

ISODISTORT SUITE HELP

## ISODISTORT: modes details

### Parent structure (139 I4/mmm)

a=5.60000, b=5.60000, c=21.59000, alpha=90.00000, beta=90.00000, gamma=90.00000

atom	site	x	y	z	occ
Pb	2a	0.00000	0.00000	0.00000	1.00000
Cl1	4c	0.00000	0.50000	0.00000	1.00000
Cl2	4e	0.00000	0.00000	0.12970	1.00000

### Subgroup details

19 P2<sub>12</sub>-12<sub>1</sub>, basis={(1,1,0),(0,0,1),(3,-3,0)}, origin=(0,0,0), s=12, i=48

### Undistorted superstructure

a=7.91960, b=21.59000, c=23.75879, alpha=90.00000, beta=90.00000, gamma=90.00000

atom	site	x	y	z	occ	displ
Pb3	4a	0.00000	0.50000	0.50000	1.00000	0.00000
Pb1	4a	0.50000	0.50000	0.66667	1.00000	0.00000
Pb2	4a	0.00000	0.50000	0.83333	1.00000	0.00000
Cl7	4a	0.75000	0.50000	0.58333	1.00000	0.00000
Cl6	4a	0.75000	0.50000	0.75000	1.00000	0.00000
Cl11	4a	0.75000	0.50000	0.91667	1.00000	0.00000
Cl2	4a	0.25000	0.50000	0.58333	1.00000	0.00000
Cl4	4a	0.25000	0.50000	0.91667	1.00000	0.00000
Cl1	4a	0.25000	0.50000	0.75000	1.00000	0.00000
Cl5	4a	0.00000	0.62970	0.50000	1.00000	0.00000
Cl12	4a	0.50000	0.37030	0.66667	1.00000	0.00000
Cl3	4a	0.00000	0.62970	0.83333	1.00000	0.00000
Cl9	4a	0.00000	0.37030	0.83333	1.00000	0.00000
Cl8	4a	0.00000	0.37030	0.50000	1.00000	0.00000
Cl10	4a	0.50000	0.62970	0.66667	1.00000	0.00000

### Distorted superstructure

a=8.31300, b=21.42592, c=21.95900, alpha=90.00000, beta=90.00000, gamma=90.00000

atom	site	x	y	z	occ	displ
Pb3	4a	-0.00945	0.49675	0.46119	1.00000	0.85867
Pb1	4a	0.50835	0.48563	0.62787	1.00000	0.90852
Pb2	4a	-0.00833	0.48856	0.79476	1.00000	0.88450
Cl7	4a	0.82140	0.48596	0.57150	1.00000	0.71436
Cl6	4a	0.67930	0.48510	0.73810	1.00000	0.71807
Cl11	4a	0.82140	0.49980	0.90490	1.00000	0.64736
Cl2	4a	0.26380	0.48866	0.53460	1.00000	1.10335
Cl4	4a	0.26460	0.49420	0.86920	1.00000	1.05669
Cl1	4a	0.23650	0.48362	0.70219	1.00000	1.11264
Cl5	4a	-0.01830	0.63090	0.47060	1.00000	0.66377
Cl12	4a	0.51910	0.35312	0.62860	1.00000	0.92706
Cl3	4a	-0.01700	0.62202	0.78806	1.00000	1.01754
Cl9	4a	-0.01880	0.35567	0.80480	1.00000	0.71782
Cl8	4a	-0.01820	0.36429	0.45279	1.00000	1.05555
Cl10	4a	0.51670	0.62010	0.62888	1.00000	0.86607

### Displacive mode definitions

atom	x	y	z	dx	dy	dz
------	---	---	---	----	----	----

I4/mmm[0,0,0]GM1+(a)[C12:e:dsp]A1(a) normfactor = 0.00945

C15	0.00000	0.62970	0.50000	0.0000	1.0000	0.0000
C112	0.50000	0.37030	0.66667	0.0000	-1.0000	0.0000
C13	0.00000	0.62970	0.83333	0.0000	1.0000	0.0000
C19	0.00000	0.37030	0.83333	0.0000	-1.0000	0.0000
C18	0.00000	0.37030	0.50000	0.0000	-1.0000	0.0000
C110	0.50000	0.62970	0.66667	0.0000	1.0000	0.0000

I4/mmm[0,0,0]GM4-(a)[C11:c:dsp]B1u(a) normfactor = 0.00945

C17	0.75000	0.50000	0.58333	0.0000	1.0000	0.0000
C16	0.75000	0.50000	0.75000	0.0000	-1.0000	0.0000
C111	0.75000	0.50000	0.91667	0.0000	1.0000	0.0000
C12	0.25000	0.50000	0.58333	0.0000	-1.0000	0.0000
C14	0.25000	0.50000	0.91667	0.0000	-1.0000	0.0000
C11	0.25000	0.50000	0.75000	0.0000	1.0000	0.0000

I4/mmm[1/6,1/6,0]DT2(0,0;0,a)[Pb:a:dsp]Eu(a) normfactor = 0.05155

Pb3	0.00000	0.50000	0.50000	-1.0000	0.0000	0.0000
Pb1	0.50000	0.50000	0.66667	-0.5000	0.0000	0.0000
Pb2	0.00000	0.50000	0.83333	0.5000	0.0000	0.0000

I4/mmm[1/6,1/6,0]DT2(0,0;0,a)[C11:c:dsp]B3u(a) normfactor = 0.02232

C17	0.75000	0.50000	0.58333	-1.0000	0.0000	-0.3333
C16	0.75000	0.50000	0.75000	0.0000	0.0000	-0.0000
C111	0.75000	0.50000	0.91667	1.0000	0.0000	0.3333
C12	0.25000	0.50000	0.58333	-1.0000	0.0000	0.3333
C14	0.25000	0.50000	0.91667	1.0000	0.0000	-0.3333
C11	0.25000	0.50000	0.75000	0.0000	0.0000	0.0000

I4/mmm[1/6,1/6,0]DT2(0,0;0,a)[C11:c:dsp]B2u(a) normfactor = 0.02232

C17	0.75000	0.50000	0.58333	1.0000	0.0000	-0.3333
C16	0.75000	0.50000	0.75000	-0.0000	0.0000	-0.0000
C111	0.75000	0.50000	0.91667	-1.0000	0.0000	0.3333
C12	0.25000	0.50000	0.58333	1.0000	0.0000	0.3333
C14	0.25000	0.50000	0.91667	-1.0000	0.0000	-0.3333
C11	0.25000	0.50000	0.75000	-0.0000	0.0000	0.0000

I4/mmm[1/6,1/6,0]DT2(0,0;0,a)[C12:e:dsp]E(a) normfactor = 0.03645

C15	0.00000	0.62970	0.50000	-1.0000	0.0000	0.0000
C112	0.50000	0.37030	0.66667	-0.5000	0.0000	0.0000
C13	0.00000	0.62970	0.83333	0.5000	0.0000	0.0000
C19	0.00000	0.37030	0.83333	0.5000	0.0000	0.0000
C18	0.00000	0.37030	0.50000	-1.0000	0.0000	0.0000
C110	0.50000	0.62970	0.66667	-0.5000	0.0000	0.0000

I4/mmm[1/6,1/6,0]DT3(0,0;0,a)[Pb:a:dsp]A2u(a) normfactor = 0.01638

Pb3	0.00000	0.50000	0.50000	0.0000	0.0000	0.0000
Pb1	0.50000	0.50000	0.66667	0.0000	-1.0000	0.0000
Pb2	0.00000	0.50000	0.83333	0.0000	-1.0000	0.0000

I4/mmm[1/6,1/6,0]DT3(0,0;0,a)[C11:c:dsp]B1u(a) normfactor = 0.01337

C17	0.75000	0.50000	0.58333	0.0000	-0.5000	0.0000
C16	0.75000	0.50000	0.75000	0.0000	-1.0000	0.0000
C111	0.75000	0.50000	0.91667	0.0000	-0.5000	0.0000
C12	0.25000	0.50000	0.58333	0.0000	-0.5000	0.0000
C14	0.25000	0.50000	0.91667	0.0000	-0.5000	0.0000
C11	0.25000	0.50000	0.75000	0.0000	-1.0000	0.0000

I4/mmm[1/6,1/6,0]DT3(0,0;a)[C12:e:dsp]A1(a) normfactor = 0.01158  
 C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 -1.0000 0.0000  
 C13 0.00000 0.62970 0.83333 0.0000 -1.0000 0.0000  
 C19 0.00000 0.37030 0.83333 0.0000 -1.0000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 -1.0000 0.0000

I4/mmm[1/6,1/6,0]DT3(0,0;a)[C12:e:dsp]E(a) normfactor = 0.01215  
 C15 0.00000 0.62970 0.50000 0.0000 0.0000 1.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 -0.5000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 -0.5000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 0.5000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 -1.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 0.5000

I4/mmm[1/3,1/3,0]DT1(0,0;a,0)[Pb:a:dsp]Eu(a) normfactor = 0.01488  
 Pb3 0.00000 0.50000 0.50000 0.0000 0.0000 0.0000  
 Pb1 0.50000 0.50000 0.66667 0.0000 0.0000 1.0000  
 Pb2 0.00000 0.50000 0.83333 0.0000 0.0000 -1.0000

I4/mmm[1/3,1/3,0]DT1(0,0;a,0)[C11:c:dsp]B3u(a) normfactor = 0.02232  
 C17 0.75000 0.50000 0.58333 1.0000 0.0000 0.3333  
 C16 0.75000 0.50000 0.75000 0.0000 0.0000 -0.0000  
 C111 0.75000 0.50000 0.91667 -1.0000 0.0000 -0.3333  
 C12 0.25000 0.50000 0.58333 -1.0000 0.0000 0.3333  
 C14 0.25000 0.50000 0.91667 1.0000 0.0000 -0.3333  
 C11 0.25000 0.50000 0.75000 -0.0000 0.0000 -0.0000

I4/mmm[1/3,1/3,0]DT1(0,0;a,0)[C11:c:dsp]B2u(a) normfactor = 0.02232  
 C17 0.75000 0.50000 0.58333 -1.0000 0.0000 0.3333  
 C16 0.75000 0.50000 0.75000 -0.0000 0.0000 -0.0000  
 C111 0.75000 0.50000 0.91667 1.0000 0.0000 -0.3333  
 C12 0.25000 0.50000 0.58333 1.0000 0.0000 0.3333  
 C14 0.25000 0.50000 0.91667 -1.0000 0.0000 -0.3333  
 C11 0.25000 0.50000 0.75000 0.0000 0.0000 -0.0000

I4/mmm[1/3,1/3,0]DT1(0,0;a,0)[C12:e:dsp]A1(a) normfactor = 0.01337  
 C15 0.00000 0.62970 0.50000 0.0000 1.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.5000 0.0000  
 C13 0.00000 0.62970 0.83333 0.0000 -0.5000 0.0000  
 C19 0.00000 0.37030 0.83333 0.0000 0.5000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 -1.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 -0.5000 0.0000

I4/mmm[1/3,1/3,0]DT1(0,0;a,0)[C12:e:dsp]E(a) normfactor = 0.01052  
 C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 1.0000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 -1.0000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 -1.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 1.0000

I4/mmm[1/3,1/3,0]DT4(0,0;a,0)[C11:c:dsp]B1u(a) normfactor = 0.01337  
 C17 0.75000 0.50000 0.58333 0.0000 -0.5000 0.0000  
 C16 0.75000 0.50000 0.75000 0.0000 -1.0000 0.0000  
 C111 0.75000 0.50000 0.91667 0.0000 -0.5000 0.0000  
 C12 0.25000 0.50000 0.58333 0.0000 0.5000 0.0000

C14 0.25000 0.50000 0.91667 0.0000 0.5000 0.0000  
 C11 0.25000 0.50000 0.75000 0.0000 1.0000 0.0000

I4/mmm[1/3,1/3,0]DT4(0,0;a,0)[C12:e:dsp]E(a) normfactor = 0.03157

C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 1.0000 0.0000 0.0000  
 C13 0.00000 0.62970 0.83333 1.0000 0.0000 0.0000  
 C19 0.00000 0.37030 0.83333 -1.0000 0.0000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 -1.0000 0.0000 0.0000

I4/mmm[1/2,1/2,0]X2+(a;0)[C11:c:dsp]B3u(a) normfactor = 0.01823

C17 0.75000 0.50000 0.58333 -1.0000 0.0000 -0.3333  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 -0.3333  
 C111 0.75000 0.50000 0.91667 -1.0000 0.0000 -0.3333  
 C12 0.25000 0.50000 0.58333 -1.0000 0.0000 0.3333  
 C14 0.25000 0.50000 0.91667 -1.0000 0.0000 0.3333  
 C11 0.25000 0.50000 0.75000 1.0000 0.0000 0.3333

I4/mmm[1/2,1/2,0]X2+(a;0)[C11:c:dsp]B2u(a) normfactor = 0.01823

C17 0.75000 0.50000 0.58333 -1.0000 0.0000 0.3333  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 0.3333  
 C111 0.75000 0.50000 0.91667 -1.0000 0.0000 0.3333  
 C12 0.25000 0.50000 0.58333 -1.0000 0.0000 -0.3333  
 C14 0.25000 0.50000 0.91667 -1.0000 0.0000 -0.3333  
 C11 0.25000 0.50000 0.75000 1.0000 0.0000 -0.3333

I4/mmm[1/2,1/2,0]X3+(0;a)[C11:c:dsp]B1u(a) normfactor = 0.00945

C17 0.75000 0.50000 0.58333 0.0000 1.0000 0.0000  
 C16 0.75000 0.50000 0.75000 0.0000 -1.0000 0.0000  
 C111 0.75000 0.50000 0.91667 0.0000 1.0000 0.0000  
 C12 0.25000 0.50000 0.58333 0.0000 1.0000 0.0000  
 C14 0.25000 0.50000 0.91667 0.0000 1.0000 0.0000  
 C11 0.25000 0.50000 0.75000 0.0000 -1.0000 0.0000

I4/mmm[1/2,1/2,0]X3+(0;a)[C12:e:dsp]E(a) normfactor = 0.00859

C15 0.00000 0.62970 0.50000 0.0000 0.0000 1.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 1.0000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 1.0000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 -1.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 -1.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 -1.0000

I4/mmm[1/2,1/2,0]X2-(a;0)[Pb:a:dsp]A2u(a) normfactor = 0.01337

Pb3 0.00000 0.50000 0.50000 0.0000 1.0000 0.0000  
 Pb1 0.50000 0.50000 0.66667 0.0000 -1.0000 0.0000  
 Pb2 0.00000 0.50000 0.83333 0.0000 1.0000 0.0000

I4/mmm[1/2,1/2,0]X2-(a;0)[C12:e:dsp]A1(a) normfactor = 0.00945

C15 0.00000 0.62970 0.50000 0.0000 1.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 -1.0000 0.0000  
 C13 0.00000 0.62970 0.83333 0.0000 1.0000 0.0000  
 C19 0.00000 0.37030 0.83333 0.0000 1.0000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 1.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 -1.0000 0.0000

I4/mmm[1/2,1/2,0]X3-(0;a)[Pb:a:dsp]Eu(a) normfactor = 0.03645

Pb3 0.00000 0.50000 0.50000 -1.0000 0.0000 0.0000

Pb1 0.50000 0.50000 0.66667 1.0000 0.0000 0.0000  
 Pb2 0.00000 0.50000 0.83333 -1.0000 0.0000 0.0000

I4/mmm[1/2,1/2,0]X3-(0;a)[C12:e:dsp]E(a) normfactor = 0.02577

C15 0.00000 0.62970 0.50000 -1.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 1.0000 0.0000 0.0000  
 C13 0.00000 0.62970 0.83333 -1.0000 0.0000 0.0000  
 C19 0.00000 0.37030 0.83333 -1.0000 0.0000 0.0000  
 C18 0.00000 0.37030 0.50000 -1.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 1.0000 0.0000 0.0000

I4/mmm[1,1,1]M5+(0,a)[C12:e:dsp]E(a) normfactor = 0.02577

C15 0.00000 0.62970 0.50000 -1.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 1.0000 0.0000 0.0000  
 C13 0.00000 0.62970 0.83333 -1.0000 0.0000 0.0000  
 C19 0.00000 0.37030 0.83333 1.0000 0.0000 0.0000  
 C18 0.00000 0.37030 0.50000 1.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 -1.0000 0.0000 0.0000

I4/mmm[1,1,1]M5-(a,0)[Pb:a:dsp]Eu(a) normfactor = 0.01215

Pb3 0.00000 0.50000 0.50000 0.0000 0.0000 -1.0000  
 Pb1 0.50000 0.50000 0.66667 0.0000 0.0000 -1.0000  
 Pb2 0.00000 0.50000 0.83333 0.0000 0.0000 -1.0000

I4/mmm[1,1,1]M5-(a,0)[C11:c:dsp]B3u(a) normfactor = 0.01823

C17 0.75000 0.50000 0.58333 -1.0000 0.0000 -0.3333  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 -0.3333  
 C111 0.75000 0.50000 0.91667 -1.0000 0.0000 -0.3333  
 C12 0.25000 0.50000 0.58333 1.0000 0.0000 -0.3333  
 C14 0.25000 0.50000 0.91667 1.0000 0.0000 -0.3333  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 -0.3333

I4/mmm[1,1,1]M5-(a,0)[C11:c:dsp]B2u(a) normfactor = 0.01823

C17 0.75000 0.50000 0.58333 -1.0000 0.0000 0.3333  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 0.3333  
 C111 0.75000 0.50000 0.91667 -1.0000 0.0000 0.3333  
 C12 0.25000 0.50000 0.58333 1.0000 0.0000 0.3333  
 C14 0.25000 0.50000 0.91667 1.0000 0.0000 0.3333  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 0.3333

I4/mmm[1,1,1]M5-(a,0)[C12:e:dsp]E(a) normfactor = 0.00859

C15 0.00000 0.62970 0.50000 0.0000 0.0000 -1.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 -1.0000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 -1.0000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 -1.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 -1.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 -1.0000

I4/mmm[1/6,5/6,0]Y2(a,0;0,0)[Pb:a:dsp]Eu(a) normfactor = 0.04464

Pb3 0.00000 0.50000 0.50000 0.0000 0.0000 0.0000  
 Pb1 0.50000 0.50000 0.66667 1.0000 0.0000 0.0000  
 Pb2 0.00000 0.50000 0.83333 1.0000 0.0000 0.0000

I4/mmm[1/6,5/6,0]Y2(a,0;0,0)[C11:c:dsp]B3u(a) normfactor = 0.02577

C17 0.75000 0.50000 0.58333 -0.5000 0.0000 -0.1667  
 C16 0.75000 0.50000 0.75000 -1.0000 0.0000 0.3333  
 C111 0.75000 0.50000 0.91667 -0.5000 0.0000 -0.1667  
 C12 0.25000 0.50000 0.58333 -0.5000 0.0000 0.1667

C14 0.25000 0.50000 0.91667 -0.5000 0.0000 0.1667  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 -0.3333

I4/mmm[1/6,5/6,0]Y2(a,0;0,0)[C11:c:dsp]B2u(a) normfactor = 0.02577  
 C17 0.75000 0.50000 0.58333 -0.5000 0.0000 0.1667  
 C16 0.75000 0.50000 0.75000 -1.0000 0.0000 -0.3333  
 C111 0.75000 0.50000 0.91667 -0.5000 0.0000 0.1667  
 C12 0.25000 0.50000 0.58333 -0.5000 0.0000 -0.1667  
 C14 0.25000 0.50000 0.91667 -0.5000 0.0000 -0.1667  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 0.3333

I4/mmm[1/6,5/6,0]Y2(a,0;0,0)[C12:e:dsp]E(a) normfactor = 0.03157  
 C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 1.0000 0.0000 0.0000  
 C13 0.00000 0.62970 0.83333 1.0000 0.0000 0.0000  
 C19 0.00000 0.37030 0.83333 1.0000 0.0000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 1.0000 0.0000 0.0000

I4/mmm[1/6,5/6,0]Y3(a,0;0,0)[Pb:a:dsp]A2u(a) normfactor = 0.01891  
 Pb3 0.00000 0.50000 0.50000 0.0000 1.0000 0.0000  
 Pb1 0.50000 0.50000 0.66667 0.0000 0.5000 0.0000  
 Pb2 0.00000 0.50000 0.83333 0.0000 -0.5000 0.0000

I4/mmm[1/6,5/6,0]Y3(a,0;0,0)[C11:c:dsp]B1u(a) normfactor = 0.01158  
 C17 0.75000 0.50000 0.58333 0.0000 1.0000 0.0000  
 C16 0.75000 0.50000 0.75000 0.0000 -0.0000 0.0000  
 C111 0.75000 0.50000 0.91667 0.0000 -1.0000 0.0000  
 C12 0.25000 0.50000 0.58333 0.0000 1.0000 0.0000  
 C14 0.25000 0.50000 0.91667 0.0000 -1.0000 0.0000  
 C11 0.25000 0.50000 0.75000 0.0000 0.0000 0.0000

I4/mmm[1/6,5/6,0]Y3(a,0;0,0)[C12:e:dsp]A1(a) normfactor = 0.01337  
 C15 0.00000 0.62970 0.50000 0.0000 1.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.5000 0.0000  
 C13 0.00000 0.62970 0.83333 0.0000 -0.5000 0.0000  
 C19 0.00000 0.37030 0.83333 0.0000 -0.5000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 1.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.5000 0.0000

I4/mmm[1/6,5/6,0]Y3(a,0;0,0)[C12:e:dsp]E(a) normfactor = 0.01052  
 C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 -1.0000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 1.0000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 -1.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 1.0000

I4/mmm[1/3,2/3,0]Y1(0,a;0,0)[Pb:a:dsp]Eu(a) normfactor = 0.01718  
 Pb3 0.00000 0.50000 0.50000 0.0000 0.0000 -1.0000  
 Pb1 0.50000 0.50000 0.66667 0.0000 0.0000 0.5000  
 Pb2 0.00000 0.50000 0.83333 0.0000 0.0000 0.5000

I4/mmm[1/3,2/3,0]Y1(0,a;0,0)[C11:c:dsp]B3u(a) normfactor = 0.02577  
 C17 0.75000 0.50000 0.58333 0.5000 0.0000 0.1667  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 -0.3333  
 C111 0.75000 0.50000 0.91667 0.5000 0.0000 0.1667  
 C12 0.25000 0.50000 0.58333 -0.5000 0.0000 0.1667

C14 0.25000 0.50000 0.91667 -0.5000 0.0000 0.1667  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 -0.3333

I4/mmm[1/3,2/3,0]Y1(0,a;0,0)[C11:c:dsp]B2u(a) normfactor = 0.02577

C17 0.75000 0.50000 0.58333 0.5000 0.0000 -0.1667  
 C16 0.75000 0.50000 0.75000 1.0000 0.0000 0.3333  
 C111 0.75000 0.50000 0.91667 0.5000 0.0000 -0.1667  
 C12 0.25000 0.50000 0.58333 -0.5000 0.0000 -0.1667  
 C14 0.25000 0.50000 0.91667 -0.5000 0.0000 -0.1667  
 C11 0.25000 0.50000 0.75000 -1.0000 0.0000 0.3333

I4/mmm[1/3,2/3,0]Y1(0,a;0,0)[C12:e:dsp]A1(a) normfactor = 0.01158

C15 0.00000 0.62970 0.50000 0.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 0.0000 -1.0000 0.0000  
 C13 0.00000 0.62970 0.83333 0.0000 -1.0000 0.0000  
 C19 0.00000 0.37030 0.83333 0.0000 1.0000 0.0000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.0000 1.0000 0.0000

I4/mmm[1/3,2/3,0]Y1(0,a;0,0)[C12:e:dsp]E(a) normfactor = 0.01215

C15 0.00000 0.62970 0.50000 0.0000 0.0000 -1.0000  
 C112 0.50000 0.37030 0.66667 0.0000 0.0000 0.5000  
 C13 0.00000 0.62970 0.83333 0.0000 0.0000 0.5000  
 C19 0.00000 0.37030 0.83333 0.0000 0.0000 0.5000  
 C18 0.00000 0.37030 0.50000 0.0000 0.0000 -1.0000  
 C110 0.50000 0.62970 0.66667 0.0000 0.0000 0.5000

I4/mmm[1/3,2/3,0]Y4(0,a;0,0)[C11:c:dsp]B1u(a) normfactor = 0.01158

C17 0.75000 0.50000 0.58333 0.0000 1.0000 0.0000  
 C16 0.75000 0.50000 0.75000 0.0000 -0.0000 0.0000  
 C111 0.75000 0.50000 0.91667 0.0000 -1.0000 0.0000  
 C12 0.25000 0.50000 0.58333 0.0000 -1.0000 0.0000  
 C14 0.25000 0.50000 0.91667 0.0000 1.0000 0.0000  
 C11 0.25000 0.50000 0.75000 0.0000 0.0000 0.0000

I4/mmm[1/3,2/3,0]Y4(0,a;0,0)[C12:e:dsp]E(a) normfactor = 0.03645

C15 0.00000 0.62970 0.50000 -1.0000 0.0000 0.0000  
 C112 0.50000 0.37030 0.66667 -0.5000 0.0000 0.0000  
 C13 0.00000 0.62970 0.83333 0.5000 0.0000 0.0000  
 C19 0.00000 0.37030 0.83333 -0.5000 0.0000 0.0000  
 C18 0.00000 0.37030 0.50000 1.0000 0.0000 0.0000  
 C110 0.50000 0.62970 0.66667 0.5000 0.0000 0.0000

#### Displacive mode amplitudes

mode	As	Ap	dmax
[0,0,0]GM1+[C12:e:dsp]A1(a)	0.38324	0.11063	0.07823
[0,0,0]GM1+ all	0.38324	0.11063	
[0,0,0]GM4-[C11:c:dsp]B1u(a)	0.02503	0.00723	0.00511
[0,0,0]GM4- all	0.02503	0.00723	
[1/6,1/6,0]DT2[Pb:a:dsp]Eu(a)	0.01436	0.00415	0.00586
[1/6,1/6,0]DT2[C11:c:dsp]B3u(a)	-0.01568	-0.00453	0.00392
[1/6,1/6,0]DT2[C11:c:dsp]B2u(a)	-0.02464	-0.00711	0.00616
[1/6,1/6,0]DT2[C12:e:dsp]E(a)	0.00640	0.00185	0.00185
[1/6,1/6,0]DT2 all	0.03317	0.00957	

[1/6,1/6,0]DT3[Pb:a:dsp]A2u(a)	0.78805	0.22749	0.27862
[1/6,1/6,0]DT3[Cl1:c:dsp]B1u(a)	1.17096	0.33803	0.33803
[1/6,1/6,0]DT3[Cl2:e:dsp]A1(a)	1.05985	0.30595	0.26496
[1/6,1/6,0]DT3[Cl2:e:dsp]E(a)	0.72207	0.20844	0.20844
[1/6,1/6,0]DT3 all	1.90705	0.55052	
[1/3,1/3,0]DT1[Pb:a:dsp]Eu(a)	-0.00750	-0.00217	0.00265
[1/3,1/3,0]DT1[Cl1:c:dsp]B3u(a)	-0.01792	-0.00517	0.00448
[1/3,1/3,0]DT1[Cl1:c:dsp]B2u(a)	-0.02688	-0.00776	0.00672
[1/3,1/3,0]DT1[Cl2:e:dsp]A1(a)	-0.00137	-0.00040	0.00040
[1/3,1/3,0]DT1[Cl2:e:dsp]E(a)	-0.04863	-0.01404	0.01216
[1/3,1/3,0]DT1 all	0.05888	0.01700	
[1/3,1/3,0]DT4[Cl1:c:dsp]B1u(a)	-0.07304	-0.02108	0.02108
[1/3,1/3,0]DT4[Cl2:e:dsp]E(a)	0.03326	0.00960	0.00832
[1/3,1/3,0]DT4 all	0.08026	0.02317	
[1/2,1/2,0]X2+[Cl1:c:dsp]B3u(a)	-2.65623	-0.76679	0.54220
[1/2,1/2,0]X2+[Cl1:c:dsp]B2u(a)	0.32066	0.09257	0.06545
[1/2,1/2,0]X2+ all	2.67552	0.77235	
[1/2,1/2,0]X3+[Cl1:c:dsp]B1u(a)	-0.00176	-0.00051	0.00036
[1/2,1/2,0]X3+[Cl2:e:dsp]E(a)	0.01533	0.00443	0.00313
[1/2,1/2,0]X3+ all	0.01543	0.00445	
[1/2,1/2,0]X2-[Pb:a:dsp]A2u(a)	-0.00798	-0.00230	0.00230
[1/2,1/2,0]X2-[Cl2:e:dsp]A1(a)	-0.00599	-0.00173	0.00122
[1/2,1/2,0]X2- all	0.00998	0.00288	
[1/2,1/2,0]X3-[Pb:a:dsp]Eu(a)	0.23895	0.06898	0.06898
[1/2,1/2,0]X3-[Cl2:e:dsp]E(a)	0.69901	0.20179	0.14268
[1/2,1/2,0]X3- all	0.73872	0.21325	
[1,1,1]M5+[Cl2:e:dsp]E(a)	0.00453	0.00131	0.00092
[1,1,1]M5+ all	0.00453	0.00131	
[1,1,1]M5-[Pb:a:dsp]Eu(a)	3.18732	0.92010	0.92010
[1,1,1]M5-[Cl1:c:dsp]B3u(a)	1.67774	0.48432	0.34247
[1,1,1]M5-[Cl1:c:dsp]B2u(a)	-3.24698	-0.93732	0.66279
[1,1,1]M5-[Cl2:e:dsp]E(a)	4.38940	1.26711	0.89598
[1,1,1]M5- all	6.54091	1.88820	
[1/6,5/6,0]Y2[Pb:a:dsp]Eu(a)	0.00022	0.00006	0.00008
[1/6,5/6,0]Y2[Cl1:c:dsp]B3u(a)	-0.01662	-0.00480	0.00480
[1/6,5/6,0]Y2[Cl1:c:dsp]B2u(a)	-0.00149	-0.00043	0.00043
[1/6,5/6,0]Y2[Cl2:e:dsp]E(a)	-0.00000	-0.00000	0.00000
[1/6,5/6,0]Y2 all	0.01669	0.00482	
[1/6,5/6,0]Y3[Pb:a:dsp]A2u(a)	-0.16623	-0.04799	0.06786
[1/6,5/6,0]Y3[Cl1:c:dsp]B1u(a)	-0.41841	-0.12078	0.10460
[1/6,5/6,0]Y3[Cl2:e:dsp]A1(a)	-0.17563	-0.05070	0.05070
[1/6,5/6,0]Y3[Cl2:e:dsp]E(a)	-0.39107	-0.11289	0.09777
[1/6,5/6,0]Y3 all	0.62168	0.17946	
[1/3,2/3,0]Y1[Pb:a:dsp]Eu(a)	0.00485	0.00140	0.00198
[1/3,2/3,0]Y1[Cl1:c:dsp]B3u(a)	-0.00369	-0.00107	0.00107
[1/3,2/3,0]Y1[Cl1:c:dsp]B2u(a)	0.00369	0.00107	0.00107
[1/3,2/3,0]Y1[Cl2:e:dsp]A1(a)	0.01360	0.00393	0.00340



[1/3,2/3,0]Y1[C12:e:dsp]E(a)	0.04883	0.01410	0.01410
[1/3,2/3,0]Y1 all	0.05119	0.01478	
[1/3,2/3,0]Y4[C11:c:dsp]B1u(a)	-0.17920	-0.05173	0.04480
[1/3,2/3,0]Y4[C12:e:dsp]E(a)	-0.00183	-0.00053	0.00053
[1/3,2/3,0]Y4 all	0.17921	0.05173	
Overall	7.39627	2.13512	

#### Parent-cell strain mode definitions

	e1	e2	e3	e4	e5	e6
I4/mmm[0,0,0]GM1+(a)strain_1(a) normfactor = 0.70711	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000
I4/mmm[0,0,0]GM1+(a)strain_2(a) normfactor = 1.00000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
I4/mmm[0,0,0]GM4+(a)strain(a) normfactor = 1.41421	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000

#### Parent-cell strain mode amplitudes

mode	amplitude
[0,0,0]GM1+strain_1(a)	-0.01844
[0,0,0]GM1+strain_2(a)	-0.00760
[0,0,0]GM4+strain(a)	0.08869