Group-Subgroup Relations of Space Groups

I. Subgroups

II. Wyckoff-position splittings

III. Supergroups of space groups

IV. Crystal-structure relationships

Subgroups: Some basic results (summary)

Subgroup H < G

1. $H=\{e,h_1,h_2,\ldots,h_k\} \subset G$
2. H satisfies the group axioms of G

Proper subgroups H < G, and

trivial subgroup: {e}, G

Index of the subgroup H in G: $[i]=|G|/|H|$

(order of G)/(order of H)

Maximal subgroup H of G

NO subgroup Z exists such that:

$$H < Z < G$$

Coset decomposition G:H

Group-subgroup pair H < G

left coset decomposition

$G=H+g_2H+\ldots+g_mH,\ g_i \notin H,$
m=index of H in G

right coset decomposition

$G=H+Hg_2+\ldots+Hg_m,\ g_i \notin H$
m=index of H in G

Normal subgroups

$Hg_j = g_jH$, for all $g_j = 1, \ldots, [i]$

Conjugate subgroups

Conjugate subgroups Let $H_1 < G$, $H_2 < G$

then, $H_1 \sim H_2$, if $\exists\, g \in G$: $g^{-1} H_1 g = H_2$

(i) Classes of conjugate subgroups: $L(H)$

(ii) If $H_1 \sim H_2$, then $H_1 \cong H_2$

(iii) $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroup

$H \lhd G$, if $g^{-1} H g = H$, for $\forall g \in G$

Subgroups of Space groups

Coset decomposition $G:T_G$

$(I,0)$	(W_2,w_2)	...	(W_m,w_m)	...	(W_i,w_i)
(I,t_1)	(W_2,w_2+t_1)	...	(W_m,w_m+t_1)	...	(W_i,w_i+t_1)
(I,t_2)	(W_2,w_2+t_2)	...	(W_m,w_m+t_2)	...	(W_i,w_i+t_2)
...	...	...	...	...	...
(I,t_j)	(W_2,w_2+t_j)	...	(W_m,w_m+t_j)	...	(W_i,w_i+t_j)
...	...	...	...	...	...

Factor group G/T_G

isomorphic to the point group P_G of G

Point group $P_G = \{I, W_1, W_2, ..., W_i\}$

Translationengleche subgroups H<G:

$$\begin{cases} T_H = T_G \\ P_H < P_G \end{cases}$$

Example: P2/m

Coset decomposition

T_G	$T_G\,2$	$T_G\,\bar{1}$	$T_G\,m$
$(I,0)$	$(2,0)$	$(\bar{1},0)$	$(m,0)$
(I,t_1)	$(2,t_1)$	$(\bar{1}, t_1)$	(m, t_1)
(I,t_2)	$(2,t_2)$	$(\bar{1}, t_2)$	(m,t_2)
...	...	...	...
(I,t_j)	$(2,t_j)$	$(\bar{1}, t_j)$	(m, t_j)
...	...	...	...

t-subgroups:

$H_1 = T_G \cup T_G 2$
P2

$H_2 = T_G \cup T_G \bar{1}$

$H_3 = T_G \cup T_G m$
Pm

EXERCISES

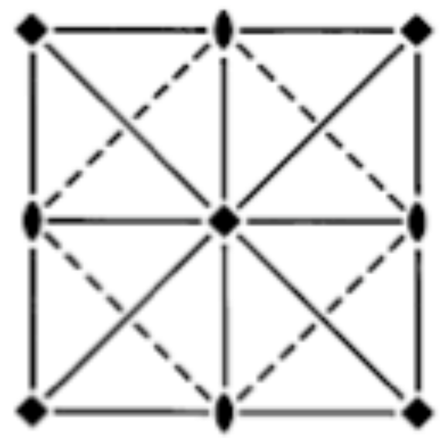
Problem 4.1

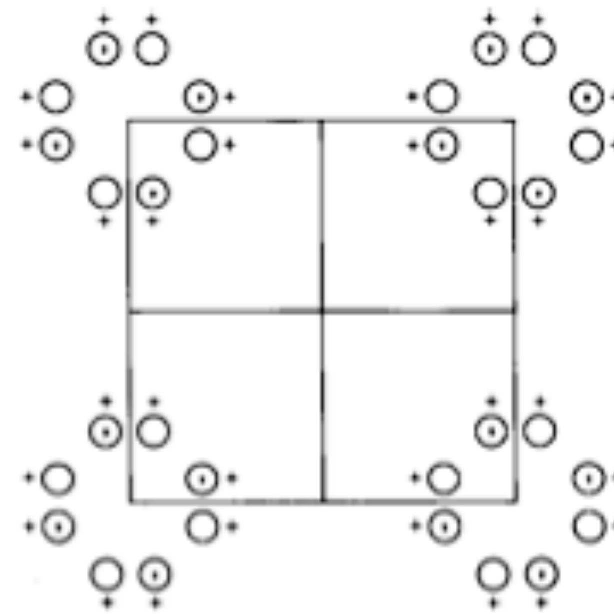
Construct the diagram of the *t*-subgroups of *P*4*mm* using the 'analogy' with the subgroup diagram of 4*mm*

International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$ $\quad C_{4v}^{1}$ $\quad 4mm$ $\quad$ Tetragonal

No. 99 $\quad P4mm$ $\quad$ Patterson symmetry $P4/mmm$





Origin on $4mm$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

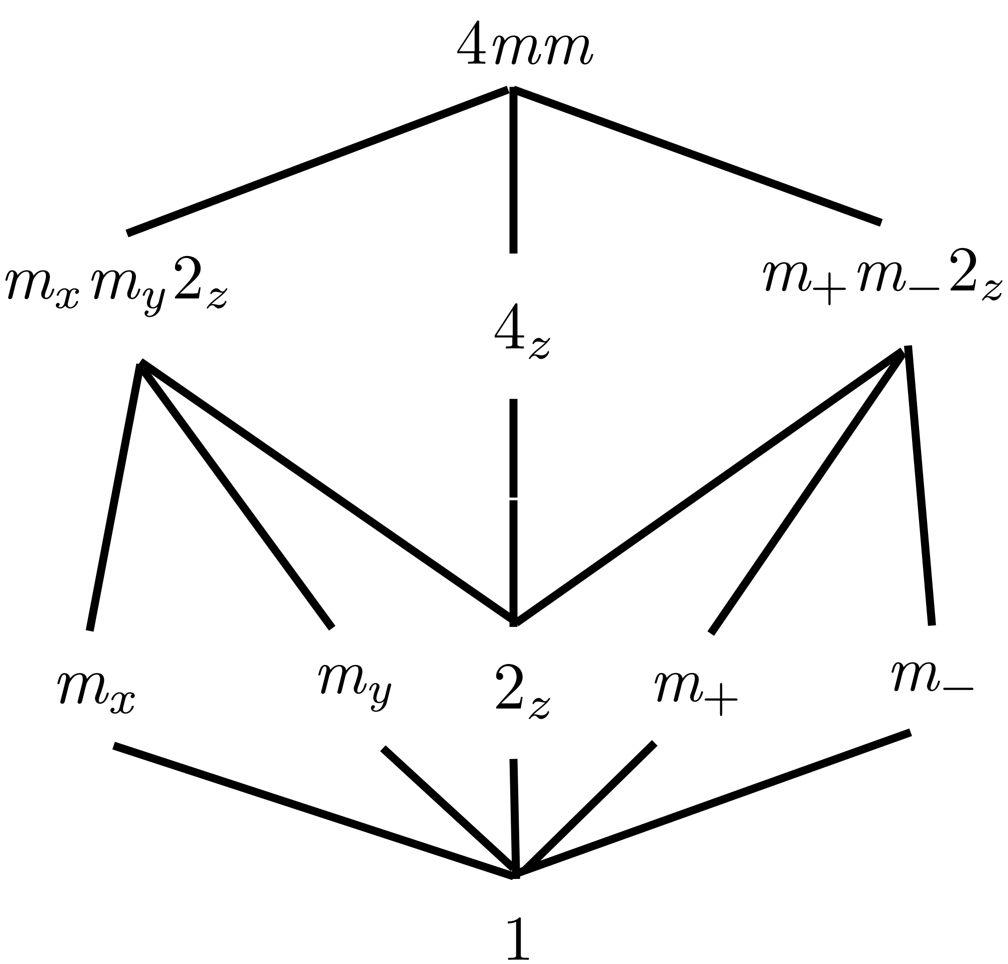
Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Problem 4.1

SOLUTION



Subgroup diagram of point group *4mm*

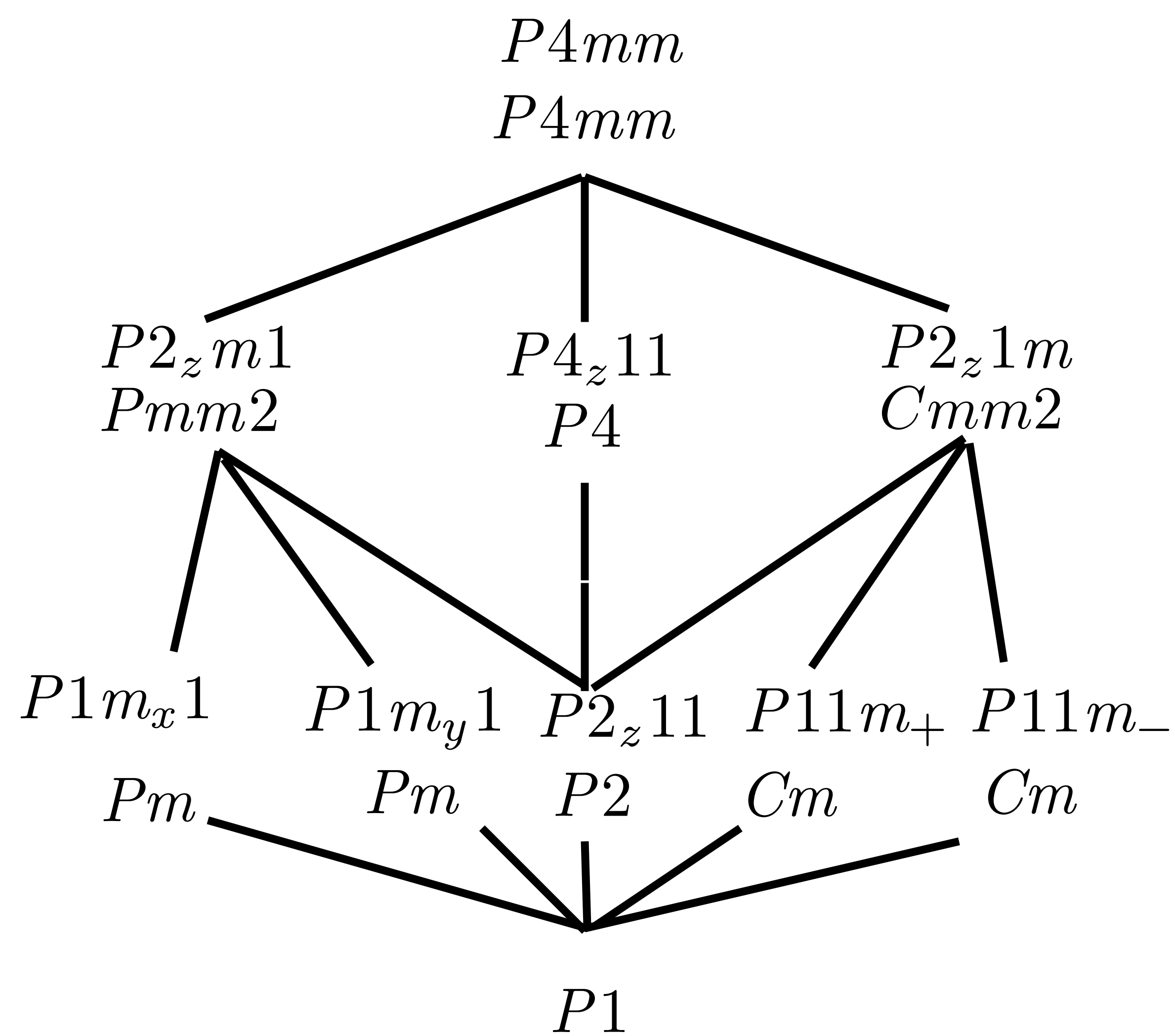
index

[1]

[2]

[4]

[8]

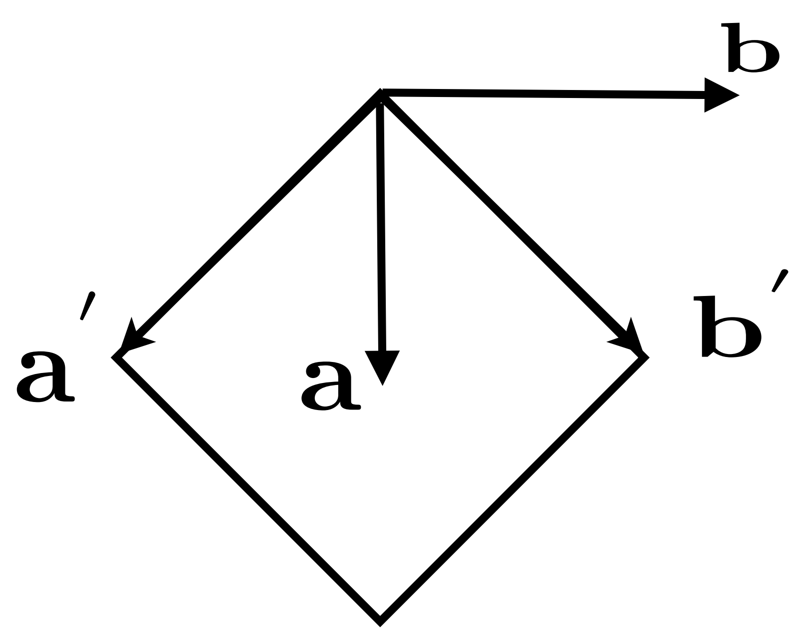


Translationengleiche subgroups of space group *P4mm*

Problem 4.1

SOLUTION

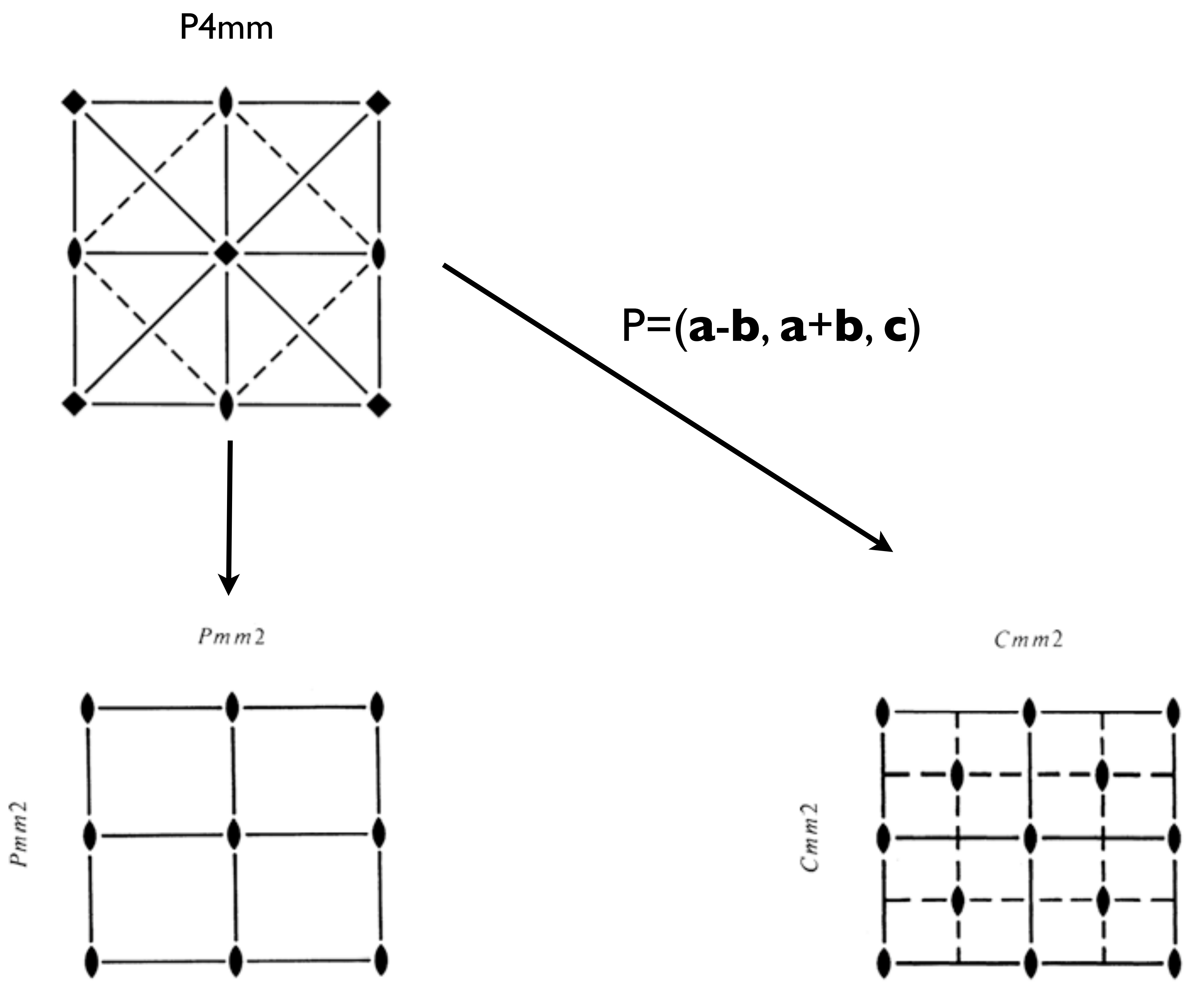
Remark 1. Due to the convention to choose the basis vectors parallel to the rotation axes, C-centered cells appear although the translation lattice has not changed. If the retained twofold axes are diagonal, the conventional basis vectors **a',b',c'** of the subgroup are **a'** $=$ **a-b, b'** $=$ **a+b, c'** $=$ **c** with respect to the basis vectors **a,b,c** of $P4mm$. Referred to **a',b',c'** the cell is C-centered



Change of basis vectors: **a**'=**a-b**, **b**'=**a+b**

Problem 4.1

SOLUTION



Klassengleiche subgroups H<G: non-isomorphic

$$\begin{cases} T_H < T_G \\ P_H = P_G \end{cases}$$

Example: C2

Coset decomposition

t_i=integer

t_c=1/2,1/2,0

T_i	$T_i t_c$	$T_i\,2$	$T_i t_c\,2$
(1,0)	(1,t_c)	(2, 0)	(2,t_c)
(1,t_1)	(1,t_1+t_c)	(2, t_1)	(2, t_1+t_c)
(1,t_2)	(1,t_2+t_c)	(2, t_2)	(2, t_2+t_c)
...	...	...	...
(1,t_j)	(1,t_j+t_c)	(2, t_j)	(2, t_j+t_c)
...	...	...	...

k-subgroups: $H_1 = T_i \cup T_i 2$ (P2) $\quad H_2 = T_i \cup T_i t_c\, 2$ ($P2_1$)

Klassengleiche subgroups H<G: isomorphic

$\begin{cases} T_H < T_G \\ P_H = P_G \end{cases}$

Example: P1

$\boldsymbol{t}$=u$\boldsymbol{a}$+v$\boldsymbol{b}$+w$\boldsymbol{c}$

Coset decomposition

$T_e=\{\boldsymbol{t}(u=2n,v,w)\}$

$\boldsymbol{t}_a(a,0,0)$

T_e	$T_e\, t_a$
(I,0)	(I,t_a)
(I,t_1)	(I,t_1+t_a)
(I,t_2)	(I,t_2+t_a)
...	...
(I,t_j)	(I,t_j+t_a)
...	...

isomorphic *k*-subgroups:

P1(2$\boldsymbol{a}$,$\boldsymbol{b}$,$\boldsymbol{c}$)

$H_1=T_e$

Problem 4.2

Determine the k-subgroups of *Pnma*, No. 53 that are obtained by doubling of the *b* lattice parameter

Hint: split the cosets of *Pnma* relative to T_G into cosets with respect to T_H

Problem 4.2

SOLUTION

Splitting of the translation subgroup T_G

$$T_G \xrightarrow{\text{splits}} T_H \cup T_H t_b$$

$T_H = \{t(u, v=2n, w)\}$

$t_b=(0,b,0)$

Splitting of the generator cosets

generator	(2)	$\longrightarrow$	$\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$	and	$\bar{x}+\frac{1}{2}, \bar{y}+1, z+\frac{1}{2}$
generator	(3)	$\longrightarrow$	$\bar{x}+\frac{1}{2}, y, \bar{z}+\frac{1}{2}$	and	$\bar{x}+\frac{1}{2}, y+1, \bar{z}+\frac{1}{2}$
generator	(5)	$\longrightarrow$	$\bar{x}, \bar{y}, \bar{z}$	and	$\bar{x}, \bar{y}+1, \bar{z}$

Referred to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}' = \mathbf{a}, 2\mathbf{b}, \mathbf{c}$, it is written as:

$(2)'$	$\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$	$(2)''$	$\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$
$(3)'$	$\bar{x}+\frac{1}{2}, y, \bar{z}+\frac{1}{2}$	$(3)''$	$\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}+\frac{1}{2}$
$(5)'$	$\bar{x}, \bar{y}, \bar{z}$	$(5)''$	$\bar{x}, \bar{y}+\frac{1}{2}, \bar{z}$

Problem 4.2

SOLUTION

k-subgroups for b'=2b

$$
\begin{array}{llll}
(2)' & (3)' & (5)' & \sim \; Pmna\,(\text{isomorphic}) \\
(2)' & (3)' & (5)'' & \sim \; Pbnn\,(Pnna) \\
(2)' & (3)'' & (5)' & \sim \; Pbna\,(Pbcn) \\
(2)' & (3)'' & (5)'' & \sim \; Pmnn\,(Pnnm) \\
(2)'' & (3)' & (5)' & \sim \; Pbnn\,(Pnna) \\
(2)'' & (3)' & (5)'' & \sim \; Pmna\,(\text{isomorphic}) \\
(2)'' & (3)'' & (5)' & \sim \; Pmnn\,(Pnnm) \\
(2)'' & (3)'' & (5)'' & \sim \; Pbna\,(Pbcn)
\end{array}
$$

Example: (2)' (5)' $\longrightarrow$ a_z

(2)'' (5)' $\longrightarrow$ n_z

Data on maximal subgroups of space groups in *International Tables for Crystallography*, Vol.A1 (*ITA1*)

$R3$ No. 146 $R3$ C_3^4

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
9	*b*	1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$

I Maximal *translationengleiche* subgroups

[3] $R1$ (1, $P1$)	1+	$\mathbf{a},\mathbf{b},1/3(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3_2$ (145)	1; $2+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; $3+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		0,1/3,0
[3] $P3_1$ (144)	1; $2+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $3+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		1/3,1/3,0
[3] $P3$ (143)	1; 2; 3		

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$

$R3$ (146)	⟨2⟩	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	

[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$

$R3$ (146)	⟨2⟩	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R3$ (146)	⟨$2+(1,-1,0)$⟩	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,0

Maximal subgroups of *P*4mm (No. 99)

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4	
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$
[2] $P2m1$ (25, $Pmm2$)	1; 2; 5; 6	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$

$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$

Remarks

[i] HMS1 (No., HMS2) Sequence matrix shift

{ braces for conjugate subgroups

***(P, p)*:** $O_H = O_G + p$

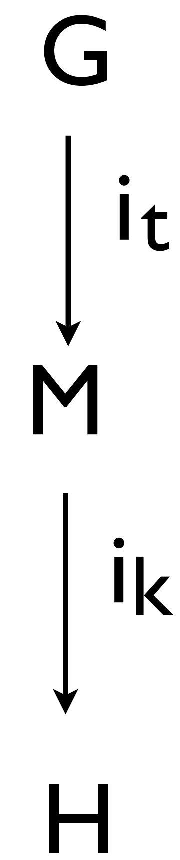
$(a_H, b_H, c_H) = (a_G, b_G, c_G)\, P$

General subgroups $H<G$:

$$\begin{cases} T_H < T_G \\ P_H < P_G \end{cases}$$

Theorem Hermann, 1929:

For each pair $G>H$, there exists a uniquely defined intermediate subgroup M, $G \geqq M \geqq H$, such that:



M is a *t-subgroup* of G

H is a *k-subgroup* of M

Corollary

A maximal subgroup is either a *t*- or *k*-subgroup

Index [i] for a group-subgroup pair G>H

Hermann, 1929:

$[i]=[i_P].[i_L]$

$\mathcal{G}$

↓ $i_P=P_G/P_H$

$\mathcal{M}$

↓ $i_L=Z_H/Z_G$

$\mathcal{H}$

Example: $Pb_3(VO_4)_2$

$[i]=3.2=6$

$R\text{-}3m$

↓ $i_P=P_G/P_H=3$

$C2/m$

↓ $i_L=Z_H/Z_G=2$

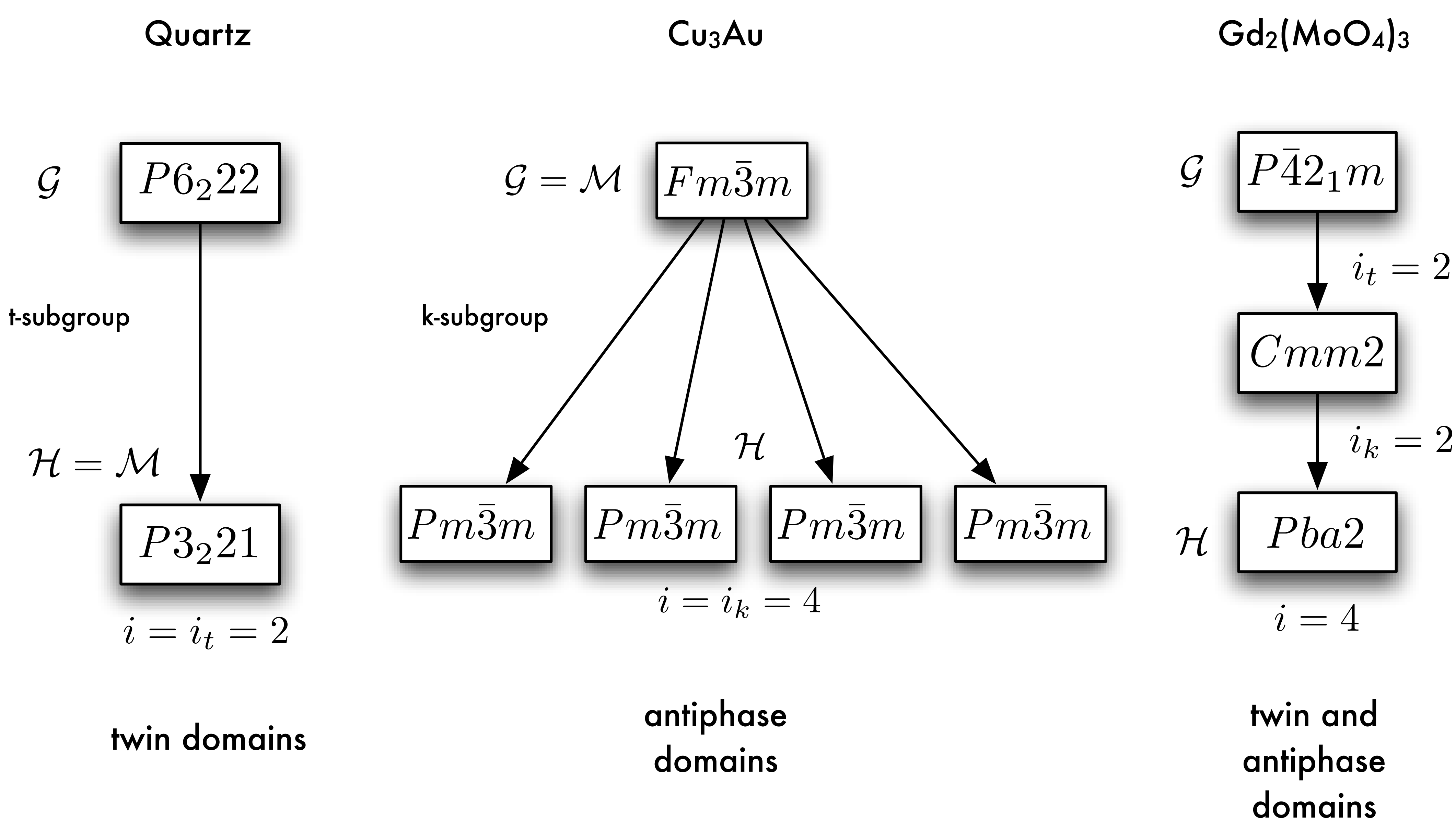
$P2_1/c$

$\mathcal{M}$ is a *t*-subgroup of $\mathcal{G}$

$\mathcal{H}$ is a *k*-subgroup of $\mathcal{M}$

Problem: CLASSIFICATION OF DOMAINS

HERMANN



Problem 4.3

At high temperatures, $BiTiO_3$ has the cubic perovskite structure, space group Pm-3m. Upon heating, it distorts to the space group P4mm. Can we expect twinned crystals of the low symmetry form? If so, how many kinds of domains?

Problem 4.4

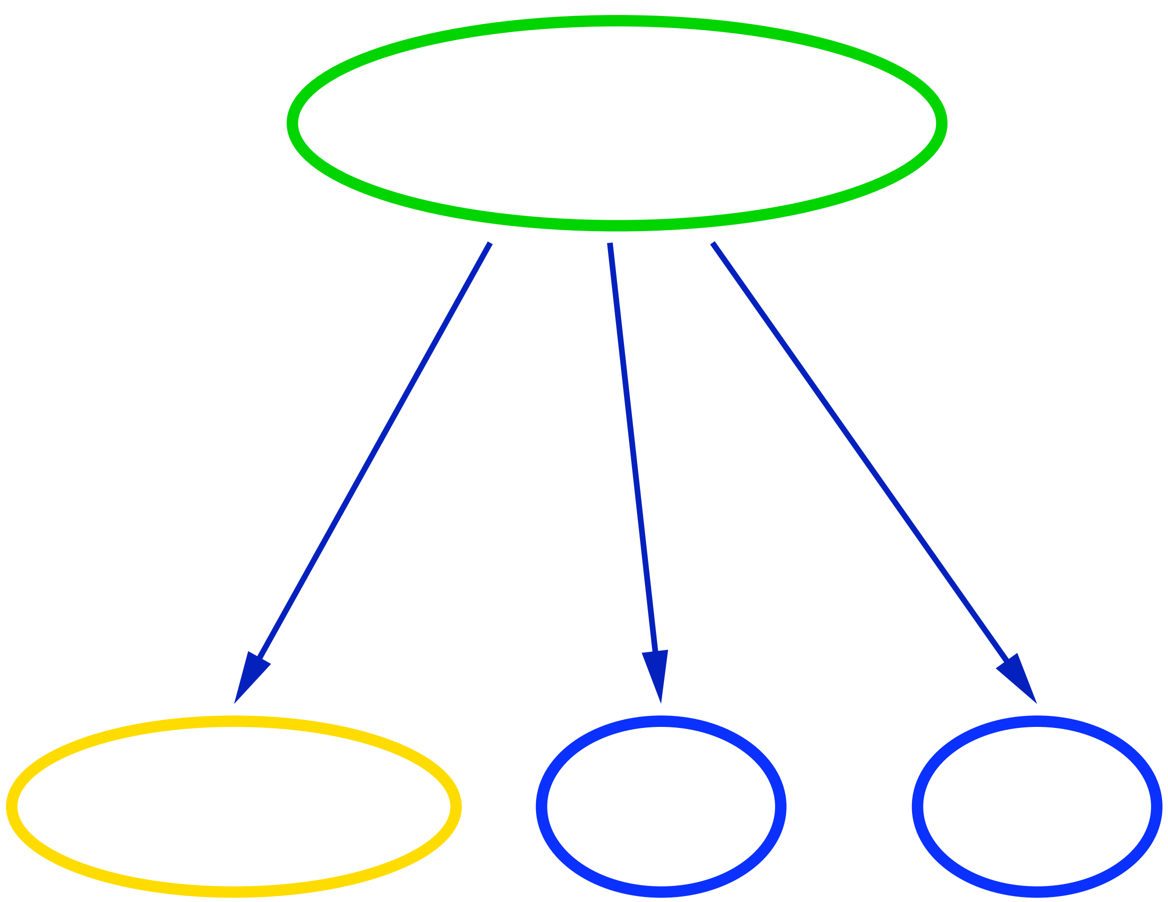
$SrTiO_3$ has the cubic perovskite structure, space group Pm-3m. Upon cooling below 105K, the coordination octahedra are mutually rotated and the space group is reduced to I4/mcm; c is doubled and the unit cell is increasd by the factor of four. Can we expect twinned crystals of the low symmetry form? If so, how many kinds of domains?

Relations between Wyckoff positions

General splitting rules

(Wondratschek 1993,1995)

$\mathcal{W}^{\mathcal{G}}$



$\mathcal{W}_i^{\mathcal{H}}$

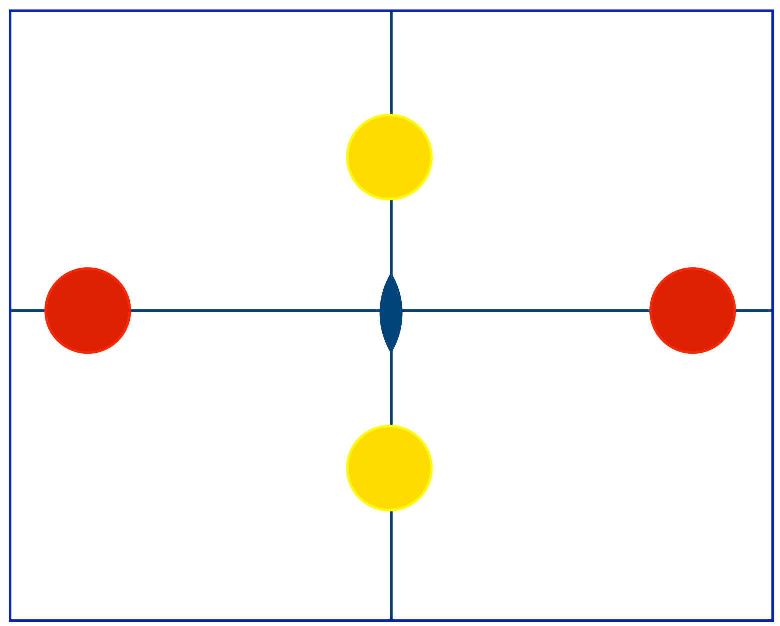
$$\mathcal{G} > \mathcal{H},\ (\mathrm{P}, \mathrm{p})$$

$$R_i = \frac{|\mathcal{S}_{\mathcal{G}}(X)|}{|\mathcal{S}_{\mathcal{H}}(X_i)|}$$

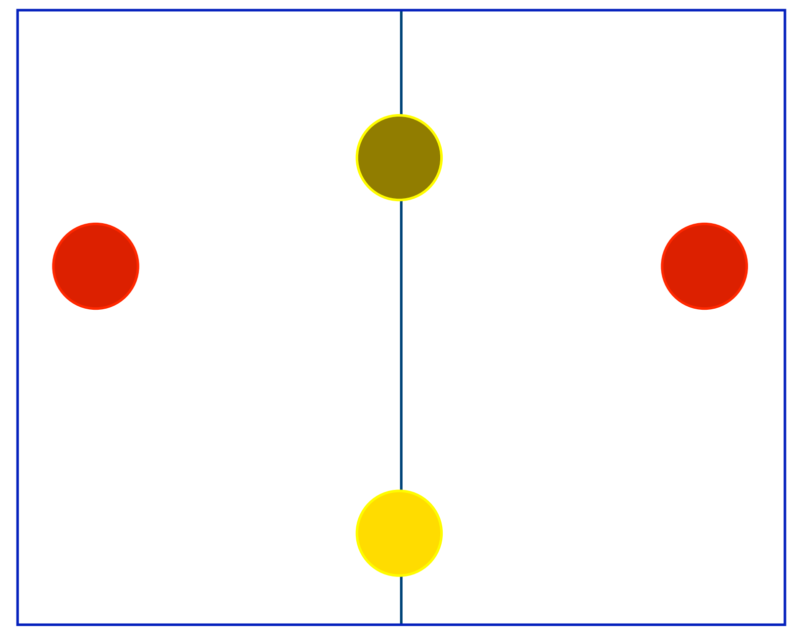
$$[i] = \sum_{i=1}^{q} R_i$$

Relations between Wyckoff positions

$$\mathcal{G} = \mathrm{P}mm2 > \mathcal{H} = \mathrm{P}m, \;\; [i] = 2$$



$S_0, \;\mathcal{G} = \mathrm{P}mm2$



$S_1, \;\mathcal{H} = \mathrm{P}m$

2*h* m.. (1/2,y,z) → 2*c* 1 (x,y,z)

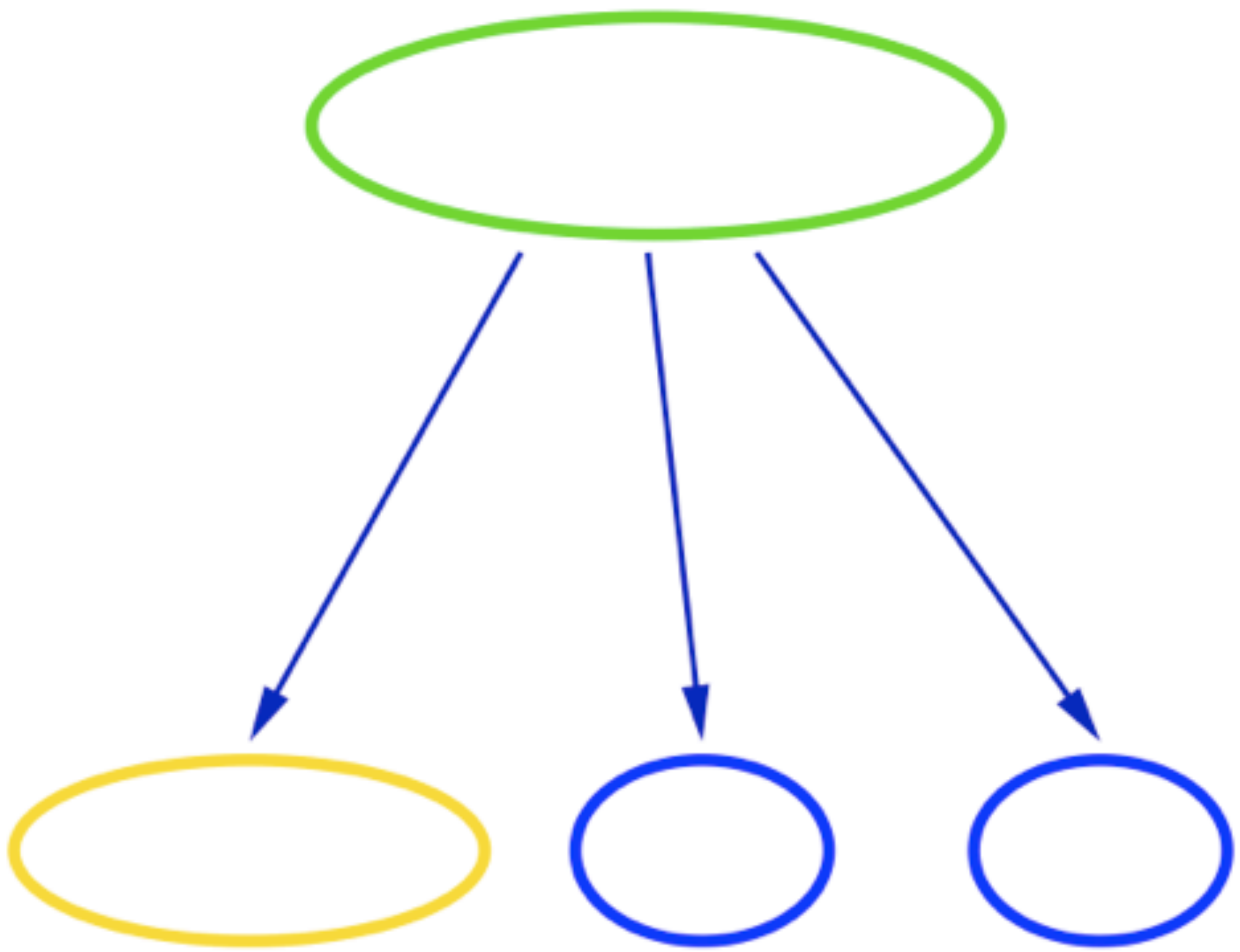
2*f* .m. (x,1/2,z) → 1*b* m (x_2,1/2,z_2)
→ 1*b* m (x_1,1/2,z_1)

SYMMETRY REDUCTION

General splitting rules

(Wondratschek 1993,1995)

$\mathcal{W}^{\mathcal{G}}$



$\mathcal{W}_i^{\mathcal{H}}$

$$\mathcal{G} > \mathcal{H},\ (\mathrm{P}, \mathbf{p})$$

$$R_i = \frac{|\mathcal{S}_{\mathcal{G}}(X)|}{|\mathcal{S}_{\mathcal{H}}(X_i)|}$$

$$[i] = \sum_{i=1}^{q} R_i$$

Restrictions on the splitting schemes:

(i) $G \triangleright H$: H a normal subgroup of G

$R_i = R$ in $[i] = \sum R_i$

(ii) $G \geq Z \geq H$:

splitting $G \longrightarrow H$ { Splitting $G \longrightarrow Z$; Splitting $Z \longrightarrow H$ }

Example: G>H, [i]=4

(i) one orbit: $R=4$

(ii) two orbits: $R_1 = R_2 = 2$

$R_1 = 3, R_2 = 1$

(iii) three orbits: $R_1 = R_2 = 1$

$R_3 = 2$

(iv) four orbits:

$R_1 = R_2 = R_3 = R_4 = 1$

General procedure:

Given G, H < G, index [i] and (P,p)

-transform $(\text{data})_G \longrightarrow (\text{data})_H$

1. Right-coset decomposition

$$G = H + Hg_2 + \ldots + Hg_k$$

2. General-position orbit splitting

$$O_G(X_o)=O_H(X_{o,1})+O_H(X_{o,2})+ \ldots +O_H(X_{o,k})$$

3. Special-position orbit splitting

(i) substitution of parameters: $O_H(X_{o,j}) \longrightarrow O_H(X_j)$

(ii)assignment of $O_H(X_j)$ to the WP of H

Example:

G=$P4_2mnm$

H=$Cmmm$ [i]=2, $a'=a-b$, $b'=a+b$, $c'=c$

1. General-orbit splitting

$$16k\ 1\ (x,y,z) \rightarrow 16r\ 1\ (x_1,y_1,z_1) \cup 16r\ 1\ (x_2,y_2,z_2)$$

Orbit 1	Orbit 2
(x,y,z)	(-y,x+1/2,z+1/2)
(-x,-y,z)	(y,-x+1/2,z+1/2)
(-x,y,-z)	(y,x+1/2,-z+1/2)
(x,-y,-z)	(-y,-x+1/2,-z+1/2)
(-x,-y,-z)	(y,-x+1/2,-z+1/2)
(x,y,-z)	(-y,x+1/2,-z+1/2)
(x,-y,z)	(-y,-x+1/2,z+1/2)
(-x,y,z)	(y,x+1/2,z+1/2)
+ t(1/2,1/2,0)	+ t(1/2,1/2,0)

coset representatives: (x,y,z) and (y,x+1/2,z+1/2)

2. Special-orbit splitting: 2a 0,0,0

(i) Substitution of parameters

general		special
x,y,z	→	0,0,0
Orbit 1: x,y,z	→	0,0,0
Orbit 2: y,x+1/2,z+1/2	→	0,1/2,1/2

(ii) Assignment

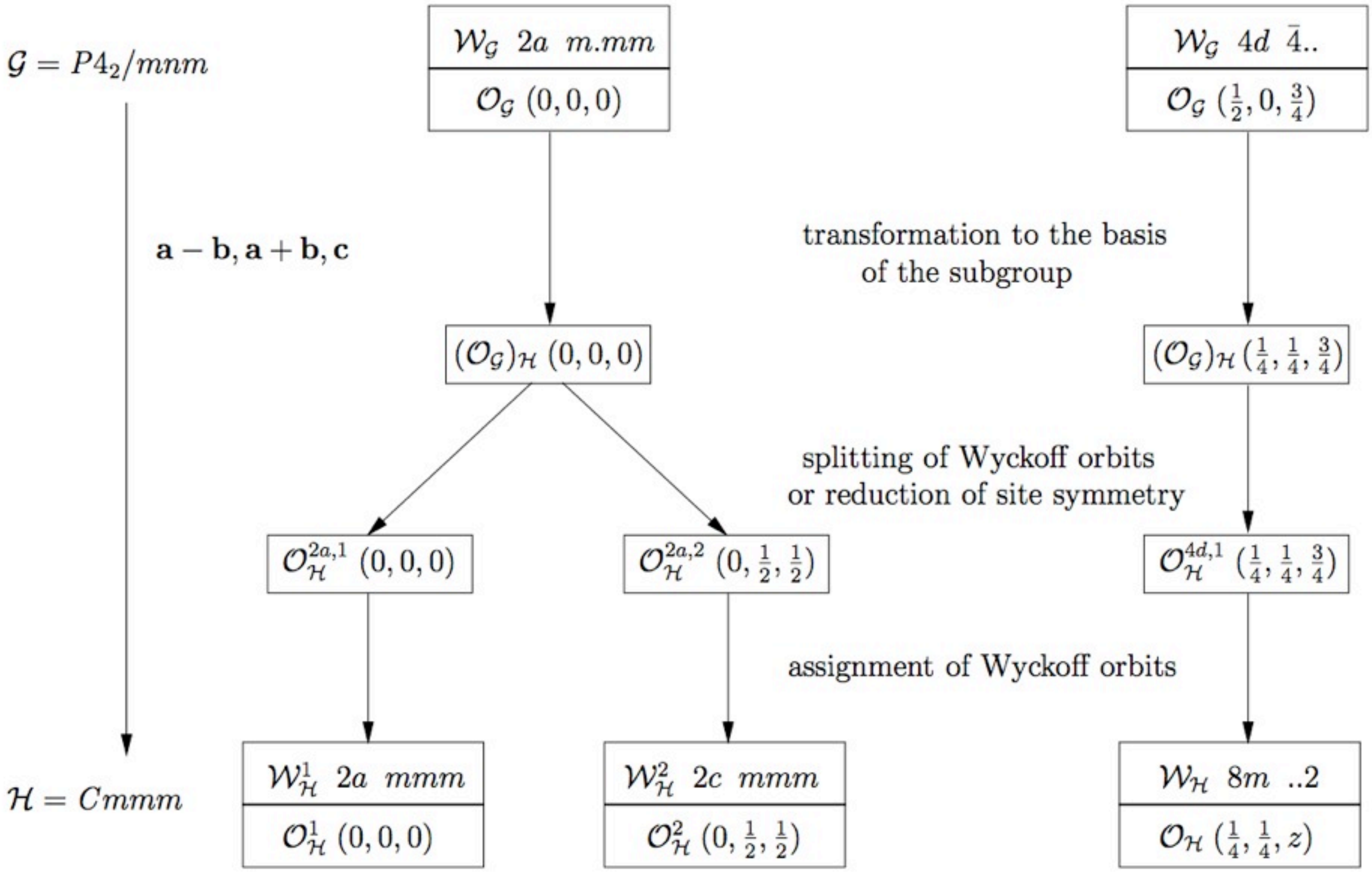
0,0,0 → $(2a)_{Cmmm}$

0,1/2,1/2 → $(2c)_{Cmmm}$

Splitting: $(2a)_{P4_2/mnm}$ → $(2a)_{Cmmm}$ + $(2c)_{Cmmm}$

Wyckoff position splitting

Example:



Example: WYCKSPLIT: $P4_2/mnm > Cmmm$, index 2

Wyckoff Positions Splitting

136 ($P4_2/mnm$) > 65 ($Cmmm$)

Splitting of Wyckoff position 4g

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, -x, 0)	(x, 0, 0)	$4g_1$	(x_1, 0, 0)
2	(-x, x, 0)	(-x, 0, 0)		($-x_1$, 0, 0)
3	(x+1, -x, 0)	(x+1/2, 1/2, 0)		(x_1+1/2, 1/2, 0)
4	(-x+1, x, 0)	(-x+1/2, 1/2, 0)		($-x_1$+1/2, 1/2, 0)
5	(x+1/2, x+1/2, 1/2)	(0, x+1/2, 1/2)	$4j_1$	(0, y_2, 1/2)
6	(-x+1/2, -x+1/2, 1/2)	(0, -x+1/2, 1/2)		(0, $-y_2$, 1/2)
7	(x+1/2, x-1/2, 1/2)	(1/2, x, 1/2)		(1/2, y_2+1/2, 1/2)
8	(-x+1/2, -x-1/2, 1/2)	(1/2, -x, 1/2)		(1/2, $-y_2$+1/2, 1/2)

Problem 5.1

Consider the group -subgroup pair *P4mm*>*Cm*

[i]=4, ***a'=a-b, b'=a+b, c'=c***

Determine the splitting schemes for WPs 1a,1b, 2c, 4d

group *P4mm*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z
4	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$
4	e	. m .	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$
4	d	. . m	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$
2	c	2 m m .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$		
1	b	4 m m	$\frac{1}{2},\frac{1}{2},z$			
1	a	4 m m	$0,0,z$			

subgroup *Cm*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$	
4	b	1	(1) x,y,z	(2) $x,\bar{y},z$
2	a	m	$x,0,z$	

Problem 5.1

SOLUTION

General-position splitting

coset 1	coset 2	coset 3	coset 4
Cm	$Cm\,(\bar{x},\bar{y},z)$	$Cm\,(\bar{y},\bar{x},z)$	$Cm\,(y,x,z)$
x,y,z	$\bar{x},\bar{y},z$	$\bar{y},\bar{x},z$	y,x,z
$x,\bar{y},z$	$\bar{x},y,z$	$\bar{y},x,z$	$y,\bar{x},z$
$x+1/2,y+1/2,z$	$\bar{x}+1/2,\bar{y}+1/2,z$	$\bar{y}+1/2,\bar{x}+1/2,z$	$y+1/2,x+1/2,z$
$x+1/2,\bar{y}+1/2,z$	$\bar{x}+1/2,y+1/2,z$	$\bar{y}+1/2,x+1/2,z$	$y+1/2,\bar{x}+1/2,z$

Special-position splittings

$1a\ 4mm\ (0,0,z) \rightarrow 2a\ m\ (x,0,z).$

$1b\ 4mm\ (0,1/2,z) \rightarrow 2a\ m\ (x,0,z),$

$2c\ 2mm.\ (1/4,1/4,z) \rightarrow 4b\ 1\ (x,y,z)$

$4d\ ..m\ (0,x,z) \rightarrow 2a\ m\ (x,0,z) \cup 2a\ m\ (\bar{x},0,z) \cup 4b\ 1\ (x,y,z).$

Problem 5.1

Splitting of the Wyckoff positions:
P4mm > *Cm* (by direct inspection)

Transformation of coordinates:

$$P = \begin{pmatrix} 1 & 1 & \\ -1 & 1 & \\ & & 1 \end{pmatrix} \quad P^{-1} = \begin{pmatrix} 1/2 & -1/2 & \\ 1/2 & 1/2 & \\ & & 1 \end{pmatrix}$$

Cm *P4mm*

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1/2 & -1/2 & \\ 1/2 & 1/2 & \\ & & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Splitting schemes:

1a 4mm (00z) ⟶ 2a m (x0z)

2c 2mm. (1/20z) ⟶ 4b 1 (xyz)

Data on Relations between Wyckoff Positions in *International Tables for Crystallography*, Vol. A1

D_{4h}^{14} $P4_2/m2_1/n2/m$ No. 136 $P4_2/mnm$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$ $4g$	$4c$ $8h$	$4d$ $8i$	$4e$ $8j$	$4f$ $16k$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}n2$ (118)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2d$	$2c$ $4f$	$4e$ $2\times4e$	$2a;2b$ $8i$	$4h$ $8i$	$4g$ $2\times8i$
[2] $P\bar{4}2_1m$ (113)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$ $4e$	$4d$ $2\times4d$	$2a;2b$ $8f$	$2\times2c$ $2\times4e$	$4e$ $2\times8f$
[2] $P4_2nm$ (102)			$2a$	$2a$ $4c$	$4b$ $2\times4b$	$4b$ $8d$	$2\times2a$ $2\times4c$	$4c$ $2\times8d$
[2] $P4_22_12$ (94)			$2a$	$2b$ $4f$	$4d$ $2\times4d$	$4d$ $8g$	$4c$ $8g$	$4e$ $2\times8g$
[2] $P4_2/m$ (84)		$x+\frac{1}{2},y,z$	$2d$	$2c$ $4j$	$2a;2b$ $4g;4h$	$2e;2f$ $2\times4j$	$4i$ $8k$	$4j$ $2\times8k$
[2] $Pnnm$ (58)			$2a$	$2b$ $4g$	$2c;2d$ $2\times4f$	$4f$ $2\times4g$	$4e$ $8h$	$4g$ $2\times8h$
[2] $Cmmm$ (65)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2c$	$2b;2d$ $4g;4j$	$4e;4f$ $2\times8m$	$8m$ $8p;8q$	$4k;4l$ $8n;8o$	$4h;4i$ $2\times16r$

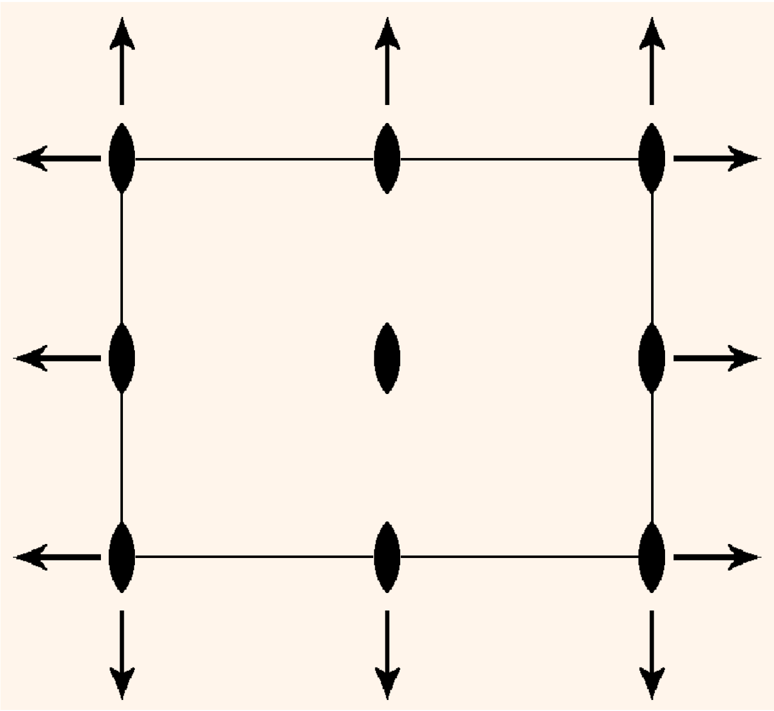
*ITA*1 Space group $P4_2/mnm$ (selection)

D_{4h}^{14} $P4_2/m2_1/n2/m$ No. 136 $P4_2/mnm$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$ $4g$	$4c$ $8h$	$4d$ $8i$	$4e$ $8j$	$4f$ $16k$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}n2$ (118)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2d$	$2c$ $4f$	$4e$ $2\times4e$	$2a;2b$ $8i$	$4h$ $8i$	$4g$ $2\times8i$
[2] $P\bar{4}2_1m$ (113)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$ $4e$	$4d$ $2\times4d$	$2a;2b$ $8f$	$2\times2c$ $2\times4e$	$4e$ $2\times8f$
[2] $P4_2nm$ (102)			$2a$	$2a$ $4c$	$4b$ $2\times4b$	$4b$ $8d$	$2\times2a$ $2\times4c$	$4c$ $2\times8d$
[2] $P4_22_12$ (94)			$2a$	$2b$ $4f$	$4d$ $2\times4d$	$4d$ $8g$	$4c$ $8g$	$4e$ $2\times8g$
[2] $P4_2/m$ (84)		$x+\frac{1}{2},y,z$	$2d$	$2c$ $4j$	$2a;2b$ $4g;4h$	$2e;2f$ $2\times4j$	$4i$ $8k$	$4j$ $2\times8k$
[2] $Pnnm$ (58)			$2a$	$2b$ $4g$	$2c;2d$ $2\times4f$	$4f$ $2\times4g$	$4e$ $8h$	$4g$ $2\times8h$
[2] $Cmmm$ (65)	**a−b,** **a+b, c**	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2c$	$2b;2d$ $4g;4j$	$4e;4f$ $2\times8m$	$8m$ $8p;8q$	$4k;4l$ $8n;8o$	$4h;4i$ $2\times16r$

Example

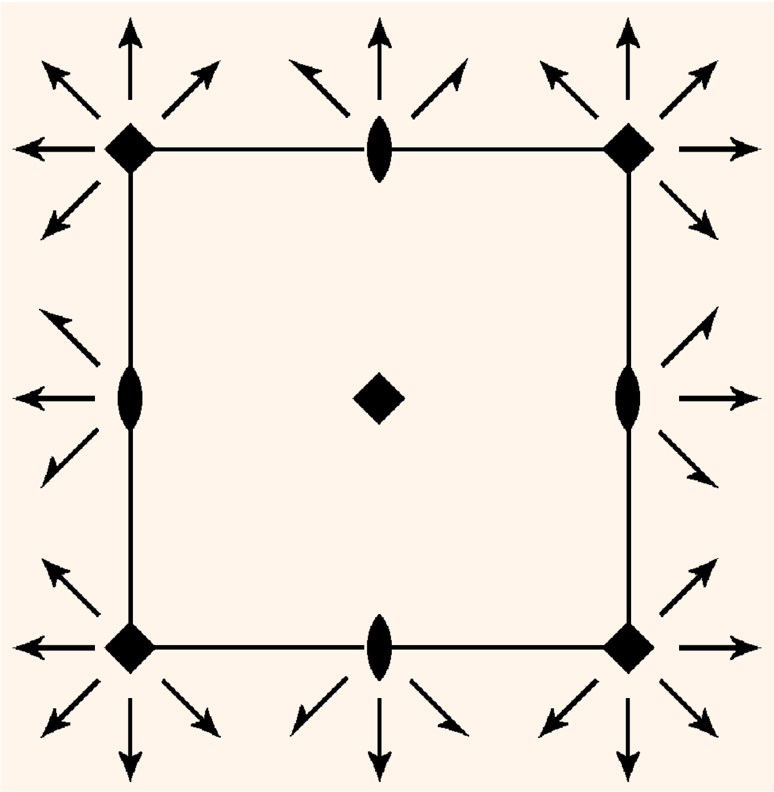
Supergroups of the same type



$$\mathcal{H} = \mathrm{P}\mathbf{222}$$

$$\mathcal{G} = \mathrm{P}\mathbf{422}$$

$$\mathrm{P}\mathbf{422} = \mathrm{P}\mathbf{222} + (\mathbf{4}|\omega)\mathrm{P}\mathbf{222}$$

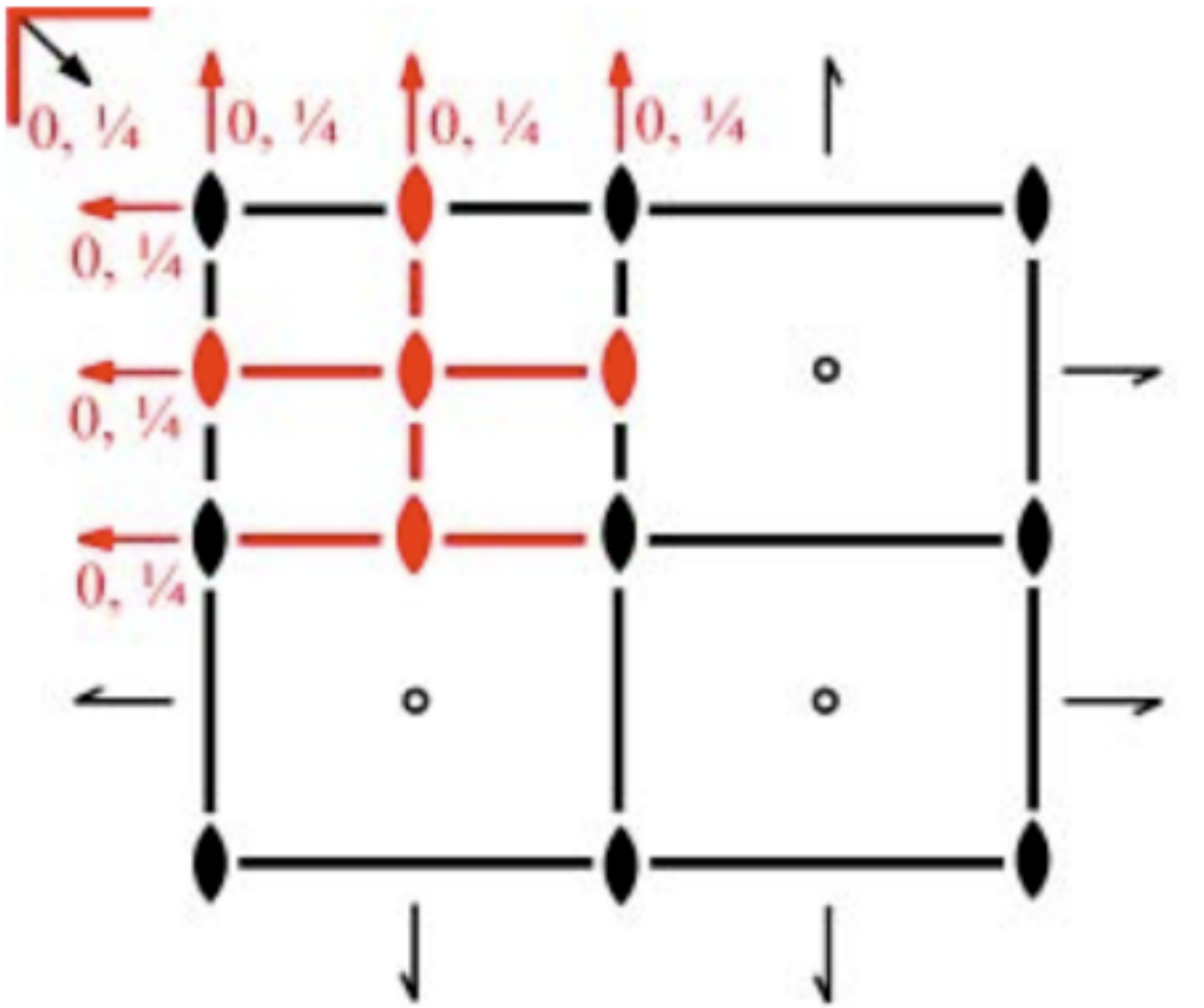


	4 en	ω	$\mathcal{G}$
4_z	$(0,0,0)$	$(0,0,0)$	$(P422)_1$
4_y	$(0,0,0)$	$(0,0,0)$	$(P422)_2$
4_x	$(0,0,0)$	$(0,0,0)$	$(P422)_3$
4_z	$(\frac{1}{2},0,0)$	$(\frac{1}{2},\frac{1}{2},0)$	$(P422)'_1$
4_y	$(\frac{1}{2},0,0)$	$(\frac{1}{2},0,\frac{1}{2})$	$(P422)'_2$
4_x	$(0,\frac{1}{2},0)$	$(0,\frac{1}{2},\frac{1}{2})$	$(P422)'_3$

Normalizers of space groups

Normalizers N(G) : $g^{-1}\{G\}g = \{G\}$ { Euclidean / Affine

the symmetry
of symmetry

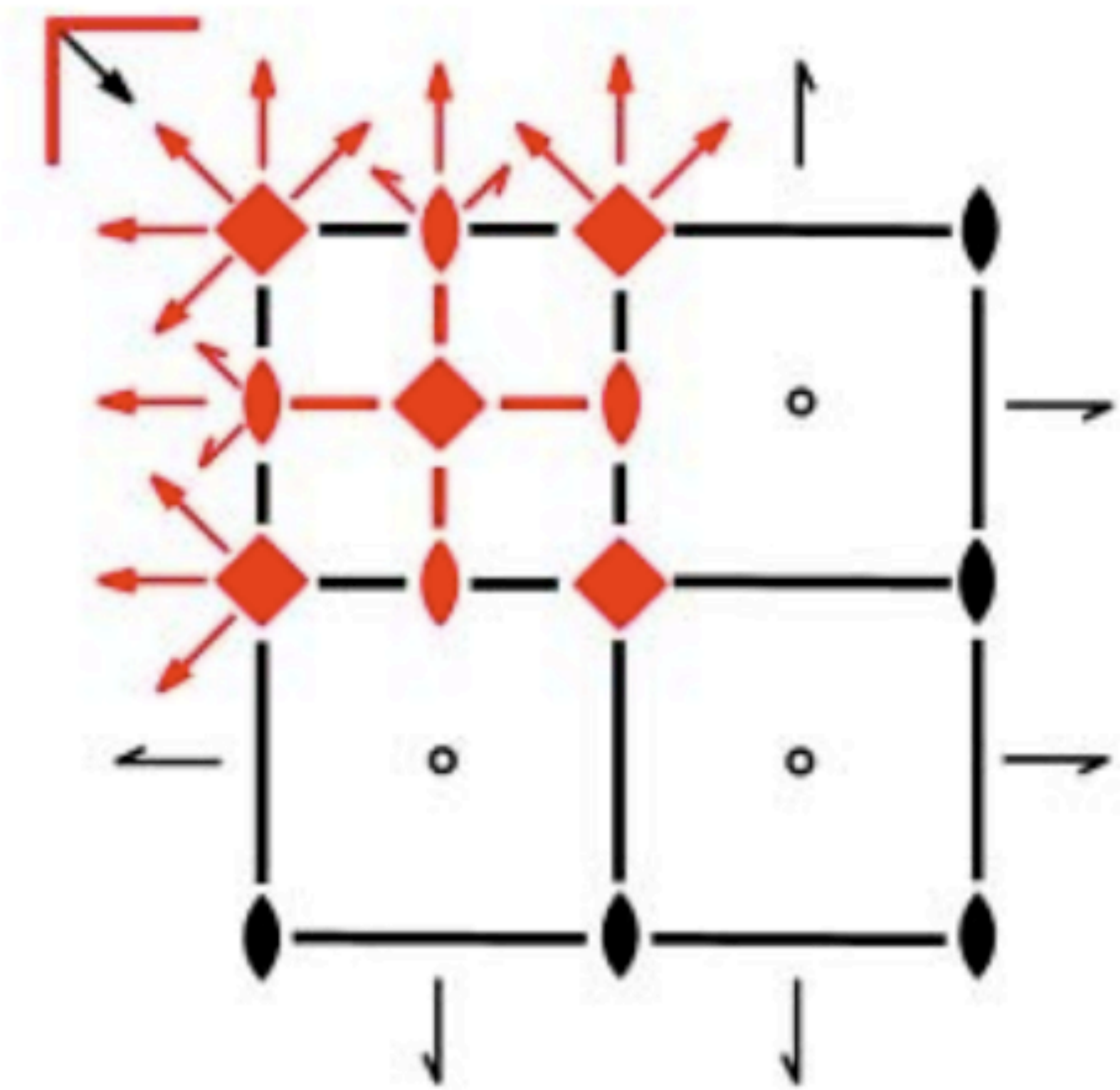


Space group: Pmmn (a,b,c)

Euclidean normalizer:
Pmmm (1/2a,1/2b,1/2c)

Normalizers for specialized metrics

Normalizers



Space group:
Pmmn (a,b,c), **a=b**

Euclidean normalizer for specialized metrics:
P4/mmm (1/2a,1/2b,1/2c)

Applications: Equivalent point configurations
Wyckoff sets
Equivalent structure descriptions

Normalizers of space groups

NORMALIZER

Cosets representatives of the Affine Normalizer with respect to the Space Group 99 (*P*4*mm*)

The Affine normalizer coincides with the *Euclidean* one.

Transformation of the Wyckoff Positions of Space Group 99 (*P*4*mm*) under Affine Normalizer N(G):

Index: 4*(infinite)

Coset Representative		Transformed WP
x,y,z	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	a b c d e f g
x+1/2,y+1/2,z	[1 0 0] [1/2] [0 1 0] [1/2] [0 0 1] [0]	b a c d f e g
-x,-y,-z	[-1 0 0] [0] [0 -1 0] [0] [0 0 -1] [0]	a b c d e f g
-x+1/2,-y+1/2,-z	[-1 0 0] [1/2] [0 -1 0] [1/2] [0 0 -1] [0]	b a c d f e g
x,y,z+t	[1 0 0] [0] [0 1 0] [0] [0 0 1] [t]	a b c d e f g

Symmetry-equivalent Wyckoff positions

WYCKOFF SETS

Additional Generators for the Normalizer of the Group 221 (*Pm-3m*)

Additional generators of Euclidean normalizer (*Im-3m*) **a,b,c**

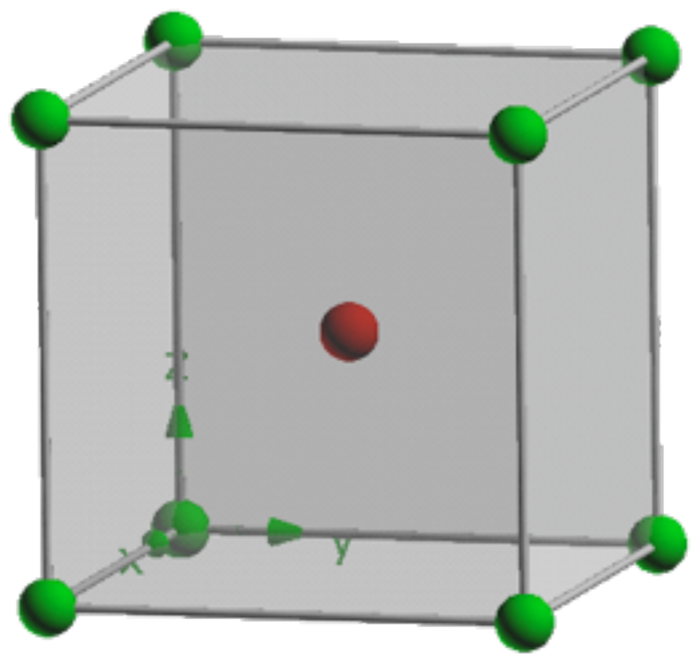
x+1/2,y+1/2,z+1/2	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$

Wyckoff Sets of Space Group 221 (*Pm-3m*)

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

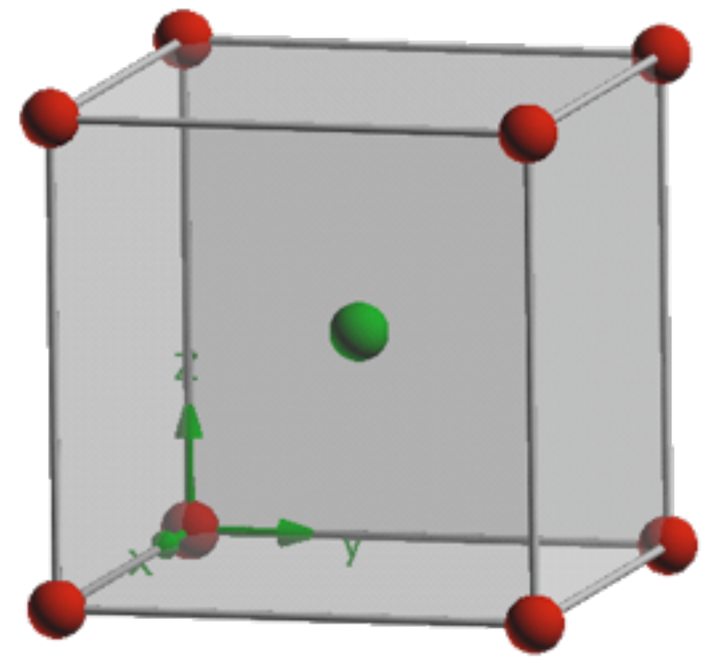
Letter	Mult	SS	Rep.	Equivalent Positions
n	48	1	(x, y, z)	n
m	24	..m	(x, x, z)	m
f	6	4m. m	(x, 1/2 , 1/2)	ef
e	6	4m. m	(x, 0, 0)	ef
d	3	4/mm. m	(1/2 , 0, 0)	cd
c	3	4/mm. m	(0, 1/2 , 1/2)	cd
b	1	m-3m	(1/2 , 1/2 , 1/2)	ab
a	1	m-3m	(0, 0, 0)	ab

Equivalent descriptions of crystal structures



CsCl

Pm-3*m* (221)



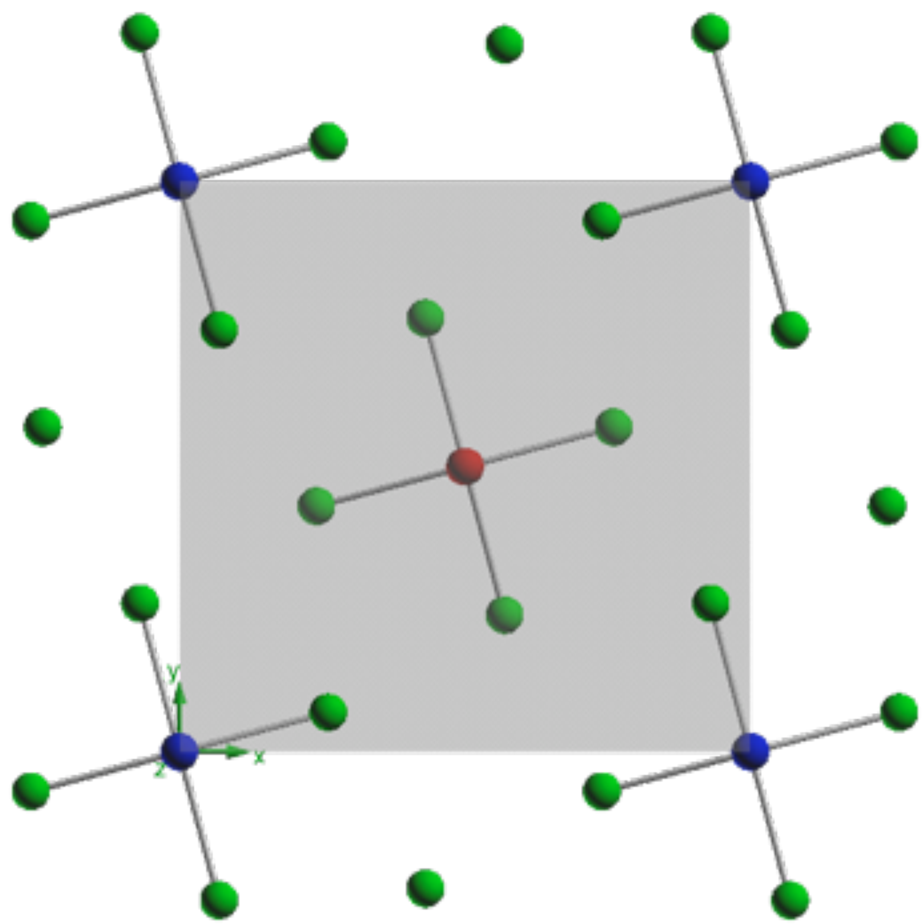
Normalizer operation: x+1/2, y+1/2, z+1/2

1*a* (0,0,0)	→	1*b* (1/2,1/2,1/2)
1*b* (1/2,1/2,1/2)	→	1a (0,0,0)

Problem: EQUIVALENT DESCRIPTIONS

EQUIVSTRU

Example: $WOBr_4$



Space Group: $I4$

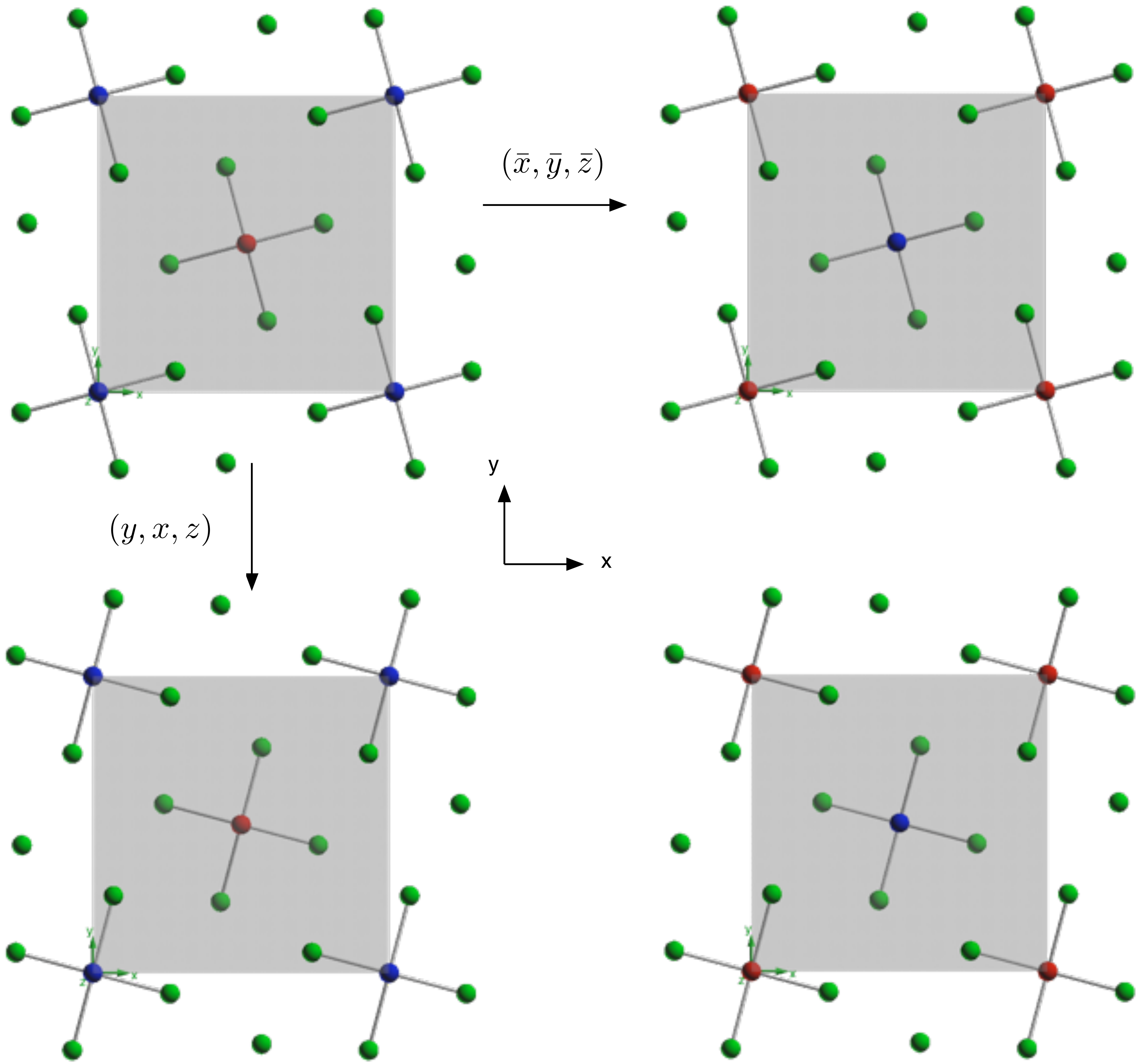
Euclidean Normalizer: $P^{1}4/mmm$

Index: 4

$$P4/mmm = I4 + (\bar{x},\bar{y},\bar{z})I4 + (y,x,z)I4 + (\bar{y},\bar{x},\bar{z})I4$$

EQUIVALENT DESCRIPTIONS

Example: $WOBr_4$



Problem: Symmetry Relations between Crystal Structures

Baernighausen Trees

Pyrite Structural family

Aristotype / **Basic structure**

$P2_1/a\bar{3}$

FeS_2

Fe:4a	S:8c
$\bar{3}$	3
0	0.386 [0.614]
0	0.386 [0.614]
0	0.386 [0.614]

t2 ↓

$P2_13$

NiAsS

Ni: 4a	S: 4a	As: 4a
3	3	3
−0.006	0.385	0.618
−0.006	0.385	0.618
−0.006	0.385	0.618

t3 ↓

Hettotypes / **Derivative structures**

$P2_1/b2_1/c2_1/a$

PdS_2

Pd:4a	S:8c
$\bar{1}$	1
0	0.393 [0.617]
0	0.388 [0.612]
0	0.425 [0.575]

t2 $-\frac{1}{4},0,0$ ↓ ; $x+\frac{1}{4},0,0$

$Pbc2_1$

PtGeSe

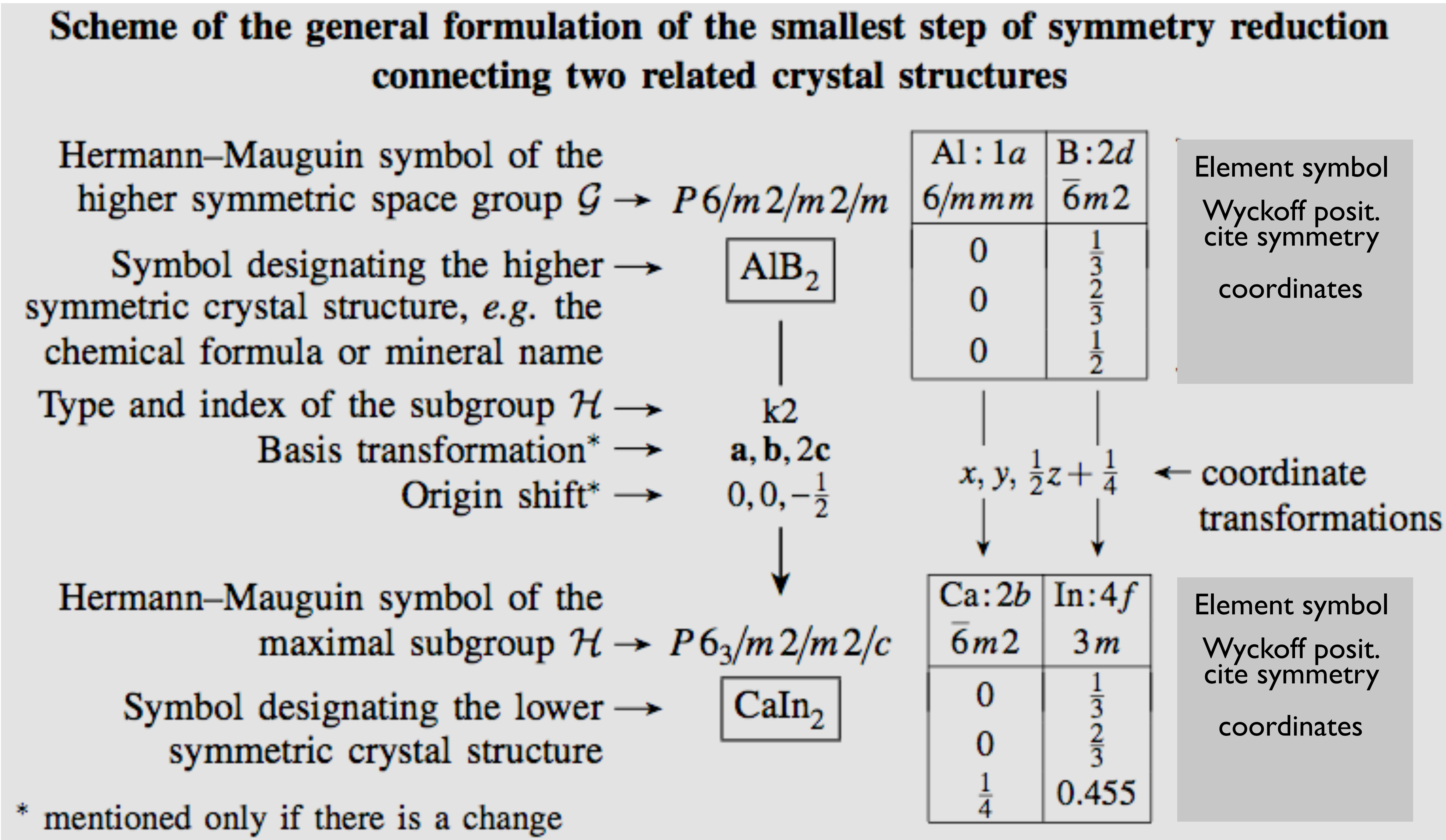
Pt:4a	Ge:4a	Se:4a
$\bar{1}$	1	1
0.242	0.633	0.876
0.009	0.383	0.620
0	0.383	0.618

lattice parameters in pm:

	a	*b*	*c*	references
pyrite	541.8	541.8	541.8	[32]
NiAsS	568.9	568.9	568.9	[33]
PdS_2	546.0	554.1	753.1	[34]
PtGeSe	607.2	601.5	599.2	[35]

U. Mueller, Gargnano 2008

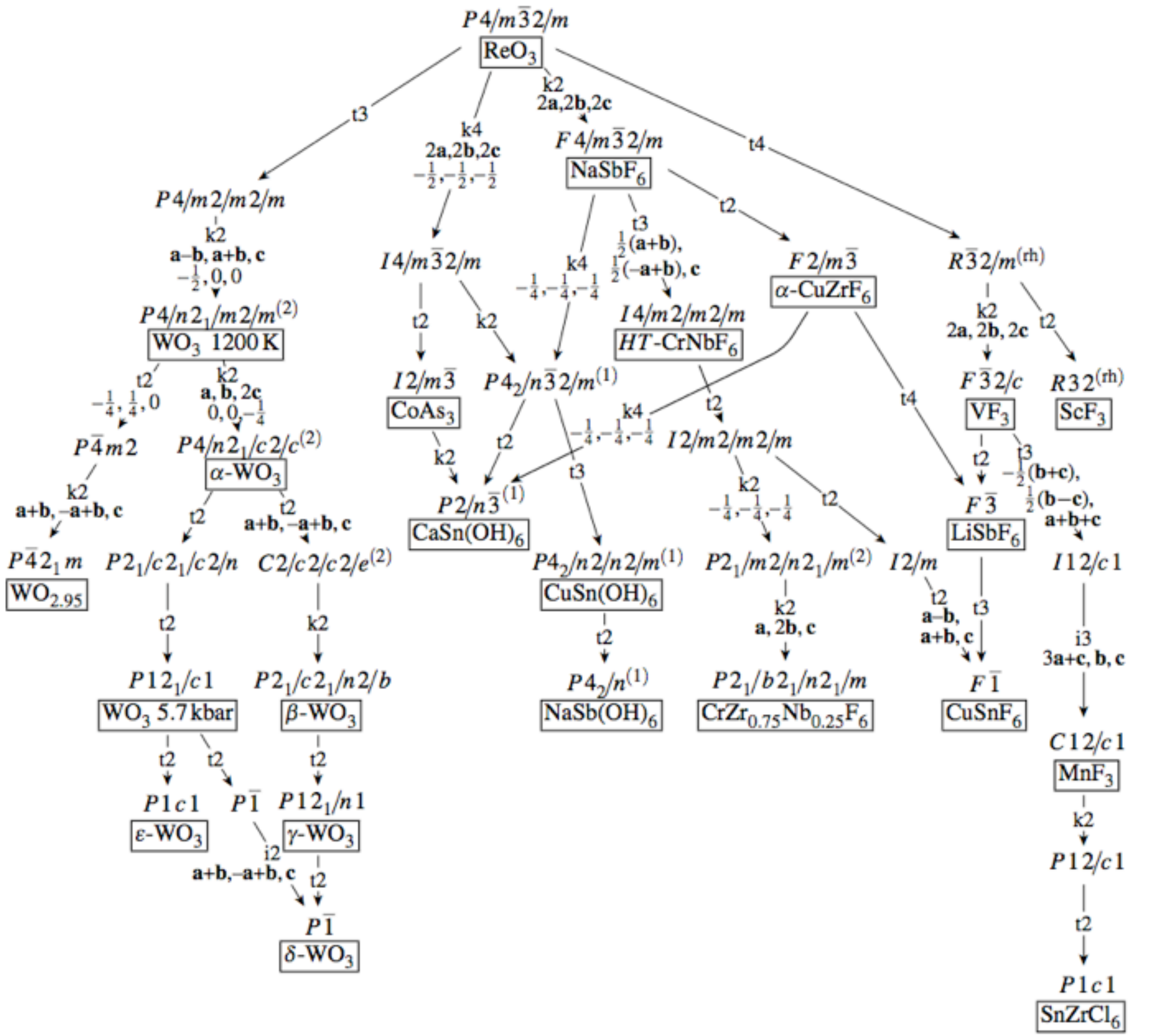
Modul design of crystal symmetry relations



U. Mueller, Gargnano 2008

Family tree of hettotypes of ReO_3

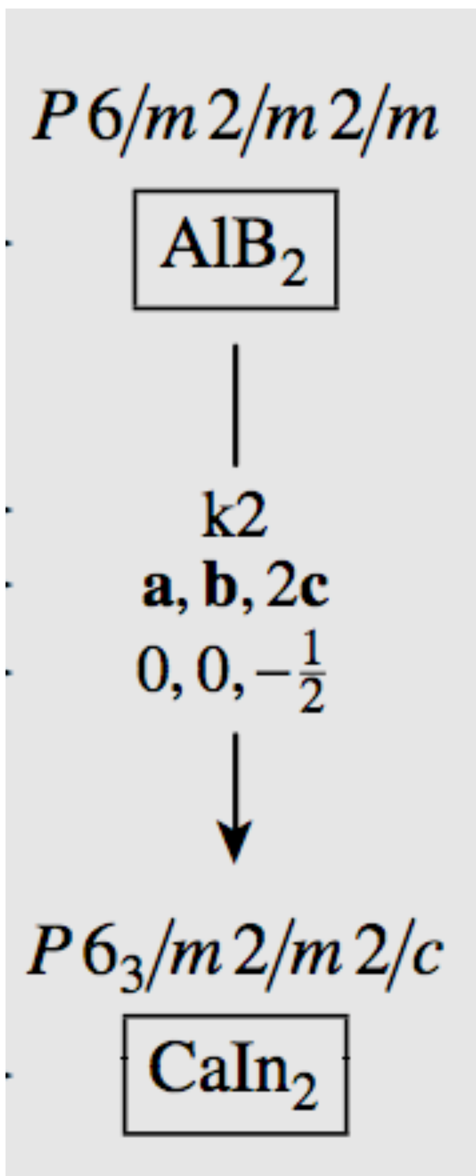
Baernighausen Trees



Baernighausen Trees

Basic tools for structure symmetry relations

Group-Subgroup relations

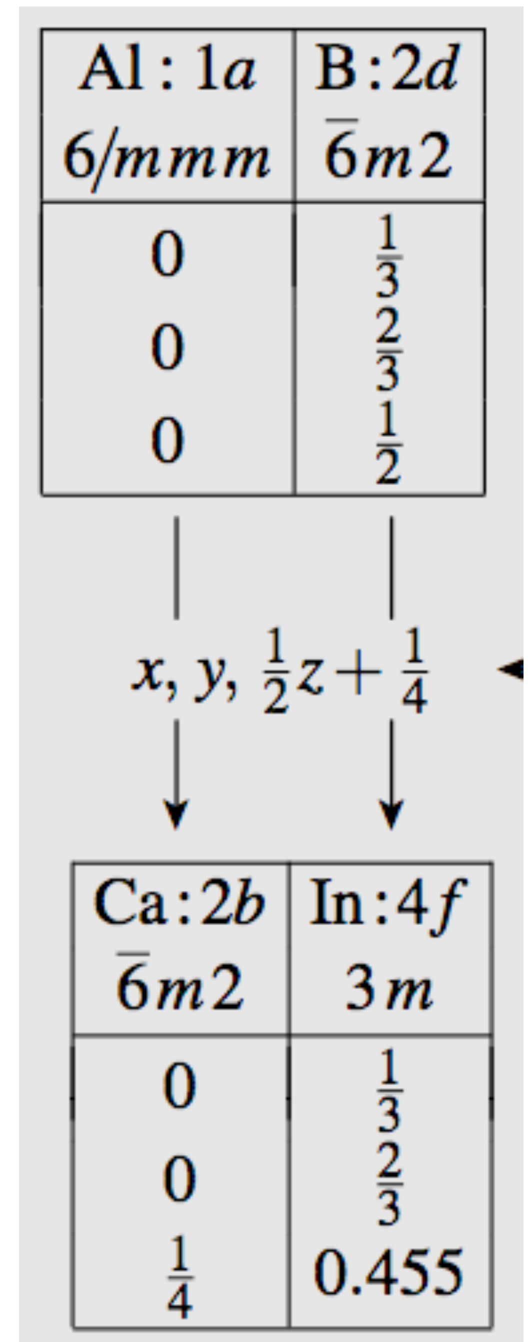


MAXSUB

SUBGROUPGRAPH

HERMANN

Wyckoff-splitting schemes



WYCKSPLIT

Problem 6.1 Cristobalite phase transitions

At low temperatures, the space-group symmetry of cristobalite is given by the space group is $P4_12_12$ (92) with lattice parameters a=4.9586A, c=6.9074A. The four silicon atoms are located in Wyckoff position 4(a) ..2 with the coordinates x, x, 0; -x, -x, 1/2; 1/2-x,1/2+x, 1/4; 1/2+x,1/2-x,3/4, x = 0.3028.

During the phase transition, the tetragonal structure is transformed into a cubic one with space group Fd-3m (227), a=7.147A. It is listed in the space-group tables with two different origins. If 'Origin choice 2' setting is used (with point symmetry -3m at the origin), then the silicon atoms occupy the position 8(a) -43m with the coordinates 1/8, 1/8, 1/8; 7/8, 3/8, 3/8 and those related by the face-centring translations.

Describe the structural distortion from the cubic to the tetragonal phase by the determination of (i) the displacements if the Si atoms in relative and absolute units, and (ii) the changes on the lattice parameters during the transition.

Ferroelastic phase transition $Pb_3(VO_4)_2$

R-3m High-symmetry phase	5.67 5.67 20.38
symmetry reduction	(P,p) $\left(\begin{array}{ccc:c} 2/3 & 0 & -2 & 0 \\ 1/3 & 1 & -1 & 0 \\ 1/3 & 0 & 0 & 0 \end{array}\right)$
$P2_1/c$	7.54 5.67 9.82 β=115.75
affine transformation	
$P2_1/c$ Low-symmetry phase	7.51 5.67 9.51 β=115.18

Example: α-Cristobalite → β-Cristobalite

2 entries selected.
CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:
Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol.

CC=44094	Details Bonds Pattern Structure Jmol
Title	First-principles study of crystalline silica.
Authors	Feng Liu;Garofalini, H.;King-Smith, D.;Vanderbilt, D.
Reference	Physical Review, Serie 3. B - Condensed Matter (1994) **49**, 12528-12534 **Link XRef SCOPUS SCIRUS Google** **Also:** Phase Transition (1992) **38**, 127-220
Compound	**Si O2** - **[Cristobalite alpha]** Silicon oxide - HT **[AX2] [tP12] [b a] [TeO2(alpha)]**
Cell	4.9586, 4.9586, 6.9074, 90., 90., 90. **P41212 (92)** V=169.84
Remarks	MIN =Cristobalite alpha : PDC =01-089-3434 : PDF =39-1425 : THE TYP =TeO2(alpha) : XDS At least one temperature factor missing in the paper. No R value given in the paper. Metastable up to 500 K (2nd ref. , Tomaszewski), above Fd3-m

Atom	(site)	Oxid.	x	y	z	B	Occupancy
Si1	(4a)	4	0.3028	0.3028	0	0	1
O1	(8b)	-2	0.2383	0.1093	0.1816	0	1

CC=44095	Details Bonds Pattern Structure Jmol
Title	First-principles study of crystalline silica.
Authors	Feng Liu;Garofalini, H.;King-Smith, D.;Vanderbilt, D.
Reference	Physical Review, Serie 3. B - Condensed Matter (1994) **49**, 12528-12534 **Link XRef SCOPUS SCIRUS Google** **Also:** Phase Transition (1992) **38**, 127-220
Compound	**Si O2** - **[Cristobalite beta]** Silicon oxide - HT **[AX2] [cF24] [h a] []**
Cell	7.147, 7.147, 7.147, 90., 90., 90. **FD3-MS (227)** V=365.07
Remarks	MIN =Cristobalite beta : PDC =01-089-3435 : PDF =4-359 : THE XDS At least one temperature factor missing in the paper. The coordinates are those given in the paper but the atomic distances do not agree with those calculated during testing.The coordinates are probably correct. No R value given in the paper. Metastable above 500 K (2nd ref. , Tomaszewski), stable above 1743 K

Atom	(site)	Oxid.	x	y	z	B	Occupancy
Si1	(8a)	4	0	0	0	0	1
O1	(96h)	-2	0.125	0.081	0.169	0	0.1667

Origin choice 2: Si 8a 1/8,1/8,1/8 7/8,3/8,3/8

Problem 6.1

SOLUTION

Symmetry break: Fd-3m→$P4_12_12$

$a_t=1/2(a_c-b_c)$, $b_t=1/2(a_c+b_c)$, $c_t=c_c$

origin shift: (-1/4,0,0)

Experiment:

Cubic phase:

a=7.147 Å

Si 8a 1/8 1/8 1/8

7/8 3/8 3/8

(P,p) →

Calculated:

a=5.053 Å, c=7.147 Å

Si 8a 0.25 0.25 0

Tetragonal phase:

a=4.9586 Å, c=6.9074

Si 4a 0.3028 0.3028 0

affine deformation

atomic displacements

Problem 6.2

The coordinates of CaF_2 are: G=Fm-3m

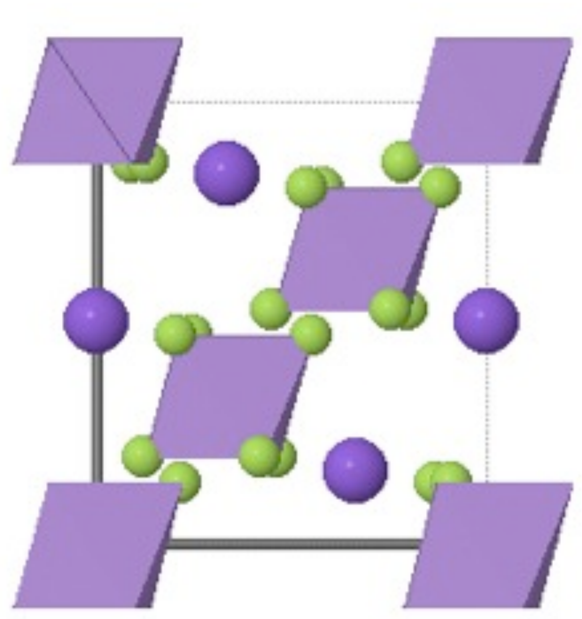
Ca	4a	$m\bar{3}m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$
F	8c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$
			$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$

(P,p)=1/2(a-b),1/2(a+b),c;-1/4, 1/4, -1/4

EXERCISES

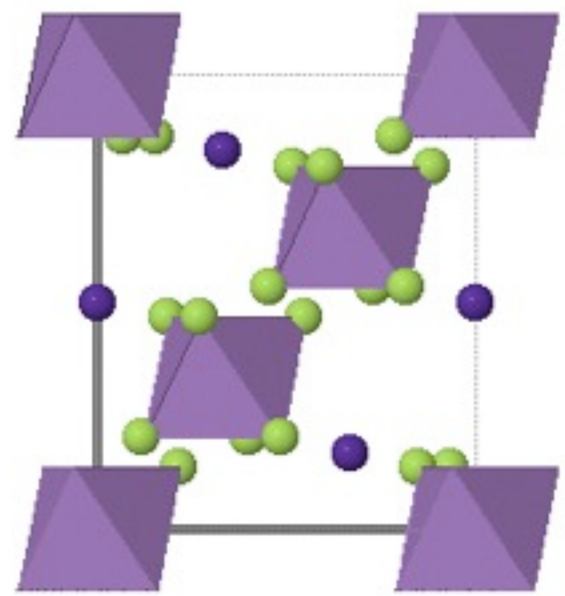
Problem 6.3

$KAsF_6$



```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K     1   3b    0.3333 0.66666 0.16667
As    1   3a    0 0 0
F     1   18f   0.1292 0.2165 0.1381
```

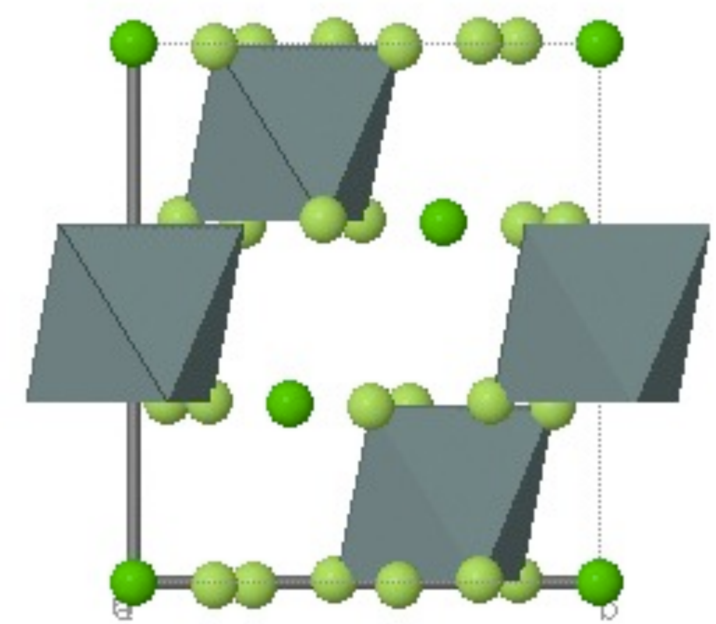
$CsSbF_6$



```
148
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs    1   3b    0. 0. 0.5
SB    1   3a    0 0 0
F     1   18f   0.06562 0.2158 0.1337
```

Maximum distance Δ: 0.4657

$BaSnF_6$



```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba    1   3a    0. 0. 0.0
Sn    1   3b    0 0 0.5
F     1   18f   0.2586 0.8262 0.0047
```

No pairing found for tolerance: 2

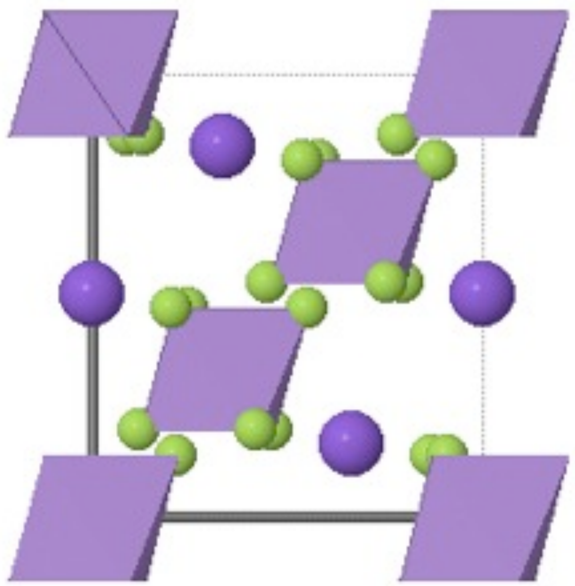
Space-group symmetry: R-3

Euclidean normalizer: R-3m(-a,-b, 1/2c)

Coset representatives: x,y,z; x,y,z+1/2;
-y,-x,z; -y,-x,z+1/2;

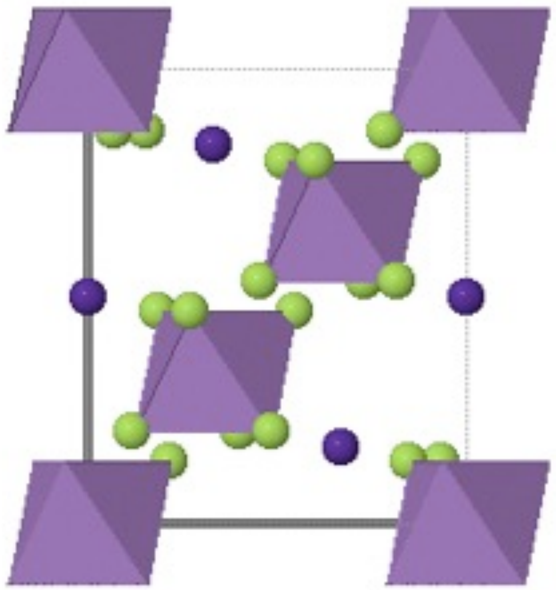
SOLUTION

KAsF$_6$



```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K       1     3b     0.3333 0.66666 0.16667
As      1     3a     0 0 0
F       1     18f    0.1292 0.2165 0.1381
```

CsSbF$_6$



```
148
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs      1     3b     0. 0. 0.5
SB      1     3a     0 0 0
F       1     18f    0.06562 0.2158 0.1337
```

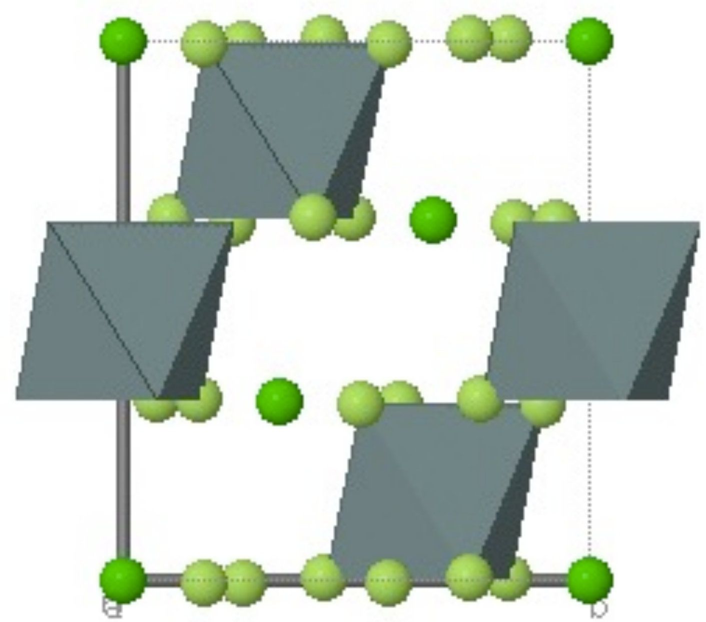
Maximum distance Δ: 0.4657

-y,-x,z

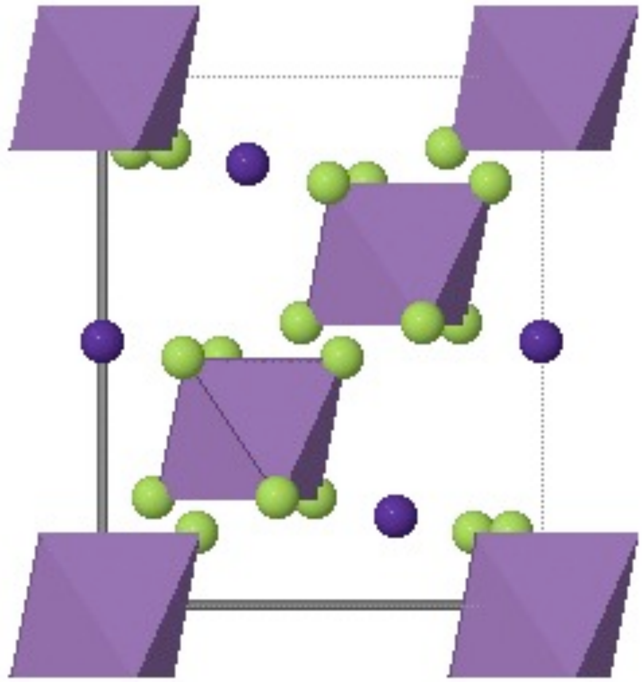
```
148
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs      1     3b     0. 0. 0.5
SB      1     3a     0 0 0
F       1     18f    0.150180 0.215800 0.133700
```

Maximum distance Δ: 0.1600

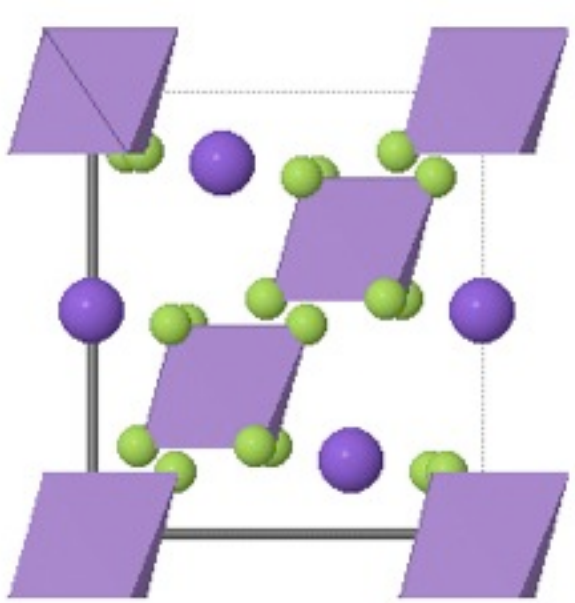
BaSnF$_6$



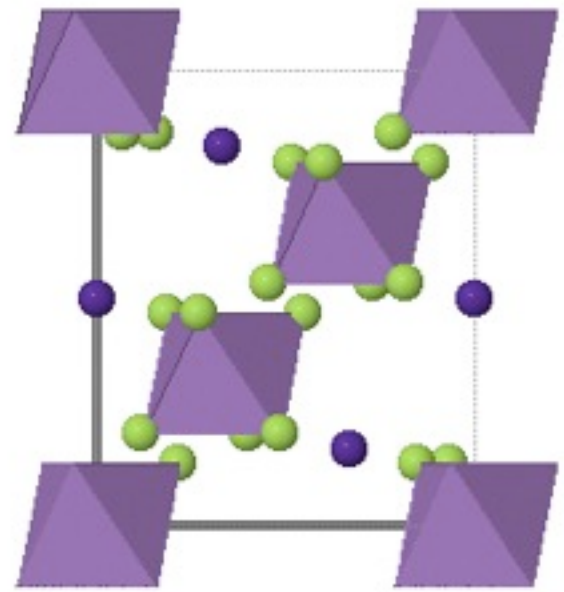
```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba      1     3a     0. 0. 0.0
Sn      1     3b     0 0 0.5
F       1     18f    0.2586 0.8262 0.0047
```



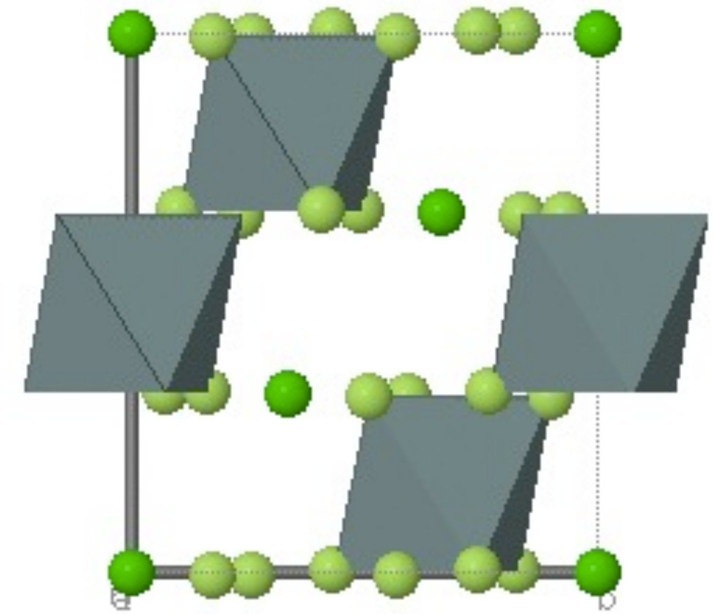
$KAsF_6$



$CsSbF_6$



$BaSnF_6$



```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K      1    3b    0.3333 0.66666 0.16667
As     1    3a    0 0 0
F      1    18f   0.1292 0.2165 0.1381
```

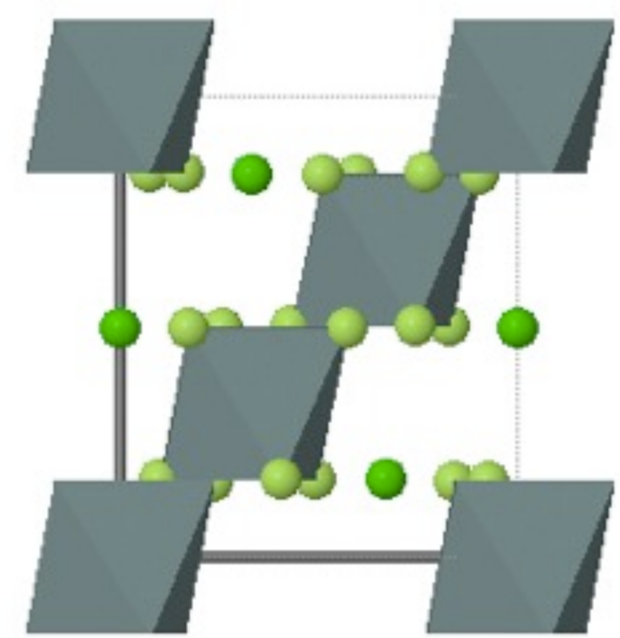
```
148
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs     1    3b    0. 0. 0.5
SB     1    3a    0 0 0
F      1    18f   0.06562 0.2158 0.1337
```

```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba     1    3a    0. 0. 0.0
Sn     1    3b    0 0 0.5
F      1    18f   0.2586 0.8262 0.0047
```

No pairing found for tolerance: 2

x,y,z+1/2

```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba     1    3b    0. 0. 0.5
Sn     1    3a    0 0 0
F      1    18f   0.159533 0.234267 0.161967
```



Maximum distance Δ: 0.2603

EXERCISES

Problem 6.4

Equivalent structure descriptions

Space group: P4/n

Exercise 6.4. $P(C_6C_5)_4[MoNCl_4]$ is tetragonal, spac

Atom	Wyckoff position	Coordinate x	triplets y	z
P	$2b$	0.25	0.75	0
Mo	$2c$	0.25	0.25	0.121
N	$2c$	0.25	0.25	−0.093
C1	$8g$	0.362	0.760	0.141
C2	$8g$	0.437	0.836	0.117
Cl	$8g$	0.400	0.347	0.191

$$N(P4/n) = P4/mmm\ (a', b', 1/2c)$$

$$a' = 1/2(a-b),\ b' = 1/2(a+b)$$

ADDITIONAL

Ferroelastic phase transition $Pb_3(VO_4)_2$

R-3m High-symmetry phase	5.67 5.67 20.38
↓ symmetry reduction	↓ (P,p) $\left(\begin{array}{ccc|c} 2/3 & 0 & -2 & 0 \\ 1/3 & 1 & -1 & 0 \\ 1/3 & 0 & 0 & 0 \end{array}\right)$
$P2_1/c$	7.54 5.67 9.82 β=115.75
↓ affine transformation	↓
$P2_1/c$ Low-symmetry phase	7.51 5.67 9.51 β=115.18

Problem: LATTICE DISTORTION — CELLTRAN STRAIN

Example: Ferroelastic phase transition $Pb_3(VO_4)_2$

High-symmetry phase
R-3m
5.67 5.67 20.38
90 90 120

CELLTRAN
1/3(2a+b+c),b,-2a-b

Low-symmetry phase
$P2_1/c$
7.51 5.67 9.51
β=115.18

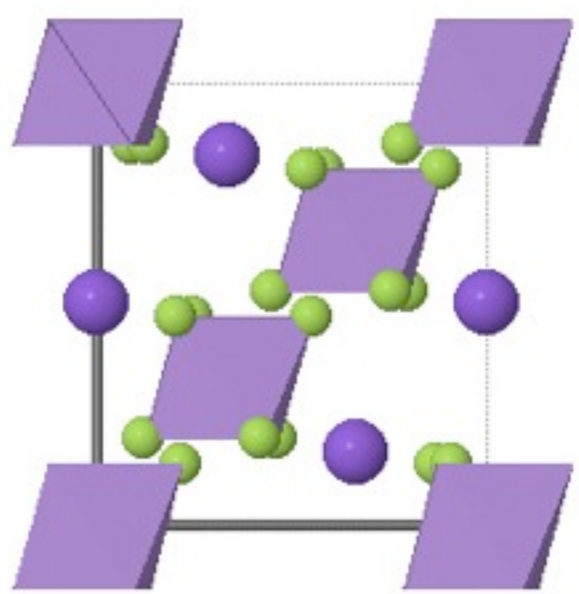
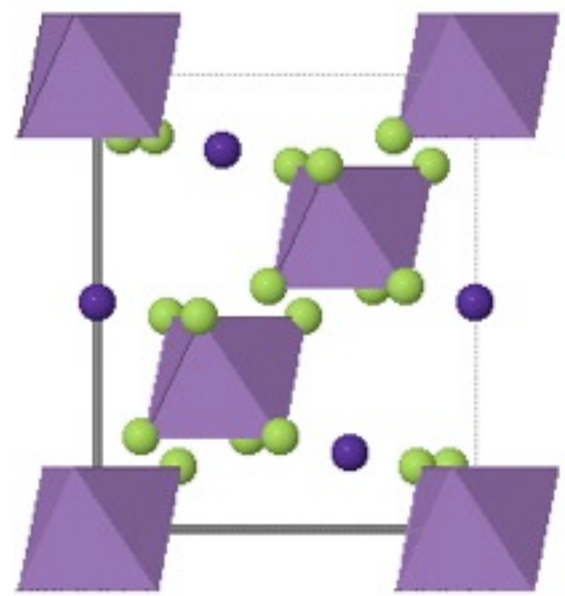
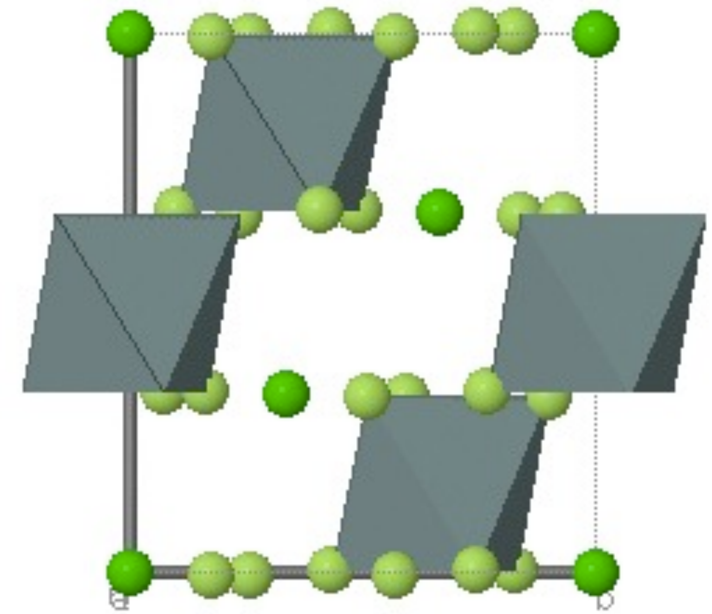
STRAIN

7.54 5.67 9.82
β=115.75

Degree of lattice distortion

Δ=0.0279

Problem: STRUCTURE TYPES

KAsF$_6$	CsSbF$_6$	BaSnF$_6$
		

```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K      1   3b     0.3333 0.66666 0.16667
As     1   3a     0  0  0
F      1   18f    0.1292 0.2165 0.1381
```

```
148
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs     1   3b     0. 0. 0.5
SB     1   3a     0 0 0
F      1   18f    0.06562 0.2158 0.1337
```

Maximum distance Δ: 0.4657

```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba     1   3a     0. 0. 0.0
Sn     1   3b     0 0 0.5
F      1   18f    0.2586 0.8262 0.0047
```

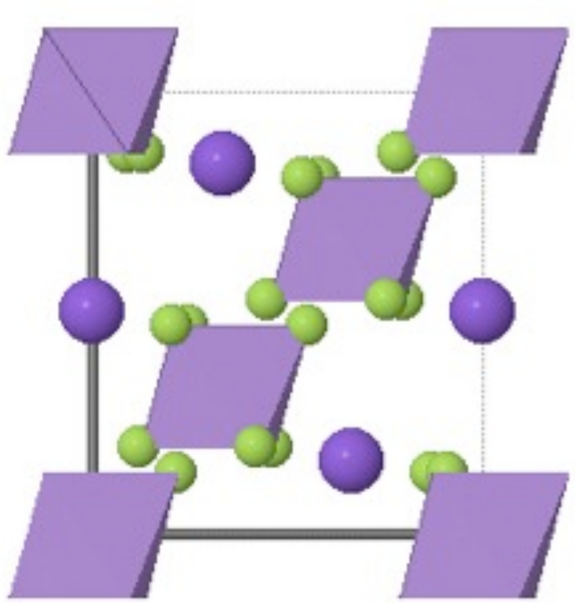
No pairing found for tolerance: 2

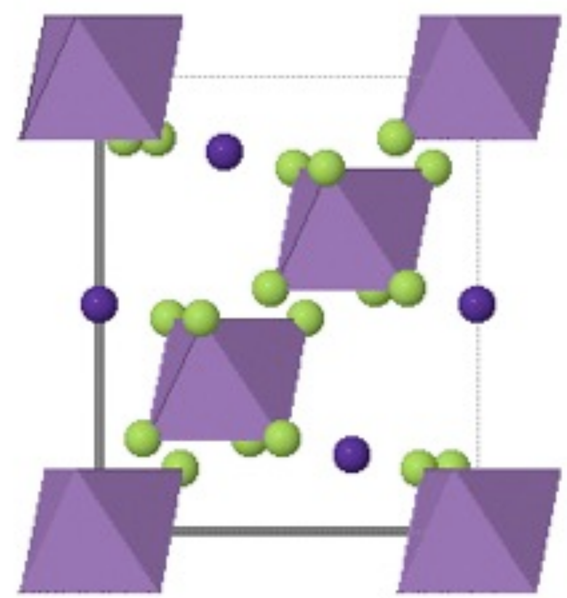
Space-group symmetry: R-3

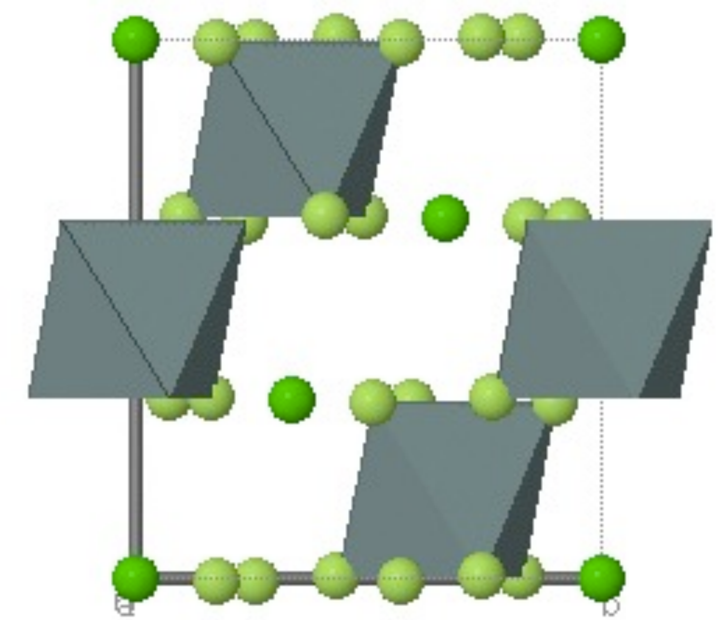
Euclidean normalizer: R-3m(-a,-b, 1/2c)

Coset representatives: x,y,z; x,y,z+1/2;
-y,-x,z; -y,-x,z+1/2;

$KAsF_6$ — $CsSbF_6$ — $BaSnF_6$







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3
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```

Maximum distance Δ: 0.4657

-y,-x,z

```
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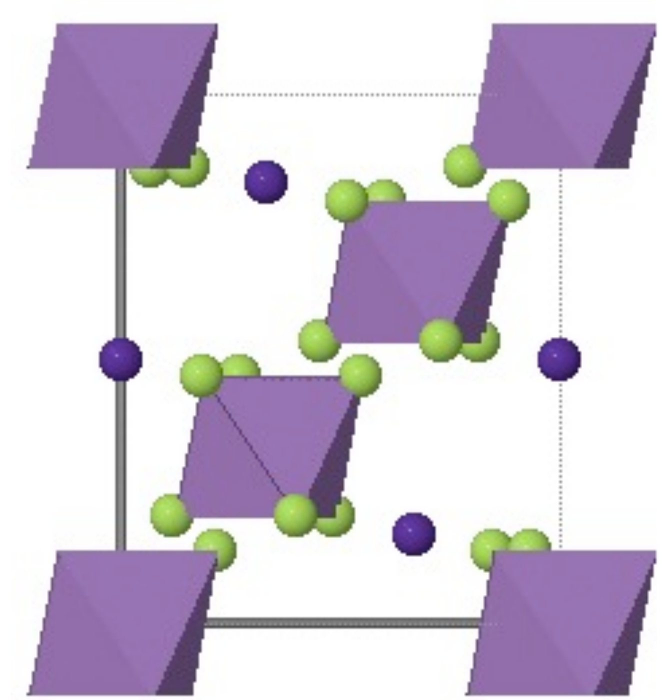
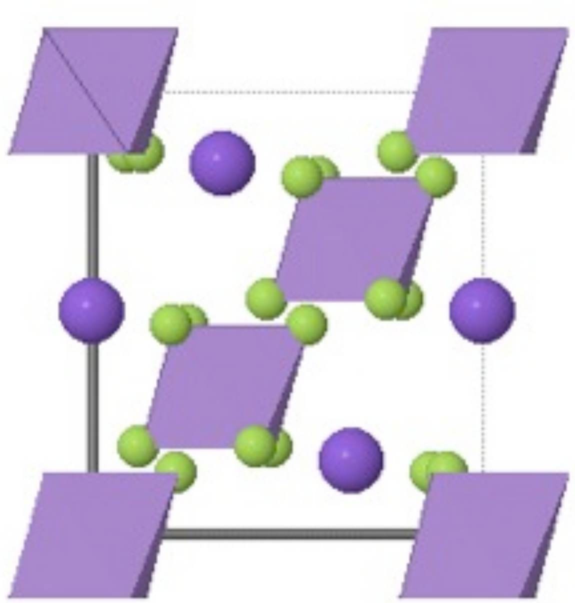
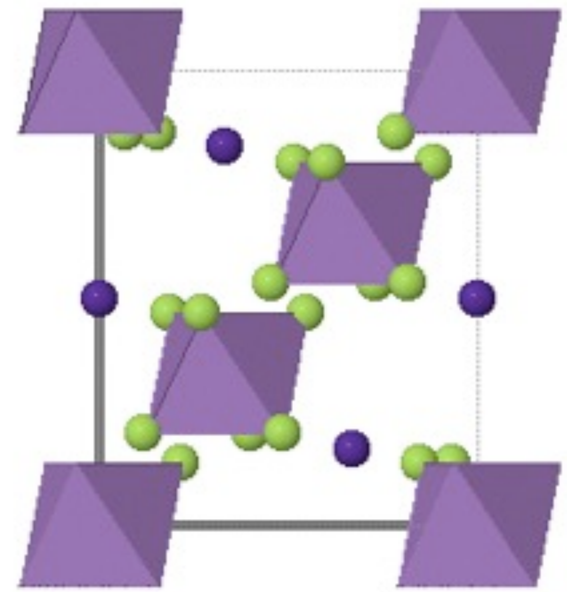
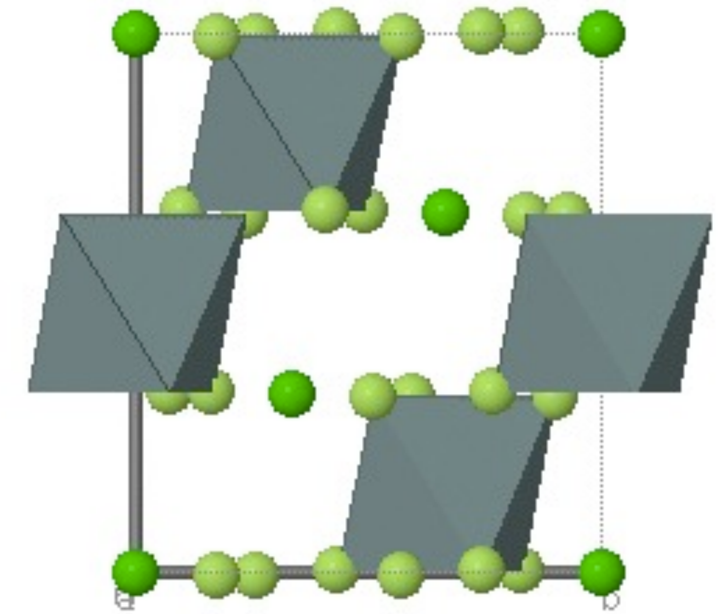
7.9040 7.9040 8.2610 90.00 90.00 120.00
3
Cs     1    3b    0. 0. 0.5
SB     1    3a    0 0 0
F      1    18f   0.150180 0.215800 0.133700
```

Maximum distance Δ: 0.1600



$KAsF_6$	$CsSbF_6$	$BaSnF_6$
		

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148
7.3480 7.3480 7.2740 90.00 90.00 120.00
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F      1    18f   0.1292 0.2165 0.1381
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7.4279 7.4279 7.4180 90.00 90.00 120.00
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F      1    18f   0.2586 0.8262 0.0047
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No pairing found for tolerance: 2

x,y,z+1/2

```
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7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba     1    3b    0. 0. 0.5
Sn     1    3a    0 0 0
F      1    18f   0.159533 0.234267 0.161967
```

Maximum distance Δ: 0.2603