BaFCl, BaHCl, BaMnGe, BiMgNa, BiCaK, BiMnK, BiMnNa, BiOF, BiZnNa, BrOGd, BrOLa, BrONd, BrOPu, BrOSm, CeClTe, CeFS, CeMnGe, CeMnSi, CeSbSe, CeSbTe, CeTiGe, CoGdSi, CsNaS, CsNaSe, CsNaTe, CuFeAs, DyFeSi, DyScSb, DyTiGe, DyTiSi, ErFS, ErTiGe, ErTiSi, EsOCl, EuFCl, EuHCl, FeCuTe, FeLiAs, FeMnAs, GaMnGe, GdBiTe, GdFS, GdMnSi, GdSbTe, GdScSb, GdTiGe, GdTiSi, GeMnGe, GeMnNd, HfGeS, HfGeSe, HfGeTe, HfSiS, HfSiSe, HfSiTe, HfVSi, HoFS, HoGeTi, HoTiSi, KAgSe, KLiSe, KLiTe, KMgAs, KMgP, KMgSb, KNaO, LaBiTe, LaClTe, LaFS, LaFSe, LaGeMn, LaGeTi, LaMnSi, LaSbTe, LiBeP, LiFeP, LuGeTi, LuTiSi, MgAgSb, MgCoGe, MgCuAs, MgSbAg, MoKNa, MnCuSb, NaAlGe, NaAlSi, NaFeAs, NaLiS, NaMgSb, NaMnP, NaMnSb, NaZnSb, NdClTe, NdFS, NdFSe, NdFTe, NdMnSi, NdOCl, NdSbTe, NdTiGe, NpAsS, NpAsSe, NpAsTe, NpOS, NpSbTe, PAsU, PbClF, PdNiGe, PrClTe, PrCoSi, PrFS, PrMnGe, PrMnSi, PrOCl, PrSbTe, PrTiGe, PuOCl, PuOIO, PuSbTe, RbNaS, SbFeZn, SbGeTi, SbGeZr, SbMnZn, SbScTb, SeGeZr, SiFeTb, SiMnSm, SiMnTb, SiMnY, SiTiTb, SmCoSi, SmFCl, SmFS, SmSbTe, SmTiGe, SnMnSr, SrFCl, SrHCl, SrHI, TbSF, TbTiGe, ThAsS, ThAsSe, ThAsTe, ThBiTe, ThOS, ThPS, ThPSe, ThSbSe, ThSbTe, TmTiGe, UAsS, UAsSe, UAsTe, UBiTe, UGeS, UNTe, UOS, UPS, UPSe, USSb, USSi, USbAs, USbSe, USbTe, USnTe, YFS, YOCl, YTiGe, YTiSi, YbFCl, ZrGeS, ZrGeTe, ZrOSiO, ZrSiS, ZrSiSe, ZrSiTe, ZrSnTe, ZrVSi

- Matlockite ($E0_1$) and PrOI have the same AFLOW prototype label, ABC_tP6_c_a_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Indeed, (Potapova, 1977) state that PrOI is a Matlockite structure, but both AFLOW and the ICSD agree that they are different enough to warrant listing them as separate prototypes.
- In both cases we have $z_3 \approx -z_2$. We somewhat arbitrarily assign structures with the $\min(z_2,z_3) < 0.199$ to the PrOI structure and those with larger values to the Matlockite structure.
- We have attempted to organize the similar compounds so that the central atom is on the (4a) site. This means that some compounds will appear twice, *e.g.*, PbFCl and PbClF.
- Binary forms of Matlockite/PrOI occur when the species on the (2a) site is the same as one of the species on the (2c) sites. We assign these structures to the prototypes:
  - Cu_2Sb ($C38$) for structures with c/a < 2,
  - UP_2 for structures with $2 <$ c/a < 3, and
  - $LaSe_{1.85}$ for structures with c/a ≈ 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
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(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).

First cited in

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