Use of the Bilbao Crystallographic Server: twinned crystals and crystal-chemical relationships

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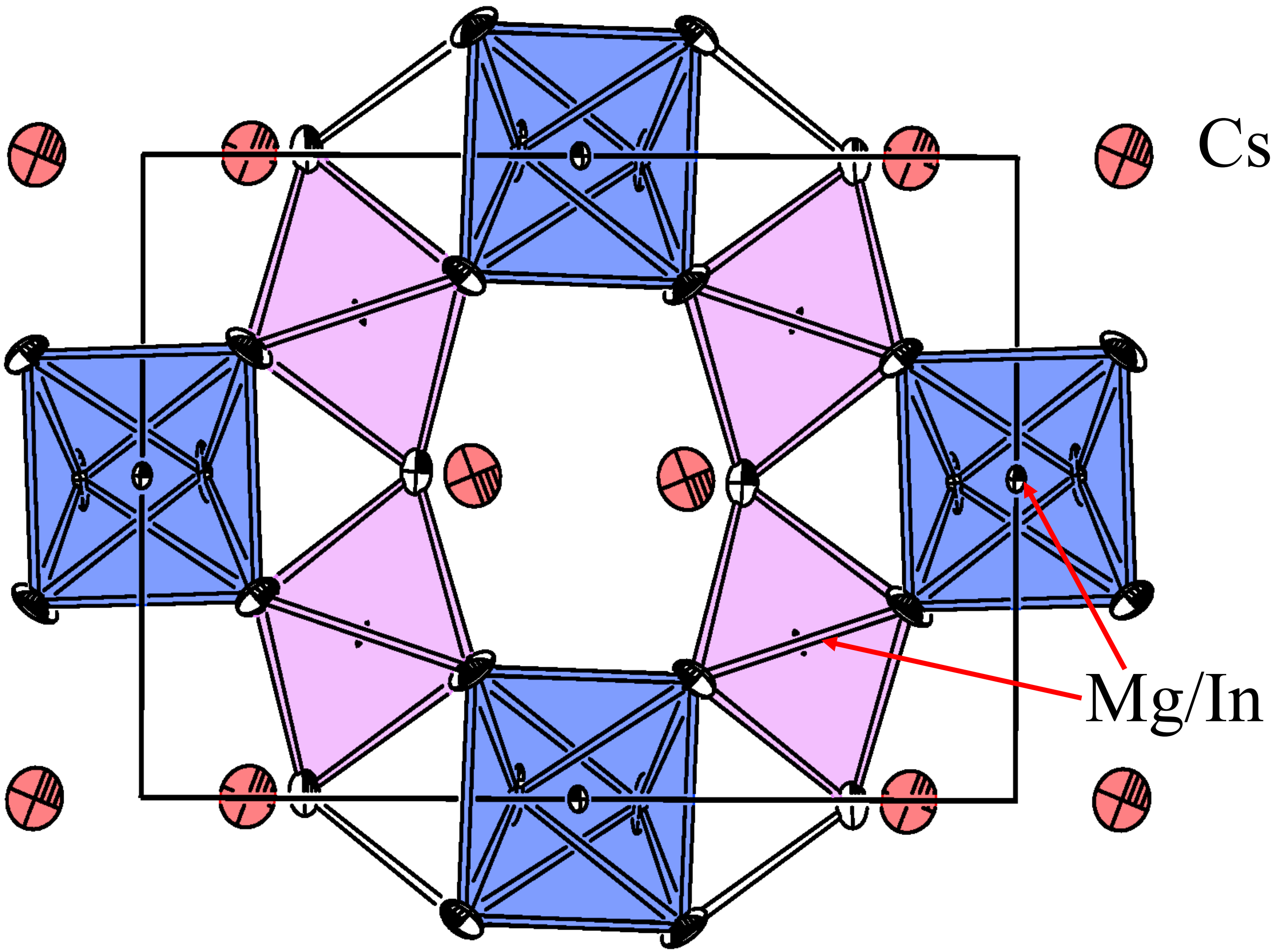
Example Pyrochlore: Twinned $CsMgInF_6$



Friese, Gesland, Grzechnik; Z. Krist. 220 (2005), 614

Pyrochlore: $ABB'F_6$

Symmetry of the archetype structure

Space group No. 227: Fd-3m
(origin choice 2, 1/8,1/8,1/8)

WYCKPOS

Wyckoff Positions of Group 227 (*Fd*-3*m*) [origin choice 2]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates	
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +	
192	i	1	(x,y,z) (-x+3/4,-y+1/4,z+1/2) (-x+1/4,y+1/2,-z+3/4) (x+1/2,-y+3/4,-z+1/4) (z,x,y) (z+1/2,-x+3/4,-y+1/4) (-z+3/4,-x+1/4,y+1/2) (-z+1/4,x+1/2,-y+3/4) (y,z,x) (-y+1/4,z+1/2,-x+3/4) (y+1/2,-z+3/4,-x+1/4) (-y+3/4,-z+1/4,x+1/2) (y+3/4,x+1/4,-z+1/2) (-y,-x,-z) (y+1/4,-x+1/2,z+3/4) (-y+1/2,x+3/4,z+1/4) (x+3/4,z+1/4,-y+1/2) (-x+1/2,z+3/4,y+1/4) (-x,-z,-y) (x+1/4,-z+1/2,y+3/4) (z+3/4,y+1/4,-x+1/2) (z+1/4,-y+1/2,x+3/4) (-z+1/2,y+3/4,x+1/4) (-z,-y,-x) (-x,-y,-z) (x+1/4,y+3/4,-z+1/2) (x+3/4,-y+1/2,z+1/4) (-x+1/2,y+1/4,z+3/4) (-z,-x,-y) (-z+1/2,x+1/4,y+3/4) (z+1/4,x+3/4,-y+1/2) (z+3/4,-x+1/2,y+1/4) (-y,-z,-x) (y+3/4,-z+1/2,x+1/4) (-y+1/2,z+1/4,x+3/4) (y+1/4,z+3/4,-x+1/2) (-y+1/4,-x+3/4,z+1/2) (y,x,z) (-y+3/4,x+1/2,-z+1/4) (y+1/2,-x+1/4,-z+3/4) (-x+1/4,-z+3/4,y+1/2) (x+1/2,-z+1/4,-y+3/4) (x,z,y) (-x+3/4,z+1/2,-y+1/4) (-z+1/4,-y+3/4,x+1/2) (-z+3/4,y+1/2,-x+1/4) (z+1/2,-y+1/4,-x+3/4) (z,y,x)	
96	h	..2	(0,y,-y) (3/4,-y+1/4,-y+1/2) (1/4,y+1/2,y+3/4) (1/2,-y+3/4,y+1/4) (-y,0,y) (-y+1/2,3/4,-y+1/4) (y+3/4,1/4,y+1/2) (y+1/4,1/2,-y+3/4) (y,-y,0) (-y+1/4,-y+1/2,3/4) (y+1/2,y+3/4,1/4) (-y+3/4,y+1/4,1/2) (0,-y,y) (1/4,y+3/4,y+1/2) (3/4,-y+1/2,-y+1/4) (1/2,y+1/4,-y+3/4) (y,0,-y) (y+1/2,1/4,y+3/4) (-y+1/4,3/4,-y+1/2) (-y+3/4,1/2,y+1/4) (-y,y,0) (y+3/4,y+1/2,1/4) (-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)	
96	g	..m	(x,x,z) (-x+3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4) (z,x,x) (z+1/2,-x+3/4,-x+1/4) (-z+3/4,-x+1/4,x+1/2) (-z+1/4,x+1/2,-x+3/4) (x,z,x) (-x+1/4,z+1/2,-x+3/4) (x+1/2,-z+3/4,-x+1/4) (-x+3/4,-z+1/4,x+1/2) (x+3/4,x+1/4,-z+1/2) (-x,-x,-z) (x+1/4,-x+1/2,z+3/4) (-x+1/2,x+3/4,z+1/4) (x+3/4,z+1/4,-x+1/2) (-x+1/2,z+3/4,x+1/4) (-x,-z,-x) (x+1/4,-z+1/2,x+3/4) (z+3/4,x+1/4,-x+1/2) (z+1/4,-x+1/2,x+3/4) (-z+1/2,x+3/4,x+1/4) (-z,-x,-x)	
48	f	2.m m	(x,1/8,1/8) (-x+3/4,1/8,5/8) (1/8,x,1/8) (5/8,-x+3/4,1/8) (1/8,1/8,x) (1/8,5/8,-x+3/4) (7/8,x+1/4,3/8) (7/8,-x,7/8) (x+3/4,3/8,3/8) (-x+1/2,7/8,3/8) (7/8,3/8,-x+1/2) (3/8,3/8,x+3/4)	F (x = 0.31)
32	e	.3m	(x,x,x) (-x+3/4,-x+1/4,x+1/2) (-x+1/4,x+1/2,-x+3/4) (x+1/2,-x+3/4,-x+1/4) (x+3/4,x+1/4,-x+1/2) (-x,-x,-x) (x+1/4,-x+1/2,x+3/4) (-x+1/2,x+3/4,x+1/4)	
16	d	.-3m	(1/2,1/2,1/2) (1/4,3/4,0) (3/4,0,1/4) (0,1/4,3/4)	
16	c	.-3m	(0,0,0) (3/4,1/4,1/2) (1/4,1/2,3/4) (1/2,3/4,1/4)	B/B’
8	b	-43m	(3/8,3/8,3/8) (1/8,5/8,1/8)	A
8	a	-43m	(1/8,1/8,1/8) (7/8,3/8,3/8)	

SAM

Raman and Infrared Investigations

(Ayala et. al, Phys. Rev. B66, 2002, 214105)

TABLE III. Wave numbers of the Raman bands observed in $CsInMgF_6$ single crystals, at room temperature in different scattering geometries.

Wave number (cm^{-1})		
$z(xx)\bar{z}$	$z(xy)\bar{z}$	$z(x'y')\bar{z}$
27	27	27
42	43	40
80	80	
134	135	136
162	165	165
189	190	189
220	223	221
257	253	253
275	273	275
322	323	320
379	382	
435	432	
564	565	

IR and Raman Modes for F d -3 m (227)

WP: 8b, 16c, 48f

IR Active Modes

WP	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_u	E_g	T_{2u}	T_{2g}	T_{1u}	T_{1g}
48f	.	.	.	.	.	.	.	.	3	.
16c	.	.	.	.	.	.	.	.	2	.
8b	.	.	.	.	.	.	.	.	1	.

Raman Active Modes

WP	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_u	E_g	T_{2u}	T_{2g}	T_{1u}	T_{1g}
48f	1	.	.	.	.	1	.	3	.	.
16c	.	.	.	.	.	.	.	.	.	.
8b	.	.	.	.	.	.	.	1	.	.

Reflection Conditions Fd-3m:

hkl:	h+k=2n, h+l=2n, k+l=2n	F
0kl:	k+l=4n, k,l=2n	d
hhl:	h+l=2n	
h00:	h=4n	4_1

WP 8b	hkl: h=2n+1 or h+k+l=4n
WP 16c	hkl: h=2n+1 or h,k,l=4n+2 or h,k,l=4n
WP 48f	hkl: h=2n+1 or h+k+l=4n

MAXSUB

$CsMgInF_6$: very weak reflections violating the reflection condition for the F-centered lattice: the correct space group is probably a subgroup of Fd-3m

Maximal Subgroups of Space Groups

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or

choose it 227

Show WP Splittings?

NOTE: the program uses the default choice for the group setting.

Show maximal subgroups

Maximal subgroups of group 227 (*Fd*-3*m*) [origin choice 2]

Note: The program uses the default choice for the group settings.

In the following table the list of maximal subgroups is given. Click over "setting..." to see the possible setting(s) for the given subgroup.

N	IT number	HM symbol	Index	Transformations
1	141	$I4_1/amd$	3	show..
2	166	$R\text{-}3m$	4	show..
3	203	$Fd\text{-}3$	2	show..
4	210	$F4_132$	2	show..
5	216	$F\text{-}43m$	2	show..

[Click here to see the Series of Maximal Subgroups]

MAXSUB

Maximal subgroup(s) of type 141 ($I4_1/amd$) [origin choice 2] of index 3

for Space Group 227 (*Fd*-3*m*) [origin choice 2]

Click over **[ChBasis]** to view the general positions of the subgroup in the basis of the supergroup.

Conjugacy class a

Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	ChBasis
group No 2	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	ChBasis
group No 3	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	ChBasis

[Click here for the Maximal Subgroups of group 141]

Reflection condition for I-centered lattice: h+k+l=2n

Fd-3m	$I4_1$/amd	
Reflections u,u,u	u,e,u or e,u,u	h+k+l=2n
Reflections e,e,e	u,u,e	h+k+l=2n
Reflections u,u,e	u,e,e or e,u,e	h+k+l=2n+1 forbidden!

The maximal subgroups are no options, as the reflections violating the F-centered lattice are forbidden also in all the maximal subgroups!

CELLSUB

Subgroup indices

$$t = \frac{\text{number of the symmetry operation of the point group of H}}{\text{number of the symmetry operation of the point group of G}}$$

$$k = \frac{\text{volume of H x number of centering operation of G}}{\text{volume of G x number of centering operations of H}}$$

Observation: very weak reflections violating the reflection condition for the F-centered lattice

The k-subgroups are the important ones!

46 k-subgroups with index k=2 and variable t-index,

Choosing the ones with low t-index (t=2 or t=3)

CELLSUB

List of subgroups of space group *Fd*-3*m*(227) for a given k-index = 2

NOTE: The program uses the default choice for the group settings.

In the following table a list of t-subgroups, k-subgroups and general subgroups is given for a given k-in
Click over "show..." to obtain the classification in conjugate classes of subgroups.

k-index $i_k = 2$

N. of subgroups (for k-index 2) found: 46

General type subgroups of space group *Fd*-3*m* (227)

N	HM Symbol	ITA	index	t-index	k-index	More info
1	~~*R*-3*c*~~	167	8	4	2	show...
2	~~*R*-3*m*~~	166	8	4	2	show...
3	*R*3*c*	161	16	8	2	show...
4	*R*3*m*	160	16	8	2	show...
5	*R*32	155	16	8	2	show...
6	*R*-3	148	16	8	2	show...
7	*R*3	146	32	16	2	show...
8	*P*-4*n*2	118	12	6	2	show...
9	*P*-4*m*2	115	12	6	2	show...
10	$P4_32_12$	096	12	6	2	show...
11	$P4_322$	095	12	6	2	show...
12	$P4_12_12$	092	12	6	2	show...
13	$P4_122$	091	12	6	2	show...
14	*P*-4	081	24	12	2	show...
15	$P4_3$	078	24	12	2	show...
16	$P4_1$	076	24	12	2	show...
17	*Pnma*	062	12	6	2	show...
18	*Pmna*	053	12	6	2	show...
19	*Pnna*	052	12	6	2	show...
20	*Pmma*	051	12	6	2	show...
21	*Pnn*2	034	24	12	2	show...
22	$Pna2_1$	033	24	12	2	show...
23	$Pmn2_1$	031	24	12	2	show...
24	*Pnc*2	030	24	12	2	show...
25	*Pma*2	028	24	12	2	show...
26	$Pmc2_1$	026	24	12	2	show...
27	*Pmm*2	025	24	12	2	show...
28	*C*222	021	24	12	2	show...
29	$C222_1$	020	24	12	2	show...
30	$P2_12_12_1$	019	24	12	2	show...
31	$P222_1$	017	24	12	2	show...
32	*C*2/*c*	015	24	12	2	show...
33	$P2_1/c$	014	24	12	2	show...
34	*P*2/*c*	013	24	12	2	show...
35	*C*2/*m*	012	24	12	2	show...
36	$P2_1/m$	011	24	12	2	show...
37	*P*2/*m*	010	24	12	2	show...
38	*Cc*	009	48	24	2	show...
39	*Cm*	008	48	24	2	show...
40	*Pc*	007	48	24	2	show...
41	*Pm*	006	48	24	2	show...
42	*C*2	005	48	24	2	show...
43	$P2_1$	004	48	24	2	show...
44	*P*2	003	48	24	2	show...
45	*P*-1	002	48	24	2	show...
46	*P*1	001	96	48	2	show...

Group-Subgroup Lattice and Chains of Maximal Subgroups

Please, enter the sequential numbers of the group and the subgroup as given in the *International Tables for Crystallography*, Vol. A:	
Enter the supergroup number (G) or choose it:	227
Enter the subgroup number (H) or choose it:	118
Enter the index [G:H]	12

Construct the lattice

Chains of maximal subgroups from 227 (*Fd*-3*m*) [origin choice 2] to 118 (*P*-4*n*2) with index 12

N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	227 141 119 118 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *I*-4*m*2 > *P*-4*n*2	6	transformation...
2	227 216 119 118 [2 3 2]	*Fd*-3*m* > *F*-43*m* > *I*-4*m*2 > *P*-4*n*2	6	transformation...

Print this table.

Draw the lattice

Classify (with complete graph) Classify (with single graphs)

Classification of the subgroups of type *P*-4*n*2(118) of group *Fd*-3*m*(227) with index 12

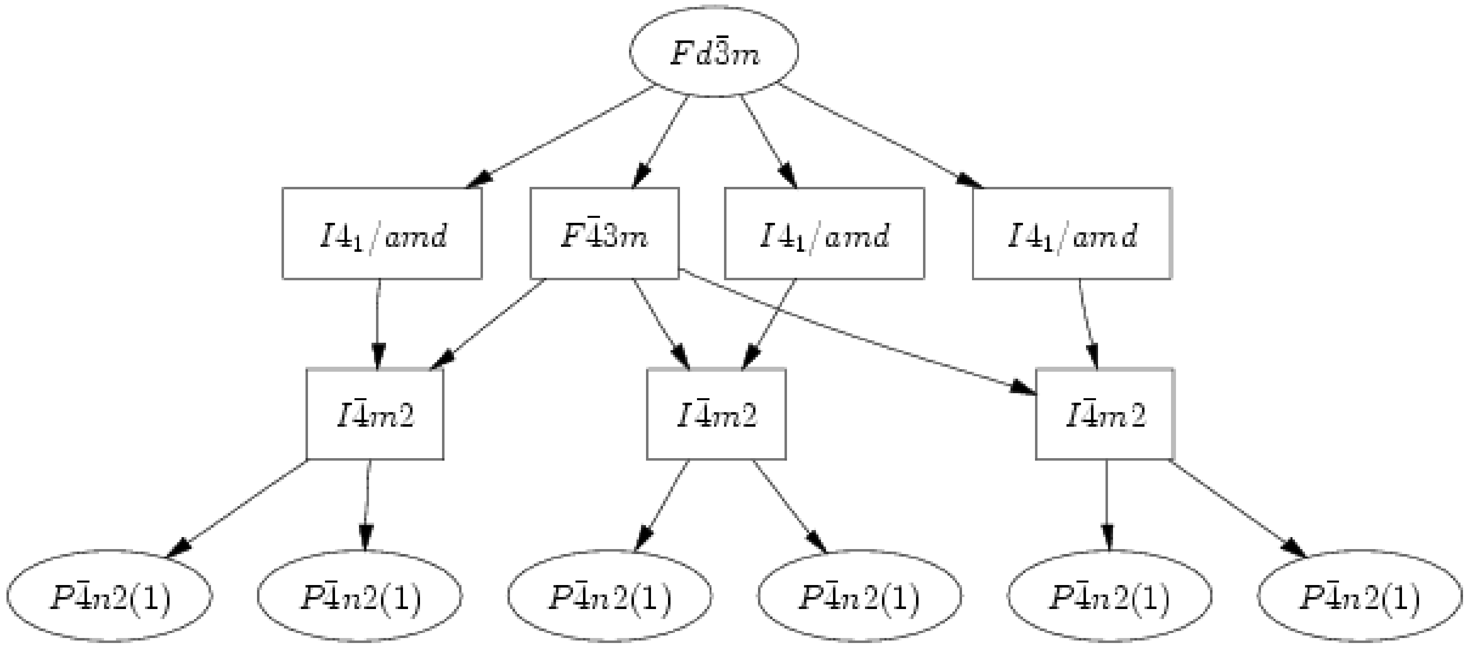
Class 1

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
1	227 141 119 118 [3 2 2]	$Fd\text{-}3m > I4_1/amd > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} 1/2 & 1/2 & 0 & 5/8 \\ -1/2 & 1/2 & 0 & 5/8 \\ 0 & 0 & 1 & 5/8 \end{pmatrix}$	matrix 1	to group 1
2	227 141 119 118 [3 2 2]	$Fd\text{-}3m > I4_1/amd > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} 0 & 0 & 1 & 5/8 \\ 1/2 & 1/2 & 0 & 5/8 \\ -1/2 & 1/2 & 0 & 5/8 \end{pmatrix}$	matrix 2	to group 2
3	227 141 119 118 [3 2 2]	$Fd\text{-}3m > I4_1/amd > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} -1/2 & 1/2 & 0 & 5/8 \\ 0 & 0 & 1 & 5/8 \\ 1/2 & 1/2 & 0 & 5/8 \end{pmatrix}$	matrix 3	to group 3
4	227 216 119 118 [2 3 2]	$Fd\text{-}3m > F\text{-}43m > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} 0 & 0 & 1 & 3/8 \\ 1/2 & 1/2 & 0 & 3/8 \\ -1/2 & 1/2 & 0 & 3/8 \end{pmatrix}$	matrix 4	to group 4
5	227 216 119 118 [2 3 2]	$Fd\text{-}3m > F\text{-}43m > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} -1/2 & 1/2 & 0 & 3/8 \\ 0 & 0 & 1 & 3/8 \\ 1/2 & 1/2 & 0 & 3/8 \end{pmatrix}$	matrix 5	to group 5
6	227 141 119 118 [3 2 2]	$Fd\text{-}3m > I4_1/amd > I\text{-}4m2 > P\text{-}4n2$	$\begin{pmatrix} 1/2 & 1/2 & 0 & 3/8 \\ -1/2 & 1/2 & 0 & 3/8 \\ 0 & 0 & 1 & 3/8 \end{pmatrix}$	matrix 6	to group 6

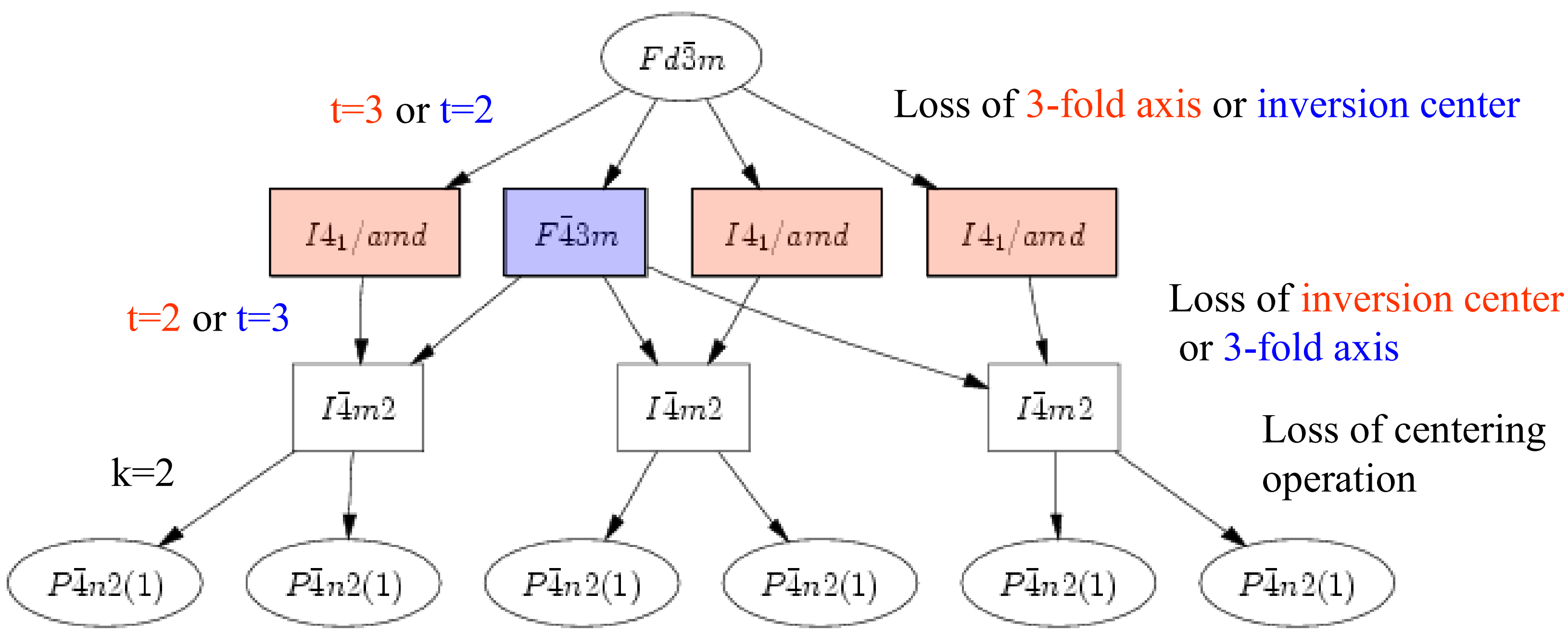
To see the graph containing all classes, click on **[Draw the lattice]**

Draw the lattice

Group-Subgroup Lattice



Group-Subgroup Lattice



Group-Subgroup Lattice and Chains of Maximal Subgroups

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup number (G) or choose it:	227
Enter subgroup number (H) or choose it:	62
Enter the index [G:H] (optional):	12

Construct the lattice

Chains of maximal subgroups from 227 (*Fd*-3*m*) [origin choice 2] to 62 (*Pnma*) with index 12

N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	227 141 074 062 [3 2 2]	*Fd*-3*m* > $I4_1/amd$ > *Imma* > *Pnma*	6	transformation...

Print this table

Draw the lattice

Classify (with complete graph) Classify (with single graphs)

Classification of the subgroups of type *Pnma*(62) of group *Fd*-3*m*(227) with index 12

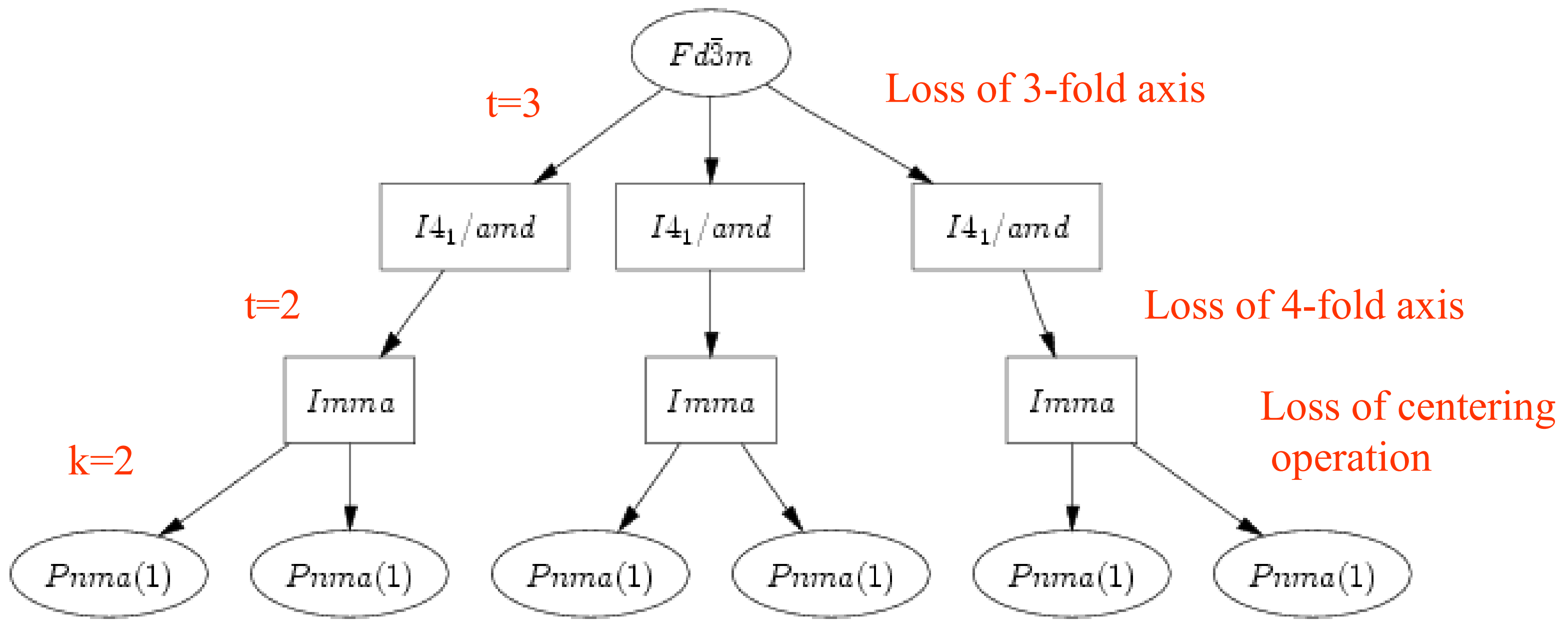
Class 1

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
1	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 1	--
2	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$	matrix 2	--
3	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	matrix 3	--
4	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \end{pmatrix}$	matrix 4	--
5	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	matrix 5	--
6	227 141 074 062 [3 2 2]	*Fd-3m* > *I4$_1$/amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \end{pmatrix}$	matrix 6	--

To see the graph containing all classes, click on **[Draw the lattice]**

Draw the lattice

Group-Subgroup Lattice



Subgroups of Fd-3m with t=6 and k=2

Six tetragonal subgroups:

$P\bar{4}n2$ $P\bar{4}m2$ $P4_3212$ $P4_322$ $P4_1212$ $P4_122$

Four orthorhombic subgroups:

Pmna Pnma Pnna Pmma

Lattice parameter:

$a = 7.5285(1), b = 7.5285(1), c = 10.6459(1)$ Å

$\alpha = \beta = \gamma = 90°$

For both tetragonal and orthorhombic system one has to take into account 6 twin domains

Classification of the subgroups of type *Pnma*(62) of group *Fd*-3*m*(227) with index 12

Class 1

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
1	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	matrix 1	--
2	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$	matrix 2	--
3	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	matrix 3	--
4	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \end{pmatrix}$	matrix 4	--
5	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	matrix 5	--
6	227 141 074 062 [3 2 2]	*Fd*-3*m* > *I*4$_1$/*amd* > *Imma* > *Pnma*	$\begin{pmatrix} -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \end{pmatrix}$	matrix 6	--

To see the graph containing all classes, click on **[Draw the lattice]**

Draw the lattice

Transformation Matrices: Fd-3m ----Pnma

	Transformation	
Matrix I	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	→ Twin Matrix I = Identity Matrix
Matrix II	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$	→ Matrix I x Twin Matrix II = Matrix II
Matrix III	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	→ Matrix I x Twin Matrix III = Matrix III
Matrix IV	$\begin{pmatrix} 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \\ -1/2 & -1/2 & 0 & 1/4 \end{pmatrix}$	→ Matrix I x Twin Matrix IV= Matrix IV
Matrix V	$\begin{pmatrix} -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \end{pmatrix}$	→ Matrix I x Twin Matrix V= Matrix V
Matrix VI	$\begin{pmatrix} -1/2 & -1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 1/2 \end{pmatrix}$	→ Matrix I x Twin Matrix VI= Matrix VI

Table 3. Details of the refinement of $CsMgInF_6$ in different space groups

Space group	Number of reflections: obs/all		
	rejected	refinement	$h+k+l=2n+1$
$Fd\bar{3}m$	806/5976	67/67	–
$Imma$	1466/1791	843/1003	–
$P\bar{4}n2$	129/967	816/1267	344/720
$P\bar{4}m2$	0/0	879/1549	407/1002
$P4_32_12$	0/83	858/1388	390/846
$P4_322$	0/30	858/1403	390/861
$P4_12_12$	0/83	858/1388	390/846
$P4_122$	0/30	858/1403	390/861
$Pnma$	0/83	1251/2013	408/1010
$Pmma$	0/0	1251/2056	408/1053
$Pmna$	0/30	1251/2041	408/1038
$Pnna$	129/967	1183/1762	340/759

Can be excluded due to violations of extinction rules

Reflections violating the I-centering (F-centering in the cubic setting)

Table 3. Details of the refinement of $CsMgInF_6$ in different space groups. Agreement factors are given in [%].

Space group	Number of reflections: obs/all rejected	refinement	$h+k+l=2n+1$	R_{int} obs/all	Number of parameters	R_w (obs)	R (all)	R_w (obs) ($h+k+l=2n+1$)	R (all)
$Fd\bar{3}m$	806/5976	67/67	–	4.60/4.60	9	1.40	2.08	–	–
$Imma$	1466/1791	843/1003	–	3.69/3.71	36	1.72	2.85	–	–
$P\bar{4}n2$	129/967	816/1267	344/720	4.40/4.60	49	1.74	7.75	36.02	49.17
$P\bar{4}m2$	0/0	879/1549	407/1002	4.42/4.67	62	1.55	9.43	25.83	56.60
$P4_32_12$	0/83	858/1388	390/846	4.44/4.68	46	1.65	5.83	21.80	30.30
$P4_322$	0/30	858/1403	390/861	4.44/4.69	49	1.74	8.87	44.53	58.11
$P4_12_12$	0/83	858/1388	390/846	4.44/4.68	49	1.63	7.00	28.93	42.88
$P4_122$	0/30	858/1403	390/861	4.44/4.69	50	1.68	9.08	34.35	60.56
$Pnma$	0/83	1251/2013	408/1010	3.93/4.22	55	1.72	3.96	10.81	18.04
$Pmma$	0/0	1251/2056	408/1053	3.93/4.22	63	1.74	5.58	17.76	39.32
$Pmna$	0/30	1251/2041	408/1038	3.93/4.22	56	1.81	6.45	28.10	50.18
$Pnna$	129/967	1183/1762	340/759	3.90/4.15	51	1.82	5.54	34.76	47.81

WYCKSPLIT

Wyckoff Positions Splitting

Conventional Settings | Non conventional Settings

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup or choose it	227
Enter subgroup or choose it	62
Please, define the transformation relating the group and the subgroup bases. (NOTE: If you don't know the transformation click here for possible workarounds)	

rotational matrix:	0.5	0.5	0
	-0.5	0.5	0
	0	0	1
origin shift:	0.25	0.25	0

Show group-subgroup data.

Wyckoff Positions Splitting

227 (*Fd*-3*m*) [origin choice 2] > 62 (*Pnma*)

Wyckoff positions:

Group Data	Subgroup Data
☐ All positions	
☐ 192i (x, y, z)	
☐ 96h (0, y, - y)	
☐ 96g (x, x, z)	8d (x, y, z)
☑ 48f (x, 1/8 , 1/8)	4c (x, 1/4 , z)
☐ 32e (x, x, x)	4b (0, 0, 1/2)
☐ 16d (1/2 , 1/2 , 1/2)	4a (0, 0, 0)
☑ 16c (0, 0, 0)	
☑ 8b (3/8 , 3/8 , 3/8)	
☐ 8a (1/8 , 1/8 , 1/8)	

Splitting

Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	48f	8d 8d 4c 4c	Relations
2	16c	4a 4c	Relations
3	8b	4c	Relations

WYCKSPLIT

Wyckoff Positions Splitting

227 (*Fd*-3*m*) [origin choice 2] > 62 (*Pnma*)

Splitting of Wyckoff position 48f

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x+1, 1/8, 1/8)	(x+7/8, x+5/8, 1/8)	$8d_1$	(x_1, y_1, z_1)
2	(-x+3/4, 1/8, 5/8)	(-x+5/8, -x+3/8, 5/8)		(-x_1+1/2, -y_1, z_1+1/2)
3	(3/8, x+1/4, 7/8)	(-x+1/8, x+1/8, 7/8)		(-x_1, y_1+1/2, -z_1)
4	(7/8, -x+1/2, 3/8)	(x+3/8, -x+7/8, 3/8)		(x_1+1/2, -y_1+1/2, -z_1+1/2)
5	(-x+1/2, 3/8, 7/8)	(-x+1/8, -x+3/8, 7/8)		(-x_1, -y_1, -z_1)
6	(x+3/4, 3/8, 3/8)	(x+3/8, x+5/8, 3/8)		(x_1+1/2, y_1, -z_1+1/2)
7	(9/8, -x+1/4, 1/8)	(x+7/8, -x+7/8, 1/8)		(x_1, -y_1+1/2, z_1)
8	(5/8, x, 5/8)	(-x+5/8, x+1/8, 5/8)		(-x_1+1/2, y_1+1/2, z_1+1/2)
9	(5/8, x+1/2, 1/8)	(-x+1/8, x+5/8, 1/8)	$8d_2$	(x_2, y_2, z_2)
10	(5/8, -x+1/4, 5/8)	(x+3/8, -x+3/8, 5/8)		(-x_2+1/2, -y_2, z_2+1/2)
11	(x+3/4, -1/8, 7/8)	(x+7/8, x+1/8, 7/8)		(-x_2, y_2+1/2, -z_2)
12	(-x+1, 3/8, 3/8)	(-x+5/8, -x+7/8, 3/8)		(x_2+1/2, -y_2+1/2, -z_2+1/2)
13	(7/8, -x, 7/8)	(x+7/8, -x+3/8, 7/8)		(-x_2, -y_2, -z_2)
14	(7/8, x+1/4, 3/8)	(-x+5/8, x+5/8, 3/8)		(x_2+1/2, y_2, -z_2+1/2)
15	(-x+3/4, 5/8, 1/8)	(-x+1/8, -x+7/8, 1/8)		(x_2, -y_2+1/2, z_2)
16	(x+1/2, 1/8, 5/8)	(x+3/8, x+1/8, 5/8)		(-x_2+1/2, y_2+1/2, z_2+1/2)
17	(5/8, 5/8, x)	(0, 3/4, x)	$4c_1$	(-x_3+1/2, 3/4, z_3+1/2)
18	(5/8, 1/8, x+1/2)	(1/2, 1/4, x+1/2)		(x_3, 1/4, z_3)
19	(3/8, 3/8, -x)	(0, 1/4, -x)		(x_3+1/2, 1/4, -z_3+1/2)
20	(7/8, 3/8, -x+1/2)	(1/2, 3/4, -x+1/2)		(-x_3, 3/4, -z_3)
21	(5/8, 1/8, -x+3/4)	(1/2, 1/4, -x+3/4)	$4c_2$	(x_4, 1/4, z_4)
22	(5/8, 5/8, -x+1/4)	(0, 3/4, -x+1/4)		(-x_4+1/2, 3/4, z_4+1/2)
23	(7/8, 3/8, x+1/4)	(1/2, 3/4, x+1/4)		(-x_4, 3/4, -z_4)
24	(3/8, 3/8, x+3/4)	(0, 1/4, x+3/4)		(x_4+1/2, 1/4, -z_4+1/2)

Wyckoff Positions Splitting

227 (*Fd*-3*m*) [origin choice 2] > 62 (*Pnma*)

Splitting of Wyckoff position 16c

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(1/2, 1/2, 0)	(0, 1/2, 0)	$4a_1$	(0, 1/2, 0)
2	(3/4, 1/4, 1/2)	(1/2, 1/2, 1/2)		(1/2, 1/2, 1/2)
3	(1/4, 1/4, 0)	(0, 0, 0)		(0, 0, 0)
4	(1/2, 0, 1/2)	(1/2, 0, 1/2)		(1/2, 0, 1/2)
5	(3/4, 0, 3/4)	(3/4, 1/4, 3/4)	$4c_1$	(x_2, 1/4, z_2)
6	(1, 1/4, 1/4)	(3/4, 3/4, 1/4)		(-x_2+1/2, 3/4, z_2+1/2)
7	(3/4, 1/2, 1/4)	(1/4, 3/4, 1/4)		(-x_2, 3/4, -z_2)
8	(1/2, 1/4, 3/4)	(1/4, 1/4, 3/4)		(x_2+1/2, 1/4, -z_2+1/2)

Wyckoff Positions Splitting

227 (*Fd*-3*m*) [origin choice 2] > 62 (*Pnma*)

Splitting of Wyckoff position 8b

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(3/8, 3/8, 3/8)	(0, 1/4, 3/8)	$4c_1$	(x_1, 1/4, z_1)
2	(7/8, 3/8, 7/8)	(1/2, 3/4, 7/8)		(-x_1+1/2, 3/4, z_1+1/2)
3	(5/8, 5/8, 5/8)	(0, 3/4, 5/8)		(-x_1, 3/4, -z_1)
4	(5/8, 1/8, 1/8)	(1/2, 1/4, 1/8)		(x_1+1/2, 1/4, -z_1+1/2)

WYCKSPLIT

Archtype structure Fd-3m		Transformed Pnma		Refined Pnma	
F1 (48f)	→	0.815, 0.065, 0.875	→	0.313,0.055, 0.868	=F1
	→	0.685, 0.435, 0.625	→	0.199, 0.440, 0.622	=F2
0.31, 1/8, 1/8	→	0.0, 0.25, 0.006	→	0.493. 0.250, 0.071	=F3
	→	0.5, 0.25, 0.81	→	0.008, 0.250, 0.813	=F4
B/B'(16c)	→	0.5, 0.0, 0.5	→	0.0, 0.0, 0.5	=In1/Mg1
0,0,0	→	0.75, 0.25, 0.75	→	0.255, 0.25, 0.75	=In2/Mg2
A(8b)	→	0.0, 0.25, 3/8	→	0.498, 0.25, 0.378	=Cs
3/8, 3/8, 3/8					

Pnma (transformed) → Pnma (refined)

Origin shift ½,0,0

EQUIVSTRU

Equivalent Descriptions of Crystal Structures

Structure Data [in CIF format]

Examinar...

HINT: [The option for a given filename is preferential]

Structure

```
62
7.5285 7.5285 10.6459 90 90 90
7
In 1     4b   0.0     0.0      0.5
In 2     4c   0.2552  0.250000 0.74758
Cs 1     4c   0.4979  0.2500   0.37811
F  1     8d   0.3126  0.0549   0.8676
F  2     8d   0.1991  0.4399   0.6220
F  3     4c   0.4931  0.25     0.0710
F  4     4c   0.0081  0.25     0.8134
```

Show

Equivalent Descriptions of Crystal Structures

Space Group: 62 (*Pnma*)

Euclidean Normalizer for General Metrics: (*Pmmm*) 1/2a,1/2b,1/2c

Additional coset representatives:

```
x,y,z
x+1/2,y,z
x,y+1/2,z
x,y,z+1/2
x+1/2,y+1/2,z
x+1/2,y,z+1/2
x,y+1/2,z+1/2
x+1/2,y+1/2,z+1/2
```

Number of crystallographic equivalent descriptions: 8

Permitted origins:

```
0,0,0
1/2,0,0
0,1/2,0
0,0,1/2
1/2,1/2,0
1/2,0,1/2
0,1/2,1/2
1/2,1/2,1/2
```

Structure number 2

EQUIVSTRU

Normalizer coset representative: x+1/2,y,z

Transformed unit cell:

7.5285 7.5285 10.6459 90.000 90.000 90.000

Transformed structure:

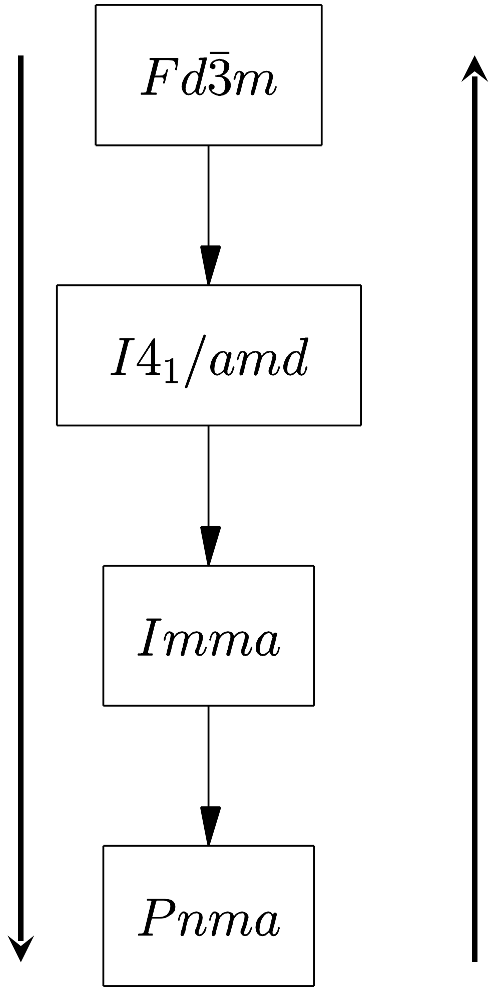
AT.	WP	SS	Representative	Atomic orbit
In1	4a (0,0,0)	-1	(0.500000,0.000000,0.500000)	(0.500000,0.000000,0.500000) (0.000000,0.000000,0.000000) (0.500000,0.500000,0.500000) (0.000000,0.500000,0.000000)
In2	4c (x,1/4,z)	.m.	(0.755200,0.250000,0.747580)	(0.755200,0.250000,0.747580) (0.744800,0.750000,0.247580) (0.244800,0.750000,0.252420) (0.255200,0.250000,0.752420)
Cs1	4c (x,1/4,z)	.m.	(0.997900,0.250000,0.378110)	(0.997900,0.250000,0.378110) (0.502100,0.750000,0.878110) (0.002100,0.750000,0.621890) (0.497900,0.250000,0.121890)
F1	8d (x,y,z)	1	(0.812600,0.054900,0.867600)	(0.812600,0.054900,0.867600) (0.687400,0.945100,0.367600) (0.187400,0.554900,0.132400) (0.312600,0.445100,0.632400) (0.187400,0.945100,0.132400) (0.312600,0.054900,0.632400) (0.812600,0.445100,0.867600) (0.687400,0.554900,0.367600)
F2	8d (x,y,z)	1	(0.699100,0.439900,0.622000)	(0.699100,0.439900,0.622000) (0.800900,0.560100,0.122000) (0.300900,0.939900,0.378000) (0.199100,0.060100,0.878000) (0.300900,0.560100,0.378000) (0.199100,0.439900,0.878000) (0.699100,0.060100,0.622000) (0.800900,0.939900,0.122000)
F3	4c (x,1/4,z)	.m.	(0.993100,0.250000,0.071000)	(0.993100,0.250000,0.071000) (0.506900,0.750000,0.571000) (0.006900,0.750000,0.929000) (0.493100,0.250000,0.429000)
F4	4c (x,1/4,z)	.m.	(0.508100,0.250000,0.813400)	(0.508100,0.250000,0.813400) (0.991900,0.750000,0.313400) (0.491900,0.750000,0.186600) (0.008100,0.250000,0.686600)

Diffraction pattern

subgroup relations
→ possible space groups and corresponding twin domain structures

Trial refinements in different space groups

Final model



Pseudosymmetry analysis

Pseudosymmetry search

PSEUDO

Formulae: CsMgInF6

Structure data [in CIF format] Examinar...

HINT: [The option for a given filename is preferential]

Initial Structure (LS)

```
62
7.5285 7.5285 10.6459 90 90 90
7
In 1       4b   0.0       0.0      0.5
In 2       4c   0.2552    0.250000 0.74758
Cs 1       4c   0.4979  0.2500  0.37811
F  1       8d   0.3126  0.0549  .8676
F  2       8d   0.1991  0.4399  0.6220
F  3       4c   0.4931  0.25    0.0710
F  4       4c   0.0081  0.25   0.8134
```

Select supergroups type for pseudosymmetry search.

1. Minimal supergroups — [Show only indices in supergroups table]
2. Supergroups with k-index — i_k: 1
3. Specify supergroup transformation — **G:** 221

Transf. Matrix (in option 3 only)	**Rotational part**			**Origin Shift**
	1	0	0	0
	0	1	0	0
	0	0	1	0

4. Lattice Pseudosymmetry with minimal supergroups — **Ang. Tol (in degrees)** 5 [*]

[*] Only for triclinics and monoclinics.

Enter the tolerance (maximum allowed distance) for pseudosymmetry search.

Maximum Δ: 1

Show

PSEUDO

Select minimal supergroups of space group *Pnma* (62)

The next step is to select the supergroups which the pseudosymmetry should be searched for. Each supergroup in the table can be selected l marking the corresponding checkbox.

No. #	Select	HM Symb.	IT Numb.	Index	Index i_k	Transformation (P,p)	Transformed Cell
1	☑	*Pbam*	055	2	2	**a,-2c,b** ; 0,0,0	7.5285 10.6459 3.7643 90.00 90.00 90.00
2	☑	*Pbcm*	057	2	2	**b,c,2a** ; 0,0,0	5.3229 7.5285 7.5285 90.00 90.00 90.00
3	☑	*Pmmn*	059	2	2	**2c,b,-a** ; 0,0,0	10.6459 7.5285 3.7643 90.00 90.00 90.00
4	☑	*Pnma*	062	3	3	**3a,b,c** ; 0,0,0	2.5095 7.5285 10.6459 90.00 90.00 90.00
5	☑	*Pnma*	062	3	3	**a,3b,c** ; 0,0,0	7.5285 2.5095 10.6459 90.00 90.00 90.00
6	☑	*Pnma*	062	3	3	**a,b,3c** ; 0,0,0	7.5285 7.5285 3.5486 90.00 90.00 90.00
7	☑	*Pnma*	062	5	5	**5a,b,c** ; 0,0,0	1.5057 7.5285 10.6459 90.00 90.00 90.00
8	☑	*Pnma*	062	5	5	**a,5b,c** ; 0,0,0	7.5285 1.5057 10.6459 90.00 90.00 90.00
9	☑	*Pnma*	062	5	5	**a,b,5c** ; 0,0,0	7.5285 7.5285 2.1292 90.00 90.00 90.00
10	☑	*Pnma*	062	7	7	**7a,b,c** ; 0,0,0	1.0755 7.5285 10.6459 90.00 90.00 90.00
11	☑	*Pnma*	062	7	7	**a,7b,c** ; 0,0,0	7.5285 1.0755 10.6459 90.00 90.00 90.00
12	☑	*Pnma*	062	7	7	**a,b,7c** ; 0,0,0	7.5285 7.5285 1.5208 90.00 90.00 90.00
13	☑	*Cmcm*	063	2	2	**b,c,a** ; 0,0,0	10.6459 7.5285 7.5285 90.00 90.00 90.00
14	☑	*Cmcm*	063	2	2	**c,a,b** ; 1/4,1/4,0	7.5285 10.6459 7.5285 90.00 90.00 90.00
15	☑	*Cmca*	064	2	2	**-b,a,c** ; 1/4,1/4,0	7.5285 7.5285 10.6459 90.00 90.00 90.00
16	☑	*Imma*	074	2	2	**a,b,c** ; 0,0,0	7.5285 7.5285 10.6459 90.00 90.00 90.00

PSEUDO

Summary search results

Pseudosymmetry search among minimal supergroups.

16	*Imma* (074)	2	2	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	0.1468	0.0734

Idealized structures

16# Supergroup *Imma* (074): a,b,c ; 0,0,0 and index 2

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
In1	(0.0000, 0.0000, 0.5000)	0.000000	0.000000	0.000000	0.0000
In2	(0.2500, 0.2500, 0.7500)	0.005200	0.000000	-0.002420	0.0469
Cs1	(0.5000, 0.2500, 0.3781)	-0.002100	0.000000	0.000000	0.0158
F1	(0.3067, 0.0575, 0.8728)	0.005850	-0.002600	-0.005200	0.0734
F2	(0.1933, 0.4425, 0.6272)	0.005850	-0.002600	-0.005200	0.0734
F3	(0.5000, 0.2500, 0.0710)	-0.006900	0.000000	0.000000	0.0519
F4	(0.0000, 0.2500, 0.8134)	0.008100	0.000000	0.000000	0.0610

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute displacement given in Å

PSEUDO

Idealized structure (subgroup setting):

```
62
7.5285 7.5285 10.6459 90.00 90.00 90.00
7
In    1   -   0.0000  0.0000  0.5000
In    2   -   0.2500  0.2500  0.7500
Cs    1   -   0.5000  0.2500  0.3781
F     1   -   0.3067  0.0575  0.8728
F     2   -   0.1933  0.4425  0.6272
F     3   -   0.5000  0.2500  0.0710
F     4   -   0.0000  0.2500  0.8134
```

Idealized structure (supergroup setting):

```
074
7.5285 7.5285 10.6459 90.00 90.00 90.00
6
In    1   -   0.0000  0.0000  0.5000
In    2   -   0.2500  0.2500  0.7500
Cs    1   -   0.5000  0.2500  0.3781
F     1   -   0.3068  0.0575  0.8728
#F     2   -   0.1933  0.4425  0.6272
F     3   -   0.5000  0.2500  0.0710
F     4   -   0.0000  0.2500  0.8134
```

Notes:

- Idealized structure with space group 074 related with the given by the transformation **a,b,c** ; 0,0,0 and index 2
- Cell parameters have not been symmetrized. They may include in general some symmetry breaking strain, to be removed by hand.
- A commented atom means a redundant atom, due to the merging of the Wyckoff orbit with another one in the supergroup

PSEUDO

Pseudosymmetry search full report

16# Supergroup *Imma* (074): a,b,c ; 0,0,0 and index 2

Transformation matrix: a,b,c ; 0,0,0 (index = 2)

```
[       1       0       0 ] [         0]
[       0       1       0 ] [         0]
[       0       0       1 ] [         0]
```

Coset representative: -x,-y+1/2,z

Maximum distance: 0.1468

Pairings and distances:

Atom in S	Coordinates in H	Atom in gS	Coordinates in gH
F1[1]	(0.312600,0.054900,0.867600)	F2[6]	(-0.312600,0.445100,0.867600)
F1[2]	(0.187400,0.945100,0.367600)	F2[5]	(-0.187400,-0.445100,0.367600)
F1[3]	(0.687400,0.554900,0.132400)	F2[8]	(-0.687400,-0.054900,0.132400)
F1[4]	(0.812600,0.445100,0.632400)	F2[7]	(-0.812600,0.054900,0.632400)
F1[5]	(0.687400,0.945100,0.132400)	F2[2]	(-0.687400,-0.445100,0.132400)
F1[6]	(0.812600,0.054900,0.632400)	F2[1]	(-0.812600,0.445100,0.632400)
F1[7]	(0.312600,0.445100,0.867600)	F2[4]	(-0.312600,0.054900,0.867600)
F1[8]	(0.187400,0.554900,0.367600)	F2[3]	(-0.187400,-0.054900,0.367600)

PSEUDO

Formulae: CsMgInF6

Structure data [in CIF format]: Examinar...

HINT: [The option for a given filename is preferential]

Initial Structure (LS)

```
74
7.5285 7.5285 10.6459 90 90 90
6
In 1     -   0.0      0.0      0.5
In 2     -   0.25     0.25     0.75
Cs 1     -   0.50     0.25     0.3781
F  1     -   0.3068   0.0575   0.8728
F  3     -   0.50     0.25     0.0710
F  4     -   0.00     0.25     0.8134
```

Summary search results

Pseudosymmetry search among minimal supergroups.

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
14	$I4_1/amd$ (141)	2	1	**a,b,c** ; 1/2,0,0	[1 0 0] [1/2] [0 1 0] [0] [0 0 1] [0]	0.0809	0.0405

PSEUDO

Formulae: CsMgInF6

Structure data [in CIF format] Examinar...

HINT: [The option for a given filename is preferential]

Initial Structure (LS)

```
141
7.5285 7.5285 10.6459 90 90 90
4
In 1        -    0.5      0.0      0.5
Cs 1        -    0.00     0.25     0.3750
F 1         -    0.8072   0.0571   0.8750
F 3         -    0.00     0.25     0.0672
```

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
7	*Fd-3m* (227)	3	1	**1/2a-1/2b,1/2a+1/2b,c** ; 1/4,1/4,0	$\begin{bmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/4 \\ 1/4 \\ 0 \end{bmatrix}$	0.0069	0.0046

Idealized structure (subgroup setting):

```
141
7.5285 7.5285 10.6459 90.00 90.00 90.00
4
In     1   -  0.5000  0.0000  0.5000
Cs     1   -  0.0000  0.2500  0.3750
F      1   -  0.8074  0.0573  0.8750
F      3   -  0.0000  0.2500  0.0676
```

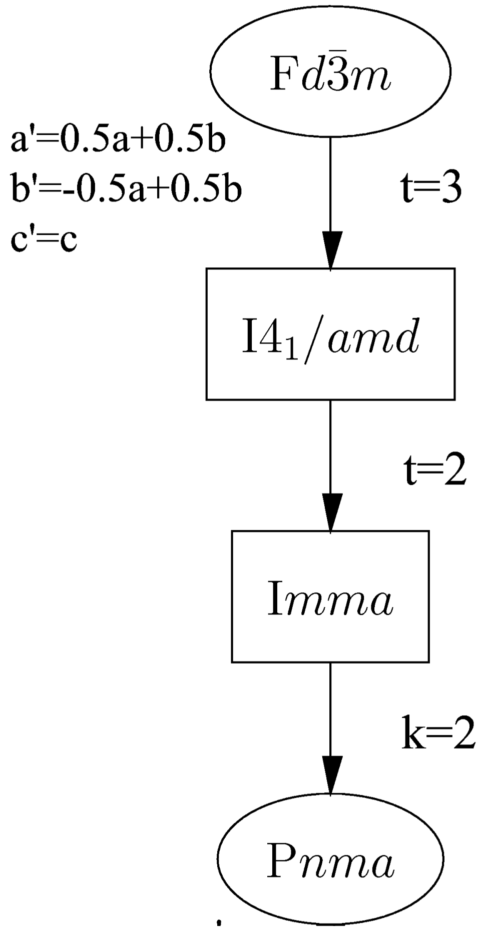
Idealized structure (supergroup setting):

```
227
10.6469 10.6469 10.6459 90.00 90.00 90.00
3
In     1   -  0.5000  0.0000  0.5000
Cs     1   -  0.3750  0.3750  0.3750
F      1   -  0.6824  0.8750  0.8750
#F      3   -  0.3750  0.3750  0.0676
```

Crystal-chemical relationships

Table 1. Selected information on ternary and quaternary fluorides with pyrochlore related structures; ratio of ionic radius (*r*) calculated on the values given by [18].

NH_4CoAlF_6	10.0487(3)			$Fd\bar{3}m$	1.17	[22]
$RbMgNiF_6$	9.978			$Fd\bar{3}m$	1.23	[2]
$RbNiCoF_6$	10.183			$Fd\bar{3}m$	1.21	[2]
$RbCoCrF_6$	10.277(5)			$Fd\bar{3}m$	1.05	[23]
$RbNiCrF_6$	10.21			$Fd\bar{3}m$	1.10	[24]
$CsNiAlF_6$	10.06			$Fd\bar{3}m$	1.23	[25]
$CsNiFeF_6$	10.35			$Fd\bar{3}m$	1.20	[25]
$CsNiNiF_6$	7.122	7.350	10.025	*Imma*	1.19	[2]
$RbNiNiF_6$	6.946	7.333	9.768	*Imma*	1.19	[2]
$CsCuCuF_6$	7.067(1)	7.277(1)	10.322(1)	*Imma*	1.28	[3]
$CsAgFeF_6$	7.338	7.564	10.554	*Pnma*	1.57	[19]
$CsAgAlF_6$	7.38	7.241	10.352	*Pnma*	1.60	[19]
$KCuAlF_6$	6.731(1)	7.040(1)	9.793(1)	*Pnma*	1.29	[3]
$RbPdAlF_6$	7.2901(1)	7.111(1)	10.065(2)	*Pnma*	1.48	[20]
$CsPdAlF_6$	7.523(1)	7.161(1)	10.258(1)	*Pnma*	1.48	[21]
NH_4CoAlF_6	7.134(1)	7.052(2)	9.930(2)	*Pnma*	1.17	[22]



Representatives

$RbMgNiF_6$, $RbNiCoF_6$, $RbCoCrF_6$, $RbNiCrF_6$, $CsNiAlF_6$, $CsNiFeF_6$, NH_4CoAlF_6

———

$RbNiNiF_6$, $CsNiNiF_6$, $CsCuCuF_6$

$KCuAlF_6$, $RbPdAlF_6$, $CsAgFeF_6$, $CsAgAlF_6$, $CsPdAlF_6$, NH_4CoAlF_6

Exercise 1: $KCuCrF_6$

Space group $P2_1/c$

Lattice parameter:

$a = 7.256$ Å, $b = 9.933$ Å, $c = 6.750$Å, $\beta = 92.61°$

		x	y	z
Cu 1	4e	0.2534	0.2660	0.8172
Cr 1	2b	0.5	0	0
Cr 2	2a	0	0	0
K 1	4e	0.2429	0.8844	0.4956
F 1	4e	0.9811	0.1663	0.8726
F 2	4e	0.5068	0.8239	0.1041
F 3	4e	0.2475	0.3290	0.0783
F 4	4e	0.7531	0.0183	0.0799
F 5	4e	0.0732	0.0851	0.2412
F 6	4e	0.5560	0.5649	0.2499

Exercise 1:

Is the structure of $KCuCrF_6$ related to the pyrochlore structures?

If yes, what is the relationship?

How many twin domains would you expect to form in this compound?

Exercise 2:

Compare the pseudosymmetry of $CsMgInF_6$, $CsPdAlF_6$ and $CsNiNiF_6$ with respect to space group Fd-3m.

If you disregard the disorder on the B/B'-site, which of the three structures has the highest pseudosymmetry?

Exercise 3: Group-subgroup relations in the Pyrochlore family

Looking at the group subgroup relationships in the fluoride pyrochlore family, it is striking that there are no compounds crystallizing in space group $I4_1/amd$.

Can you find an explanation?

Exercise 4: Twinning in $Ag_4Mn_3O_8$

$Ag_4Mn_3O_8$ is a Ag ionic conductor. It crystallizes in space group P3121 with lattice parameter a=12.5919(1) and c=15.4978(1)Å.

The investigated crystal is a fourfold twin.

Can you find a relationship between the crystal structure and the formation of twins?