A hybrid fluoride layered perovskite, $(enH_2)MnF_4$

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Supplementary Information

Table S3. ISODISTORT mode decomposition for $(enH_2)MnF_4$ at 93 K.

ISODISTORT: modes details

Parent structure (123 P4/mmm)

a=4.23500, b=4.23500, c=8.16000, alpha=90.00000, beta=90.00000, gamma=90.00000

atom	site	x	y	z	occ
Mn1	1a	0.00000	0.00000	0.00000	1.00000
F1	2f	0.00000	0.50000	0.00000	1.00000
F2	2g	0.00000	0.00000	0.25700	1.00000

Subgroup details

14 P2_1/c, basis={(0,0,1),(1,1,0),(-1,1,0)}, origin=(0,0,1/2), s=2, i=8

Undistorted superstructure

a=8.16000, b=5.98919, c=5.98919, alpha=90.00000, beta=90.00000, gamma=90.00000

atom	site	x	y	z	occ	displ
Mn1	2b	0.50000	0.50000	0.50000	1.00000	0.00000
F1	4e	0.50000	0.75000	0.75000	1.00000	0.00000
F2	4e	0.75700	0.50000	0.50000	1.00000	0.00000

Distorted superstructure

a=8.17349, b=5.98682, c=5.96372, alpha=90.00000, beta=90.28722, gamma=90.00000

atom	site	x	y	z	occ	displ
Mn1	2b	0.50000	0.50000	0.50000	1.00000	0.00000
F1	4e	0.52763	0.78515	0.71488	1.00000	0.37367
F2	4e	0.75458	0.45781	0.53033	1.00000	0.31136

Displacive mode definitions

atom	x	y	z	dx	dy	dz
P4/mmm[0,0,0]GM1+(a)[F2:g:dsp]A1(a) normfactor = 0.06127						
F2	0.75700	0.50000	0.50000	1.0000	0.0000	0.0000

P4/mmm[0,0,0]GM5+(a,a)[F2:g:dsp]E(a) normfactor = 0.08348

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F2    0.75700  0.50000  0.50000  0.0000  0.0000 -1.0000

P4/mmm[1/2,1/2,0]M2+(a)[F1:f:dsp]B2u(a) normfactor = 0.05903
F1    0.50000  0.75000  0.75000  0.0000 -1.0000 -1.0000

P4/mmm[1/2,1/2,0]M3+(a)[F1:f:dsp]B3u(a) normfactor = 0.05903
F1    0.50000  0.75000  0.75000  0.0000 -1.0000  1.0000

P4/mmm[1/2,1/2,0]M5+(0,a)[F1:f:dsp]B1u(a) normfactor = 0.06127
F1    0.50000  0.75000  0.75000  1.0000  0.0000  0.0000

P4/mmm[1/2,1/2,0]M5+(0,a)[F2:g:dsp]E(a) normfactor = 0.08348
F2    0.75700  0.50000  0.50000  0.0000 -1.0000  0.0000
```

Displacive mode amplitudes

mode	**As**	**Ap**	**dmax**
[0,0,0]GM1+[F2:g:dsp]A1(a)	-0.03949	-0.02792	0.01975
[0,0,0]GM1+ all	0.03949	0.02792	
[0,0,0]GM5+[F2:g:dsp]E(a)	-0.36330	-0.25689	0.18165
[0,0,0]GM5+ all	0.36330	0.25689	
[1/2,1/2,0]M2+[F1:f:dsp]B2u(a)	-0.00025	-0.00018	0.00013
[1/2,1/2,0]M2+ all	0.00025	0.00018	
[1/2,1/2,0]M3+[F1:f:dsp]B3u(a)	-0.59519	-0.42086	0.29760
[1/2,1/2,0]M3+ all	0.59519	0.42086	
[1/2,1/2,0]M5+[F1:f:dsp]B1u(a)	0.45092	0.31885	0.22546
[1/2,1/2,0]M5+[F2:g:dsp]E(a)	0.50537	0.35735	0.25269
[1/2,1/2,0]M5+ all	0.67729	0.47892	
Overall	0.97290	0.68794	

Parent-cell strain mode definitions

```
    e1      e2      e3      e4      e5      e6
P4/mmm[0,0,0]GM1+(a)strain_1(a) normfactor = 0.70711
  1.0000  1.0000  0.0000  0.0000  0.0000  0.0000
P4/mmm[0,0,0]GM1+(a)strain_2(a) normfactor = 1.00000
  0.0000  0.0000  1.0000  0.0000  0.0000  0.0000
P4/mmm[0,0,0]GM4+(a)strain(a) normfactor = 1.41421
  0.0000  0.0000  0.0000  0.0000  0.0000  1.0000
P4/mmm[0,0,0]GM5+(a,a)strain(a) normfactor = 1.00000
  0.0000  0.0000  0.0000  1.0000 -1.0000  0.0000
```

Parent-cell strain mode amplitudes

mode	**amplitude**
[0,0,0]GM1+strain_1(a)	-0.00329
[0,0,0]GM1+strain_2(a)	0.00165
[0,0,0]GM4+strain(a)	0.00273
[0,0,0]GM5+strain(a)	-0.00354

Table S4. ISODISTORT derivatives of $TlAlF_4$ aristotype (*P*4/*mmm*), based on all combinations of M_3^+, M_5^+ and X_3^+ tilt modes.

M3+ only

P1 (a) 127 P4/mbm, basis={(1,1,0),(-1,1,0),(0,0,1)}, origin=(0,0,0), s=2, i=2, k-active= (1/2,1/2,0)

M5+ only

P1 (a,0) 53 Pmna, basis={(1,1,0),(0,0,1),(1,-1,0)}, origin=(0,0,0), s=2, i=4, k-active= (1/2,1/2,0)

P3 (a,a) 67 Cmma, basis={(2,0,0),(0,2,0),(0,0,1)}, origin=(1/2,1/2,0), s=2, i=4, k-active= (1/2,1/2,0)

C1 (a,b) 13 P2/c, basis={(-1,1,0),(0,0,1),(2,0,0)}, origin=(0,0,0), s=2, i=8, k-active= (1/2,1/2,0)

X3+ only

P1 (a;-a) 129 P4/nmm, basis={(2,0,0),(0,2,0),(0,0,1)}, origin=(1,0,0), s=4, i=4, k-active= (0,1/2,0),(1/2,0,0)

P3 (0;a) 51 Pmma, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,0,0), s=2, i=4, k-active= (1/2,0,0)

C1 (a;b) 59 Pmmn, basis={(2,0,0),(0,2,0),(0,0,1)}, origin=(0,0,0), s=4, i=8, k-active= (0,1/2,0),(1/2,0,0)

M3+ and M5+

P1(1)P3(1) (a|b,b) 12 C2/m, basis={(0,-2,0),(2,0,0),(0,0,1)}, origin=(1/2,-1/2,0), s=2, i=8, k-active= (1/2,1/2,0);(1/2,1/2,0)

P1(1)P1(1) (a|b,0) 14 P2_1/c, basis={(0,0,1),(1,-1,0),(1,1,0)}, origin=(0,0,0), s=2, i=8, k-active= (1/2,1/2,0);(1/2,1/2,0)

P1(1)C1(1) (a|b,c) 2 P-1, basis={(1,1,0),(-1,1,0),(0,0,1)}, origin=(0,0,0), s=2, i=16, k-active= (1/2,1/2,0);(1/2,1/2,0)

M3+ and X3+

P1(1)C1(1) (a|b;c) 59 Pmmn, basis={(2,0,0),(0,2,0),(0,0,1)}, origin=(0,0,0), s=4, i=8, k-active= (1/2,1/2,0);(0,1/2,0),(1/2,0,0)

M5+ and X3+

P3(1)P3(1) (a,a|0;b) 51 Pmma, basis={(2,0,0),(0,2,0),(0,0,1)}, origin=(0,0,0), s=4, i=8, k-active= (1/2,1/2,0);(1/2,0,0)

P3(1)P3(2) (a,a|b;0) 57 Pbcm, basis={(0,0,1),(0,2,0),(-2,0,0)}, origin=(0,0,0), s=4, i=8, k-active= (1/2,1/2,0);(0,1/2,0)

C1(1)P3(1) (a,b|0;c) 13 P2/c, basis={(0,2,0),(0,0,1),(2,0,0)}, origin=(0,0,0), s=4, i=16, k-active= (1/2,1/2,0);(1/2,0,0)

 P1(1)P1(1) (a,0|b;-b) 12 C2/m, basis={(2,-2,0),(2,2,0),(0,0,1)}, origin=(0,0,0), s=4, i=16, k-active= (1/2,1/2,0);(0,1/2,0),(1/2,0,0)

 P3(1)C1(1) (a,a|b;c) 11 P2_1/m, basis={(0,0,-1),(-2,0,0),(0,2,0)}, origin=(0,0,0), s=4, i=16, k-active= (1/2,1/2,0);(0,1/2,0),(1/2,0,0)

 C1(1)C1(1) (a,b|c;d) 2 P-1, basis={(0,0,1),(0,2,0),(-2,0,0)}, origin=(0,0,0), s=4, i=32, k-active= (1/2,1/2,0);(0,1/2,0),(1/2,0,0)