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Commission on Mathematical and Theoretical Crystallography

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Facultad de Ciencias

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Workshop on the Applications of Group Theory in the Study of Phase Transitions

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SYMMETRY RELATIONS OF SPACE GROUPS

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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

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

MAXIMAL SUBGROUPS OF SPACE GROUPS

I. MAXIMAL TRANSLATIONENGLEICHE SUBGROUPS

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)
...	...	...	...	...	...

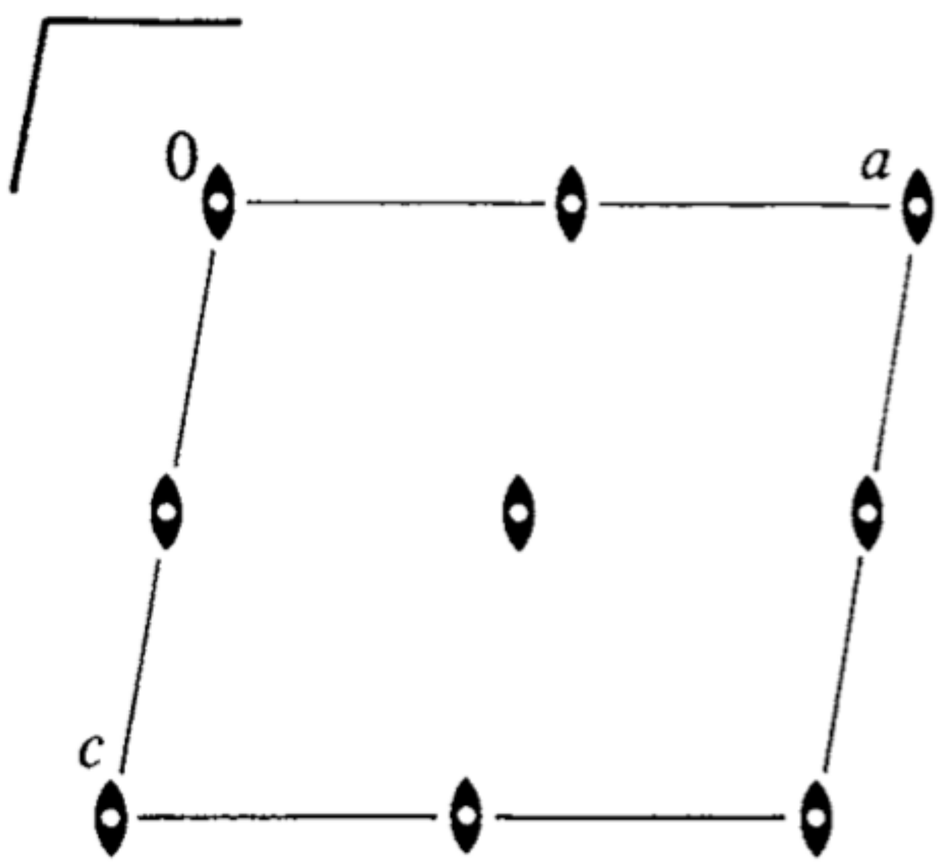
Factor group G/T_G

isomorphic to the point group P_G of G

Point group $P_G = \{I, W_2, W_3, \ldots, W_i\}$

Example: P12/m1

Factor group $G/T_G \simeq P_G$



Coset decomposition $G:T_G$

$P_G = \{1, 2, \bar{1}, m\}$

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

inversion centres $(\bar{1},t)$:

$$\left(\begin{array}{ccc|c} -1 & & & n_1 \\ & -1 & & n_2 \\ & & -1 & n_3 \end{array}\right) \xrightarrow{\bar{1}\ \text{at}} \begin{pmatrix} n_1/2 \\ n_2/2 \\ n_3/2 \end{pmatrix}$$

Translationengleche subgroups H<G:

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

Example: P12/m1

Coset decomposition

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

t-subgroups:

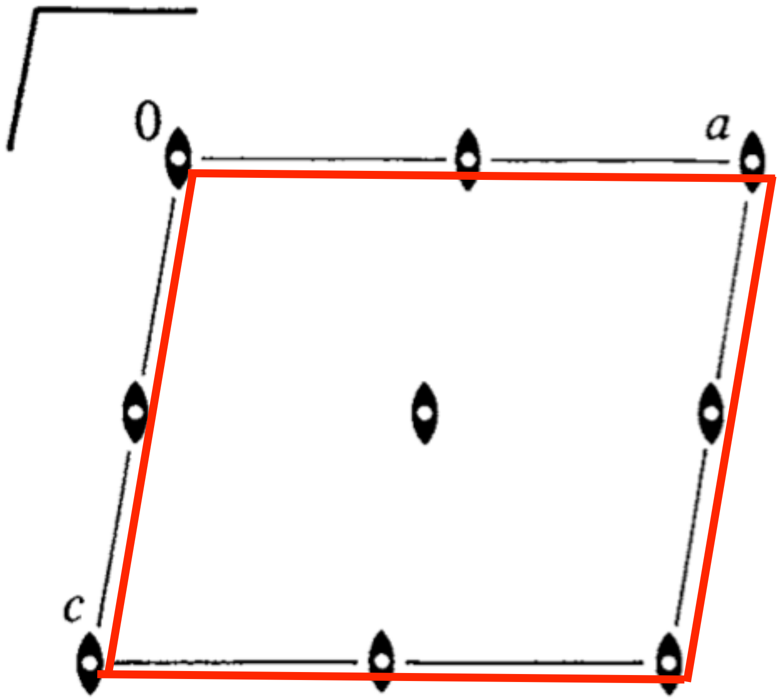
$H_1 = T_G \cup T_G 2$
P121

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

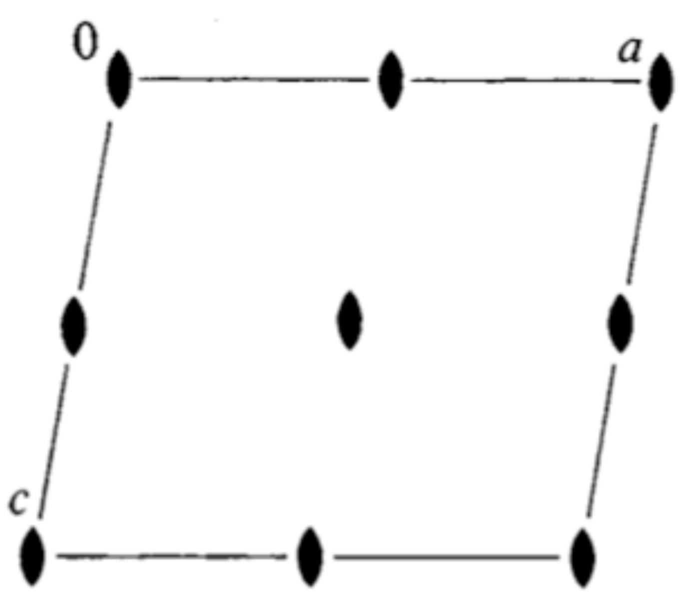
$H_3 = T_G \cup T_G m$
Pm

Example: P12/m1

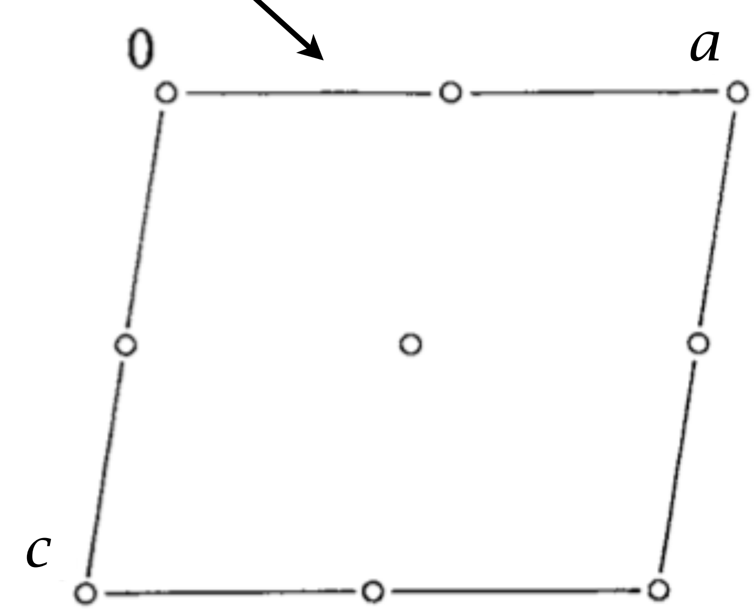
Translationengleche subgroups H<G:



P121 = $T_G \cup T_G 2$

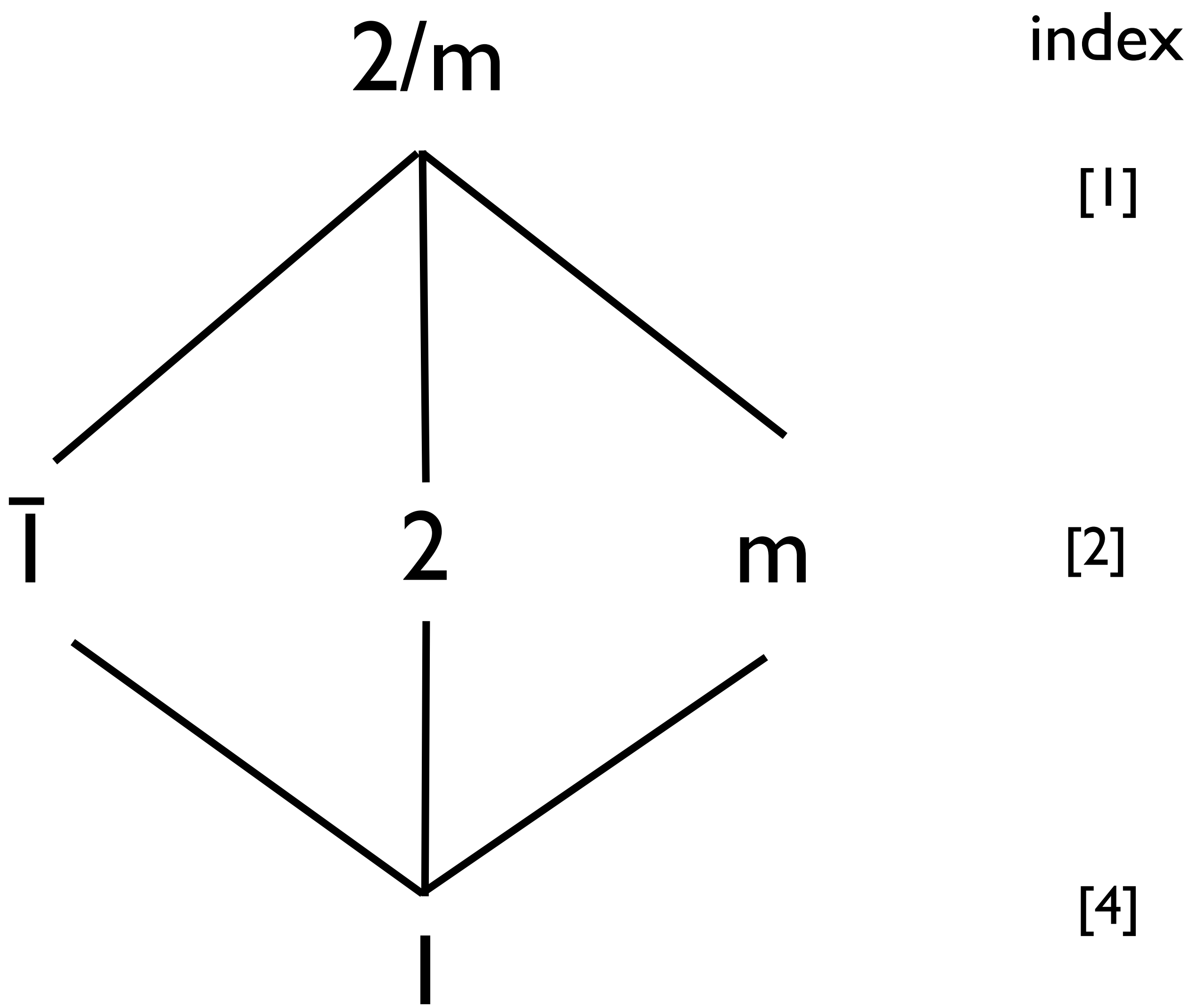


$P\bar{1} = T_G \cup T_G \bar{1}$

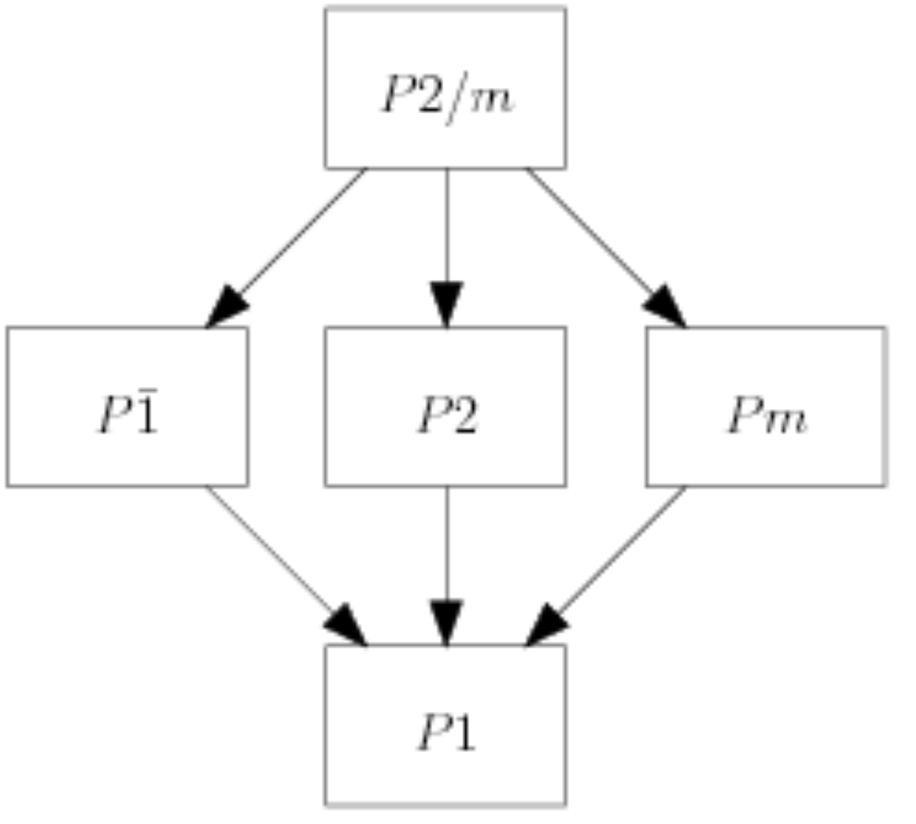


Example: P12/m1

Translationengleche subgroups H<G:



Subgroup diagram of point group 2/m



Translationengleiche subgroups of space group *P*2/m

EXERCISES

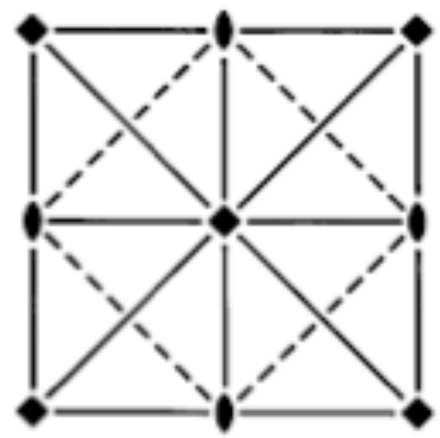
Problem 2.25

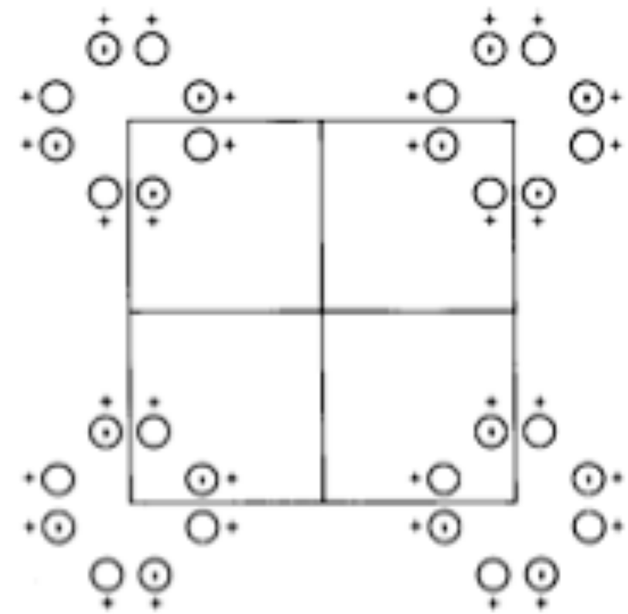
Construct the diagram of the
t-subgroups of *P*4*mm* using the ‘analogy’
with the subgroup diagram of 4*mm*

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

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

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





Origin on $4mm$

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

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 (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

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Example: P4mm

Maximal subgroups of space groups

C_{4v}^1 $P4mm$ No. 99 $P4mm$

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)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$

- **Series of maximal isomorphic subgroups**

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

$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	

$[p^2]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$P4mm$ (99)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

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

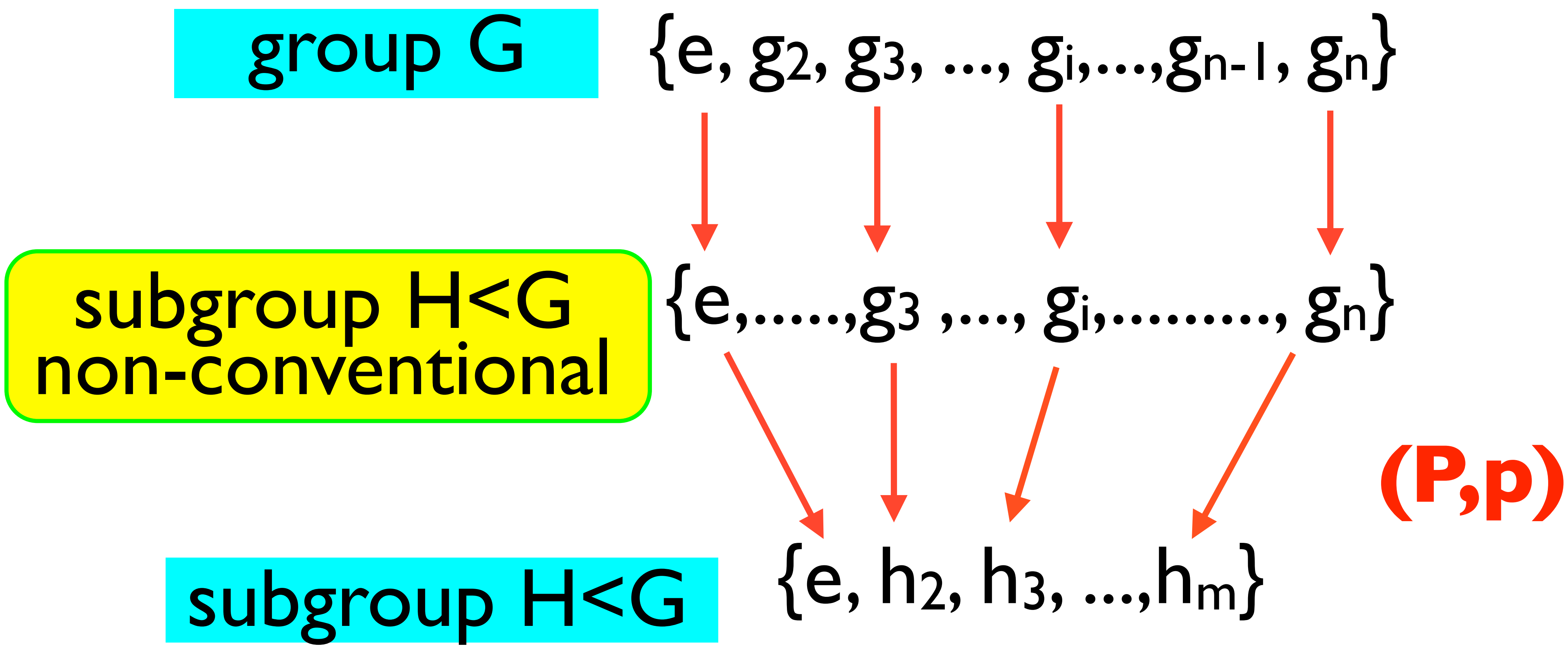
[*i*] HMS1 (No., HMS2) Sequence matrix shift

{ braces for conjugate subgroups

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

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

Transformation matrix: (P,p)



Subgroup specification: HM symbol, [i], (P,p)

Crystallographic computing programs

THE GROUP-SUBGROUPS SUITE

Group - Subgroup Relations of Space Groups	
SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	More group-subgroup relations
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
COMMONSUBS	Common Subgroups of Two Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

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Problem: SUBGROUPS OF SPACE GROUPS

SUBGROUPGRAPH

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Group-Subgroup Lattice and Chains of Maximal Subgroups

Lattice and chains ...

For a given group and supergroup the program SUBGROUPGRAPH will give the lattice of maximal subgroups that relates these two groups and, in the case that the index is specified, all of the possible chains of maximal subgroup that relate the two groups. In the latter case, also there is a possibility to obtain all of the different subgroups of the same type.

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:	99
Enter subgroup number (H) or choose it:	4
Enter the index [G:H] (optional):	

Construct the lattice

subgroup index

EXERCISES

Problem 2.28

With the help of the program SUBGROUPGRAPH obtain the graph of the *t*-subgroups of *P4mm* (No. 99). Explain the difference between the *contracted* and *complete* graphs of the *t*-subgroups of *P4mm* (No. 99).

Explain why the *t*-subgroup graphs of all 8 space groups from No. 99 *P4mm* to No. 106 $P4_2bc$ have the same `topology' (i.e. the same type of `family tree'), only the corresponding subgroup entries differ.

MAXIMAL SUBGROUPS OF SPACE GROUPS

II. MAXIMAL KLASSENGLEICHE SUBGROUPS

Klassengleiche subgroups H<G:

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

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)
...	...

$H=T_e$

isomorphic *k*-subgroups:

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

Klassengleiche subgroups H<G:

Subgroups of space groups

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

Example: P1

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

$H = T_e \quad t_a(1,0,0)$

Coset decomposition

$$P1 = T_e + T_e t_a$$

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

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*-subgroup:

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

Series of isomorphic *k*-subgroups:

$P1(p\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})$: p>1, prime

$P1(\boldsymbol{a},q\boldsymbol{b},\boldsymbol{c})$: q>1, prime

... *etc.*

INFINITE number of maximal isomorphic subgroups

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Example: P-1

Series of maximal isomorphic subgroups

$P\bar{1}$ No. 2 $P\bar{1}$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = q\mathbf{a}+\mathbf{b},\ \mathbf{c}' = r\mathbf{a}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2+(2u,0,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le r<p;\ 0\le u<p$ p conjugate subgroups for each triplet of q, r, and prime p	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, r\mathbf{a}+\mathbf{c}$	$u,0,0$

[p] $\mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = q\mathbf{b}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2+(0,2u,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}, p\mathbf{b}, q\mathbf{b}+\mathbf{c}$	$0,u,0$

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

$P\bar{1}$ (2)	$\langle 2+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

Klassengleiche subgroups H<G: **non-isomorphic**

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

Example: C2

Coset decomposition

$C2 = T_c + T_c 2$

$(T_i + T_i t_c)$

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)
...	...	...	...

non-isomorphic *k*-subgroups:

$H_1 = T_i \cup T_i 2$

P2

$H_2 = T_i \cup T_i t_c\,2$

P2$_1$

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Example: P4mm

Maximal subgroups of space groups

C_{4v}^1 | $P4mm$ | No. 99 | $P4mm$

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)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
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$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$

- **Series of maximal isomorphic subgroups**

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

$P4mm$ (99) $\langle 2;\ 3;\ 5\rangle$ $\mathbf{a}, \mathbf{b}, p\mathbf{c}$

$p > 1$

no conjugate subgroups

[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$P4mm$ (99) $\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $u,v,0$

$p > 2;\ 0 \le u < p;\ 0 \le v < p$

p^2 conjugate subgroups for the prime p

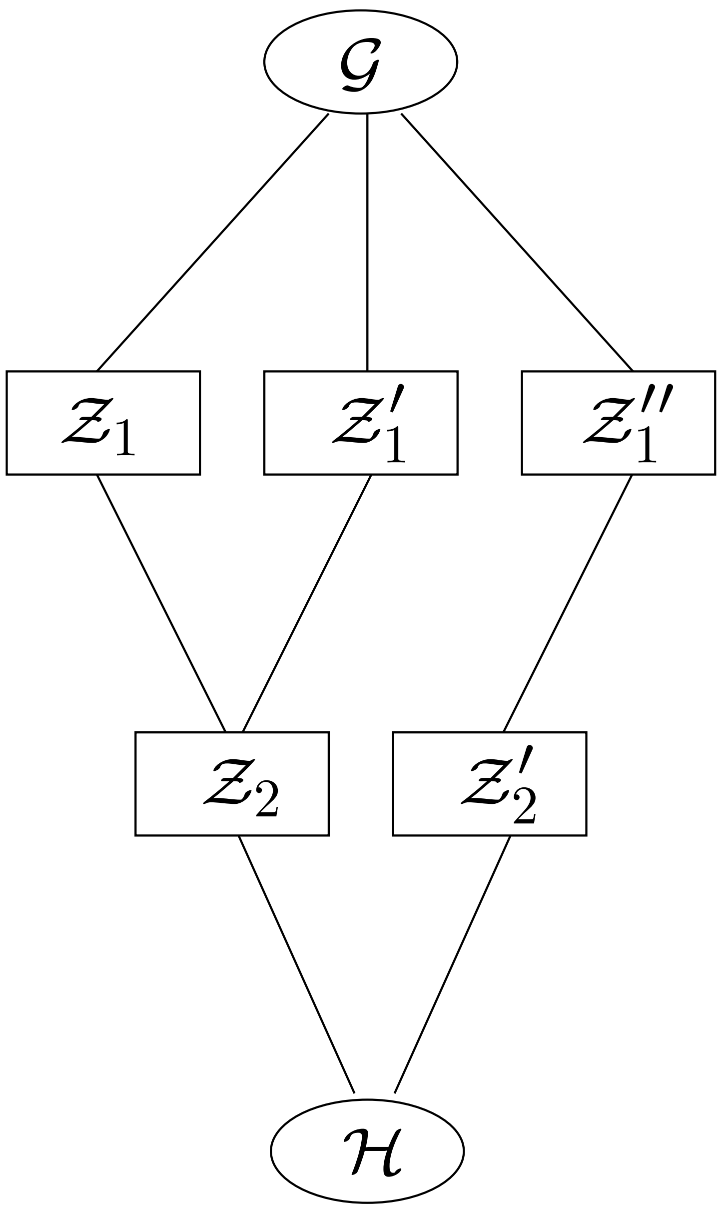
Problem 2.26

The retrieval tool MAXSUB gives an access to the database on maximal subgroups of space groups as listed in *ITA*1. Consider the maximal subgroups of the group *P*4*mm*, (No.99) and compare them with the maximal subgroups of *P*4*mm* derived in Problem 2.17 (*ITA* Exercises). Comment on the differences, if any.

GENERAL SUBGROUPS OF SPACE GROUPS

General subgroups H<G:

Graph of maximal subgroups



Group-subgroup pair

$$\mathcal{G} > \mathcal{H} \ : \ \mathcal{G},\ \mathcal{H},\ [i],\ (\mathrm{P},\mathbf{p})$$

Pairs: group - maximal subgroup

$$\mathcal{Z}_k > \mathcal{Z}_{k+1},\ (\mathrm{P},\mathbf{p})_k$$

$$(\mathrm{P},\mathbf{p}) = \prod_{k=1}^{n} (\mathrm{P},\mathbf{p})_k$$

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 ≧ M ≧ H, such that:

M is a *t*-subgroup of G

H is a *k*-subgroup of M

$$G \xrightarrow{i_P} M \xrightarrow{i_L} H$$

$$[i]=[i_P]\cdot[i_L]$$

Corollary

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

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Problem: SUBGROUPS OF SPACE GROUPS

SUBGROUPGRAPH

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Lattice and chains ...

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Enter subgroup number (H) or choose it:	4
Enter the index [G:H] (optional):	

Construct the lattice

subgroup index

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

Problem 2.27

Study the group--subgroup relations between the groups G=$P4_12_12$, No.92, and H=$P2_1$, No.4 using the program SUBGROUPGRAPH. Consider the cases with specified index e.g. [i]=4, and not specified index of the group-subgroup pair.

What is [i_L] for $P4_12_12$ > $P2_1$, [i]=4 ?

PROBLEM: **Domain-structure analysis**

$$G \xrightarrow{[i]} H$$

number of domain states

twins and antiphase domains

twinning operation

symmetry groups of the domain states; multiplicity and degeneracy

Phase transitions domain structures

Homogeneous (parent) phase G —symmetry reduction→ H Deformed (daughter) phase

Domain structure

Domain

A connected homogeneous part of a domain structure or of a twinned crystal is called a *domain*. Each domain is a single crystal.

The number of such crystals is not limited; they differ in their locations in space, in their orientations, in their shapes and in their space groups but all belong to the same space-group type of H.

Domain states

The domains belong to a finite (small) number of *domain states*. Two domains belong to the same *domain state* if their crystal patterns are identical, *i.e.* if they occupy different regions of space that are part of the *same* crystal pattern.

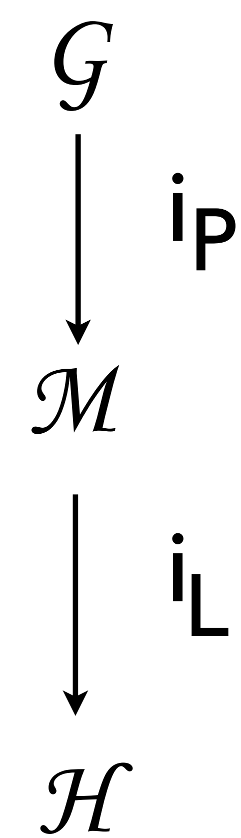
The number of domain states which are observed after a phase transition is limited and determined by the group-subgroup relations of the space groups G and H.

SUBGROUPS CALCULATIONS: HERMANN

Hermann, 1929:

For each pair $\mathcal{G}>\mathcal{H}$, index [i], there exists a uniquely defined intermediate subgroup $\mathcal{M}$, $\mathcal{G} \geqq \mathcal{M} \geqq \mathcal{H}$, such that:

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



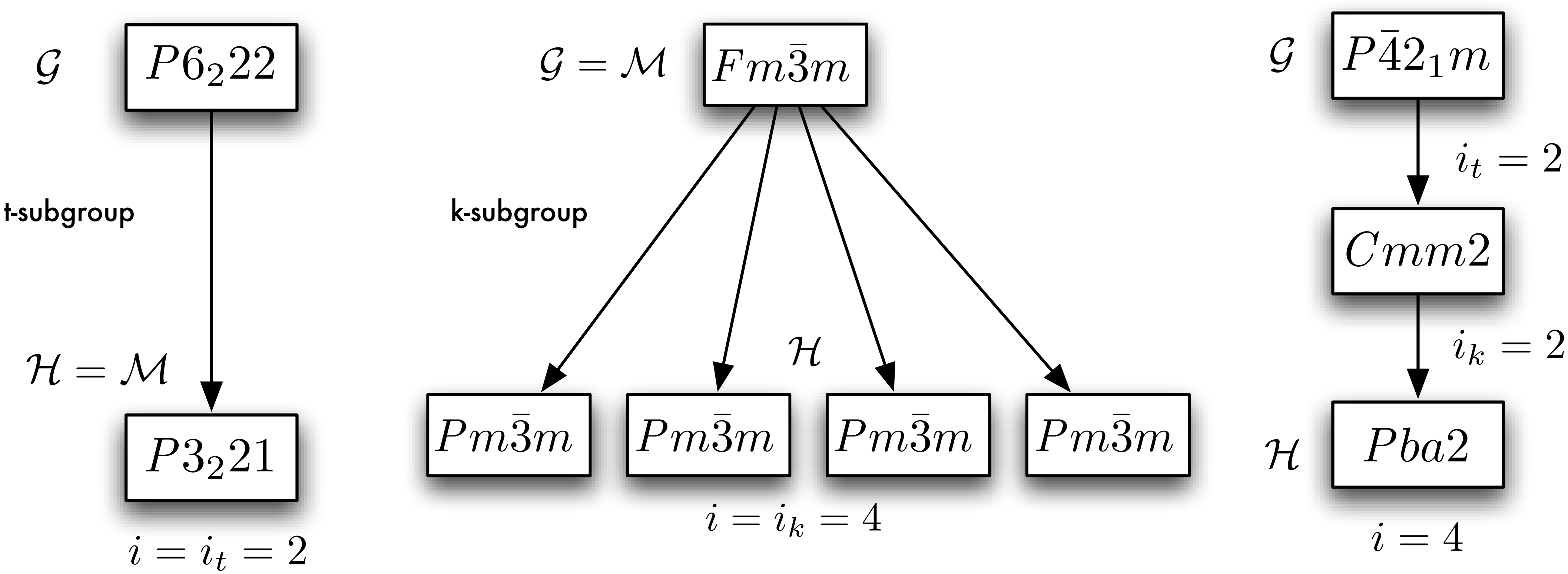
with $[i]=[i_P].[i_L]$

$i_P=P_G/P_H$ twins

$i_L=Z_{H,p}/Z_{G,p}=V_{H,p}/V_{G,p}$ antiphase

Problem: CLASSIFICATION OF DOMAINS **HERMANN**

Quartz | Cu_3Au | $Gd_2(MoO_4)_3$



twin domains | antiphase domains | twin and antiphase domains

EXAMPLE

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

Lead vanadate $Pb_3(VO_4)_2$

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

R-3m

$i_P=P_G/P_H$ **$[i_P]=3$**

C2/m

$i_L=Z_{H,p}/Z_{G,p}$ **$[i_L]=2$**

$P2_1/c$

High-symmetry phase R-3m

```
166
5.6748 5.6748 20.3784 90 90 120
5
Pb    1    3a    0.000000    0.000000    0.000000
Pb    2    6c    0.000000    0.000000    0.207100
PV    3    6c    0.000000    0.000000    0.388400
O     4    6c    0.000000    0.000000    0.324000
O     5    18i   0.842400    0.157600    0.430100
```

$Z_{G,p}=1$ $|P_G|=12$

Low-symmetry phase $P2_1/c$

```
14
7.5075 6.0493 9.4814 90. 115.162 90.
7
Pb 1 2a 0 0 0
Pb 2 4e 0.3835 0.5815 0.2879
PV 1 4e 0.2071 0.0143 0.3999
O  1 4e 0.2872 0.2559 0.0159
O  2 4e 0.2598 0.7979 0.0216
O  3 4e 0.3194 0.9784 0.2823
O  4 4e 0.0335 0.5431 0.2091
```

$|P_H|=?$

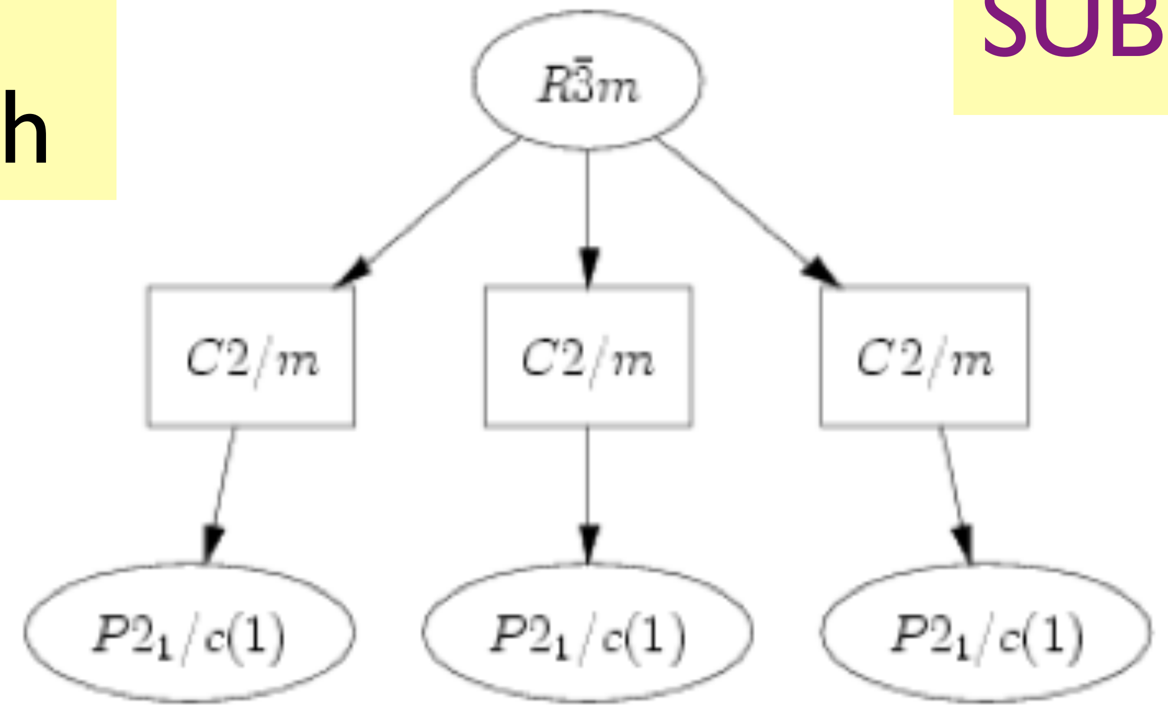
$Z_{H,p}=?$

$Pb_3(VO_4)_2$: Ferroelastic Domains in $P2_1/c$ phase

Group-Subgroup Lattice

Maximal-subgroup graph

SUBGROUPGRAPH



number of domains= index [i] = [i_P].[i_L]=6

number of ferroelastic domains: i_P = 12:4=3

number of different subgroups $P2_1/c$: 3

EXERCISES

Problem 2.29

(A) High symmetry phase: P2/m

Low symmetry phase: P1, small unit-cell deformation

How many and what kind of domain states?

Hint: Determine the index $[i]=[i_P].[i_L]$

(B) High symmetry phase: P2/m

Low symmetry phase: P1, duplication of the unit cell

How many and what kind of domain states?

(C) High symmetry phase: P4mm

Low symmetry phase: P2, index 8

How many and what kind of domain states?

(D) High symmetry phase: $P4_2bc$

Low symmetry phase: $P2_1$, index 8

How many and what kind of domain states?

Problem 2.30

At high temperatures, $BiTiO_3$ has the cubic perovskite structure, space group Pm-3m (No. 221). Upon cooling, it distorts to three slightly deformed structures, all three being ferroelectric, with space groups P4mm (No. 99), Amm2 and R3m. Can we expect twinned crystals of the low symmetry forms? If so, how many kinds of domains?

What program can be used?

What INPUT data should be introduced?

Hint: The program INDEX could be useful

Problem: INDEX [i] for G>H INDEX

INDEX: Index of a group-subgroup pair

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A : choose 227

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A : choose 92

space-group identification

- **Option A: Introduce the formula units (conventional) of the high and low symmetry structure.**

formula units

The formula units (conventional) on the high symmetry structure:

The formula units (conventional) on the low symmetry structure:

- **Option B: Introduce the lattice parameters of the high and low symmetry structure.**

The lattice parameters on the high symmetry structure: 7.12637 7.12637 7.12637 90. 90. 90.

The lattice parameters on the low symmetry structure: 4.9501 4.9501 6.8760 90. 90. 90.

Show index

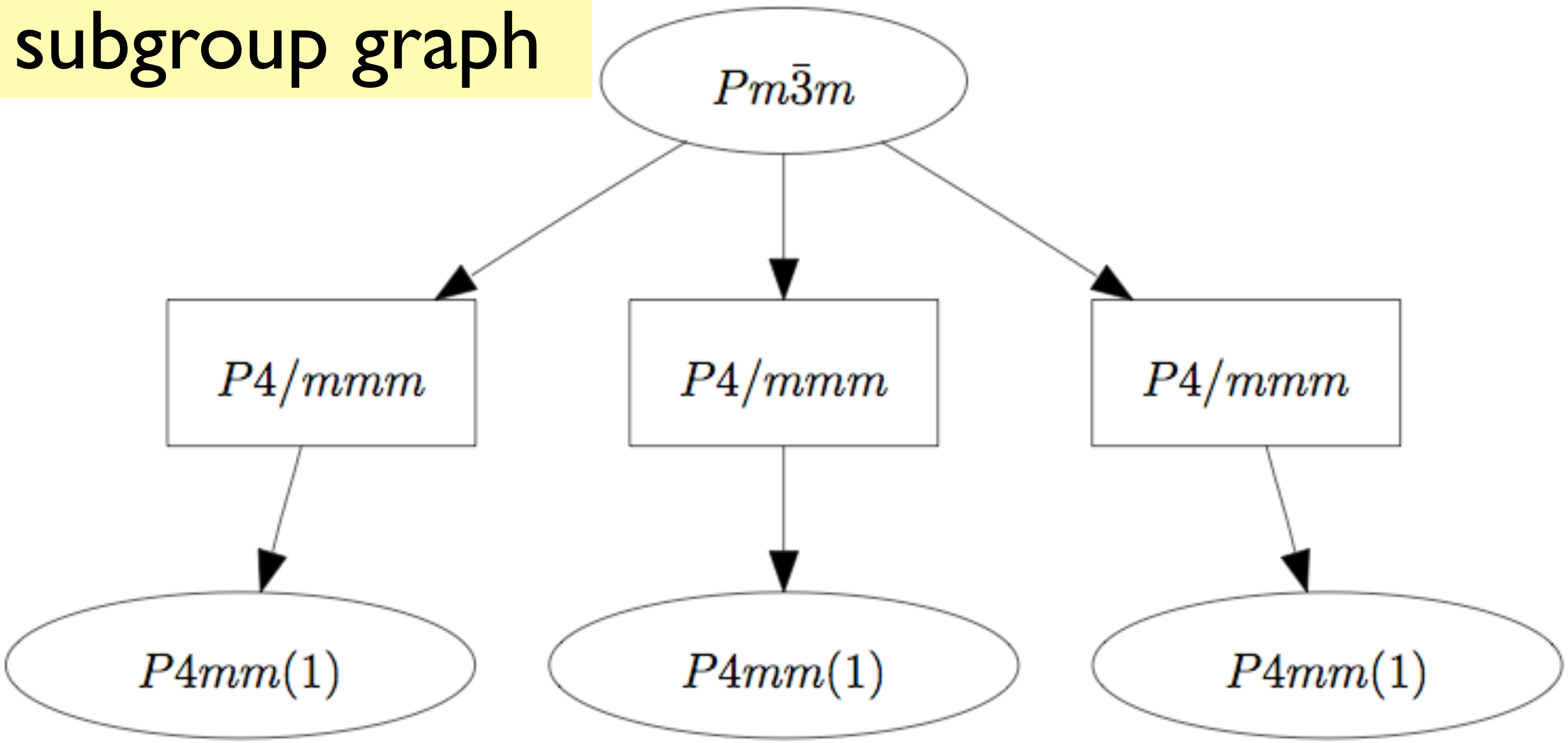
index $[i_L]$

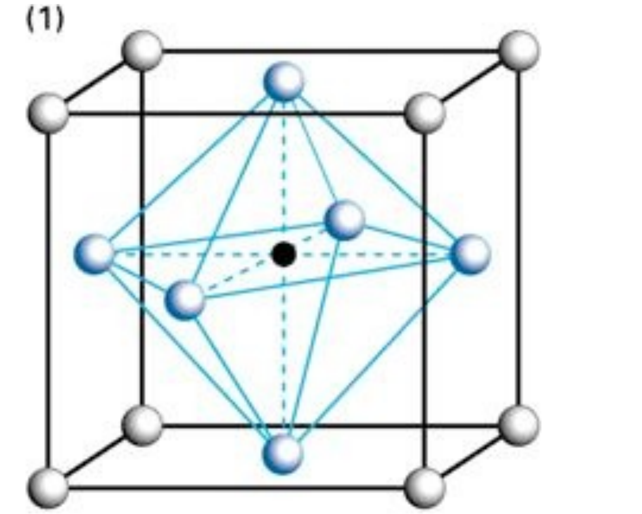
$$i_L = Z_{H,p}/Z_{G,p} = (f_G/f_H) Z_{H,c}/Z_{G,c}$$

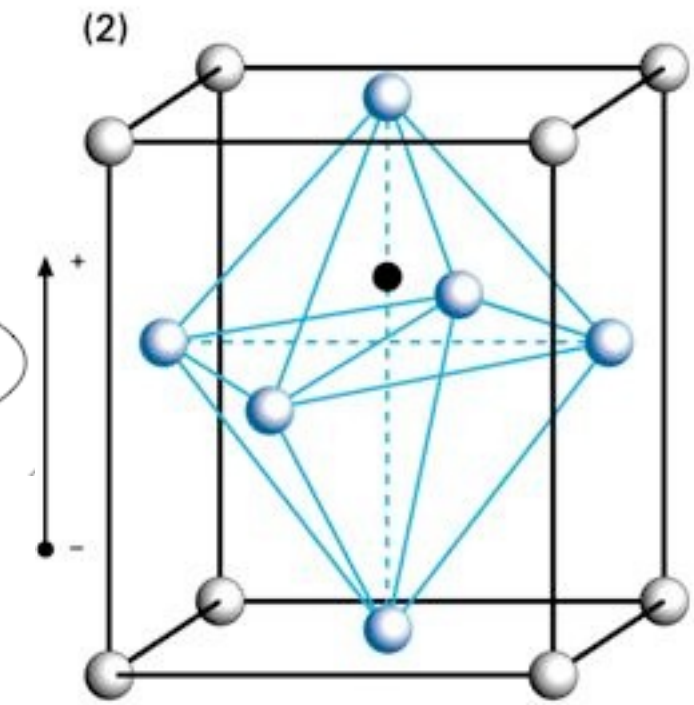
$$i_L = V_{H,p}/V_{G,p} = (f_G/f_H) V_{H,c}/V_{G,c}$$

$BaTiO_3$: Ferroelectric Domains in P4mm phase

Maximal-subgroup graph







index [i] = i_P= 48 : 8=6

number of ferroelectric domains: 6

number of different subgroups P4mm: 3

Domain-structure analysis: Twinning operation

Coset decomposition of G:H

left: G>H, $G=H+(V_2,v_2)H + \ldots + (V_n,v_n)H$

right: G>H, $G=H+H(W_2,w_2) + \ldots + H(W_n,w_n)$

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: 221

Enter subgroup number (H) or choose it: 99

Please, define the transformation that relates the group and the subgroup bases.

Enter transformation matrix :

Rotational part			Origin Shift
1	0	0	0
0	1	0	0
0	0	1	0

Decomposition: left (selected) right

$BaTiO_3$: Ferroelectric Domains in P4mm phase

Twinning operations

Coset decomposition: $Pm\bar{3}m : P4_zmm$, index 6

Coset 1:	Coset 2:	Coset 3:	Coset 4:	Coset 5:	Coset 6:
(x,y,z)	(-x,y,-z)	**(z,x,y)**	(-z,-x,y)	**(y,z,x)**	(y,-z,-x)
(-x,-y,z)	(x,-y,-z)	(z,-x,-y)	(-z,x,-y)	(-y,z,-x)	(-y,-z,x)
(-y,x,z)	(y,x,-z)	(z,-y,x)	(-z,y,x)	(x,z,-y)	(x,-z,y)
(y,-x,z)	(-y,-x,-z)	(z,y,-x)	(-z,-y,-x)	(-x,z,y)	(-x,-z,-y)
(x,-y,z)	**(-x,-y,-z)**	(z,x,-y)	**(-z,-x,-y)**	(-y,z,x)	**(-y,-z,-x)**
(-x,y,z)	(x,y,-z)	(z,-x,y)	(-z,x,y)	(y,z,-x)	(y,-z,x)
(-y,-x,z)	(y,-x,-z)	(z,-y,-x)	(-z,y,-x)	(-x,z,-y)	(-x,-z,y)
(y,x,z)	(-y,x,-z)	(z,y,x)	(-z,-y,x)	(x,z,y)	(x,-z,-y)

coset representatives: q_i

$(1,0)$ $(\bar{1},0)$ $(3,0)$ $(\bar{3},0)$ $(3^{-1},0)$ $(\bar{3}^{-1},0)$

polarization: $P_i = q_i P$

0	0	V	-V	0	0
0	0	0	0	V	-V
V	-V	0	0	0	0

Problem 2.31

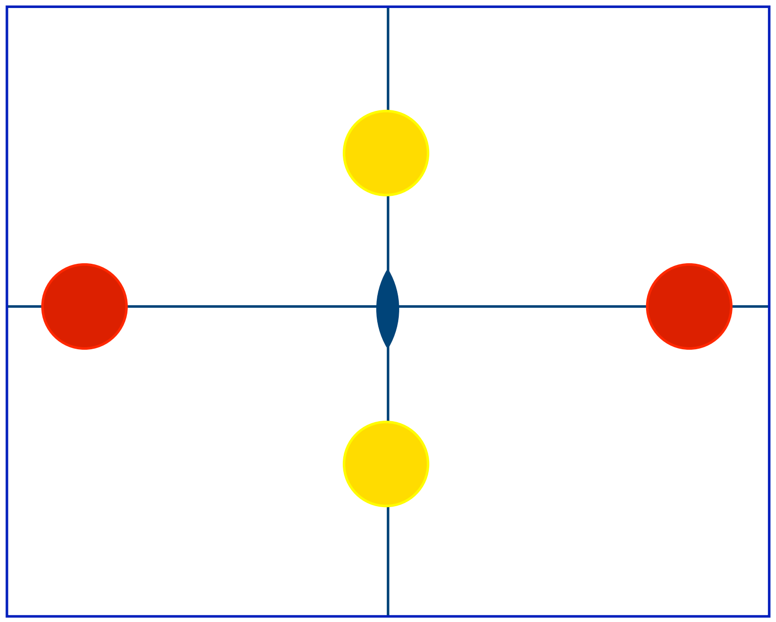
$SrTiO_3$ has the cubic perovskite structure, space group *Pm-3m*. Upon cooling below 105K, the coordination octahedra are mutually rotated and the space group is reduced to *I4/mcm*; *c* is doubled and the conventional unit cell is increased by a factor of four.

Determine the number and the type of domains of the low-temperature form of $SrTiO_3$ using the computer tools of the Bilbao Crystallographic server.

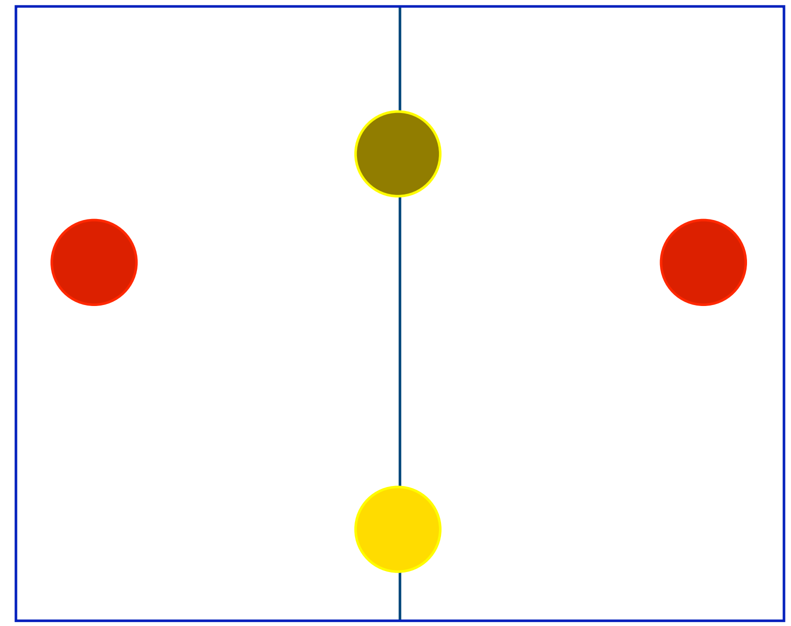
RELATIONS BETWEEN WYCKOFF POSITIONS

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.. (0,y,z) → 2*c* 1 (x,y,z)

2*f* .m. (x,0,z) → 1*b* m (x_2,0,z_2)
→ 1*b* m (x_1,0,z_1)

SYMMETRY REDUCTION

EXAMPLE

Consider the group-subgroup pair *P4mm*>*Pmm2*

[i]=2, ***a'=a, b'=b, c'=c***

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

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*	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$		
1	*b*	$4mm$	$\frac{1}{2},\frac{1}{2},z$			
1	*a*	$4mm$	$0,0,z$			

subgroup *Pmm2*

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	*h*	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	*g*	$m..$	$0,y,z$	$0,\bar{y},z$		
2	*f*	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	*e*	$.m.$	$x,0,z$	$\bar{x},0,z$		
1	*d*	$mm2$	$\frac{1}{2},\frac{1}{2},z$			
1	*c*	$mm2$	$\frac{1}{2},0,z$			
1	*b*	$mm2$	$0,\frac{1}{2},z$			
1	*a*	$mm2$	$0,0,z$			

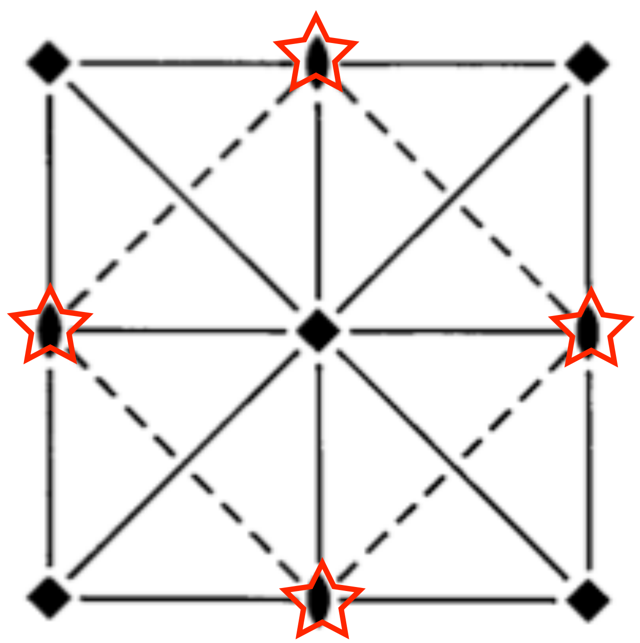
EXAMPLE

Group-subgroup pair

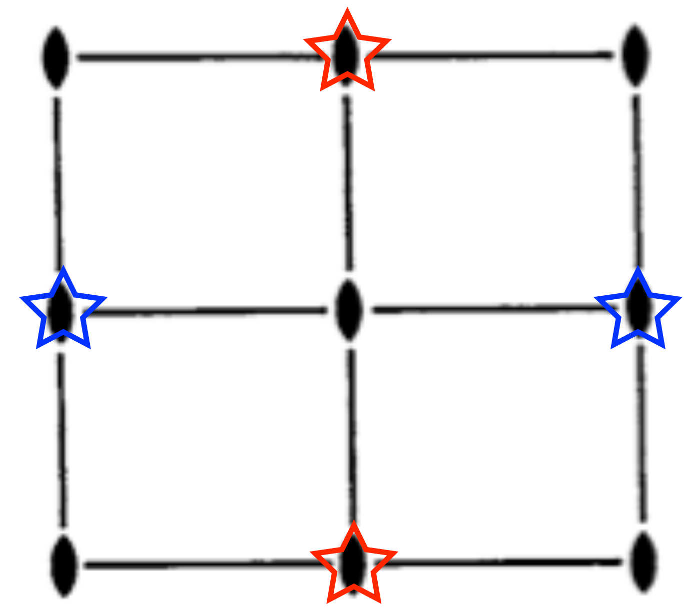
*P*4*mm*>*Pmm*2, [i]=2

a'=a, b'=b, c'=c

*P*4*mm*



*Pmm*2



2c 2mm. 1/2 0 z ☆ → ☆ 1/2 0 z 1c mm2

0 1/2 z → ☆ 0 1/2 z' 1b mm2

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

C_{4v}^{1} | No. 99 | *P*4*mm*

	Axes	Coordinates	Wyckoff positions 1*a*	1*b*	2*c*	4*d*	4*e*	4*f*	8*g*
I Maximal *translationengleiche* subgroups									
[2] *P*4 (75)			1*a*	1*b*	2*c*	4*d*	4*d*	4*d*	2×4*d*
[2] *Pmm*2 (25)			1*a*	1*d*	1*b*;1*c*	4*i*	2*e*;2*g*	2*f*;2*h*	2×4*i*
[2] *Cmm*2 (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	2*a*	2*b*	4*c*	4*d*;4*e*	8*f*	8*f*	2×8*f*
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] *I*4*cm* (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	4*a*	4*b*	8*c*	16*d*	16*d*	2×8*c*	2×16*d*
[2] *I*4*cm* (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	4*b*	4*a*	8*c*	16*d*	2×8*c*	16*d*	2×16*d*
[2] *I*4*mm* (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	2×2*a*	4*b*	8*c*	2×8*d*	2×8*c*	16*e*	2×16*e*
[2] *I*4*mm* (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	4*b*	2×2*a*	8*c*	2×8*d*	16*e*	2×8*c*	2×16*e*
[2] $P4_2mc$ (105)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*a*	2*b*	2×2*c*	8*f*	2×4*d*	2×4*e*	2×8*f*
[2] *P*4*cc* (103)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*a*	2*b*	4*c*	8*d*	8*d*	8*d*	2×8*d*
[2] $P4_2cm$ (101)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*a*	2*b*	4*c*	2×4*d*	8*e*	8*e*	2×8*e*
[2] *P*4*bm* (100)	**a**−**b**,	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$	2*a*	2*b*	4*c*	8*d*	8*d*	2×4*c*	2×8*d*

Example

Bilbao Crystallographic Server

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	136 group
Enter subgroup or choose it	subgroup 65
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:	Transformation matrix (P,p)
origin shift:	0 0 0

1	1	0
-1	1	0
0	0	1

Show group-subgroup data.

Two-level input:

Choice of the Wyckoff positions

Wyckoff Positions Splitting

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

Group Data	Subgroup Data
	16r (x, y, z)
	8q (x, y, 1/2)
	8p (x, y, 0)
☐ All positions	8o (x, 0, z)
☐ 16k (x, y, z)	8n (0, y, z)
☐ 8j (x, x, z)	8m (1/4 , 1/4 , z)
☐ 8i (x, y, 0)	4l (0, 1/2 , z)
☐ 8h (0, 1/2 , z)	4k (0, 0, z)
☐ 4g (x, - x, 0)	4j (0, y, 1/2)
☐ 4f (x, x, 0)	4i (0, y, 0)
☐ 4e (0, 0, z)	4h (x, 0, 1/2)
☐ 4d (0, 1/2 , 1/4)	4g (x, 0, 0)

Bilbao Crystallographic Server

Wyckoff Positions Splitting

99 (*P4mm*) > 8 (*Cm*) [unique axis b]

Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	8g	4b 4b 4b 4b	Relations
2	4f	4b 4b	Relations
3	4e	4b 4b	Relations
4	4d	4b 2a 2a	Relations
5	2c	4b	Relations
6	1b	2a	Relations
7	1a	2a	Relations

Two-level output:

Relations between coordinate triplets

Splitting of Wyckoff position 4d

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, x, z)	(0, x, z)	$4b_1$	(x_1, y_1, z_1)
2	(-x, -x, z)	(0, -x, z)		(x_1, -y_1, z_1)
3	(x+1, x, z)	(1/2, x+1/2, z)		(x_1+1/2, y_1+1/2, z_1)
4	(-x+1, -x, z)	(1/2, -x+1/2, z)		(x_1+1/2, -y_1+1/2, z_1)
5	(-x, x, z)	(-x, 0, z)	$2a_1$	(x_2, 0, z_2)
6	(-x+1, x, z)	(-x+1/2, 1/2, z)		(x_2+1/2, 1/2, z_2)
7	(x, -x, z)	(x, 0, z)	$2a_2$	(x_3, 0, z_3)
8	(x+1, -x, z)	(x+1/2, 1/2, z)		(x_3+1/2, 1/2, z_3)

Problem 2.32

Consider the group-subgroup pair P4mm (No.99) > Cm (No.8) of index [i]=4 and the relation between the bases ***a'=a-b, b'=a+b, c'=c***. Study the splittings of the Wyckoff positions for the group-subgroup pair by the program WYCKSPLIT.

SUPERGROUPS
OF
SPACE GROUPS

Supergroups of space groups

Definition:

The group G is a supergroup of H if H is a subgroup of G, $G \geq H$

If H is a proper subgroup of G, $H < G$, then G is a proper supergroup of H, $G > H$

If H is a maximal subgroup of G, $H < G$, then G is a minimal supergroup of H, $G > H$

Types of minimal supergroups:

translationengleiche (t-type)
klassengleiche (k-type)

- non-isomorphic
- isomorphic

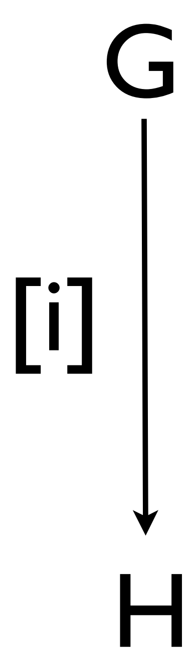
ITA1 data:

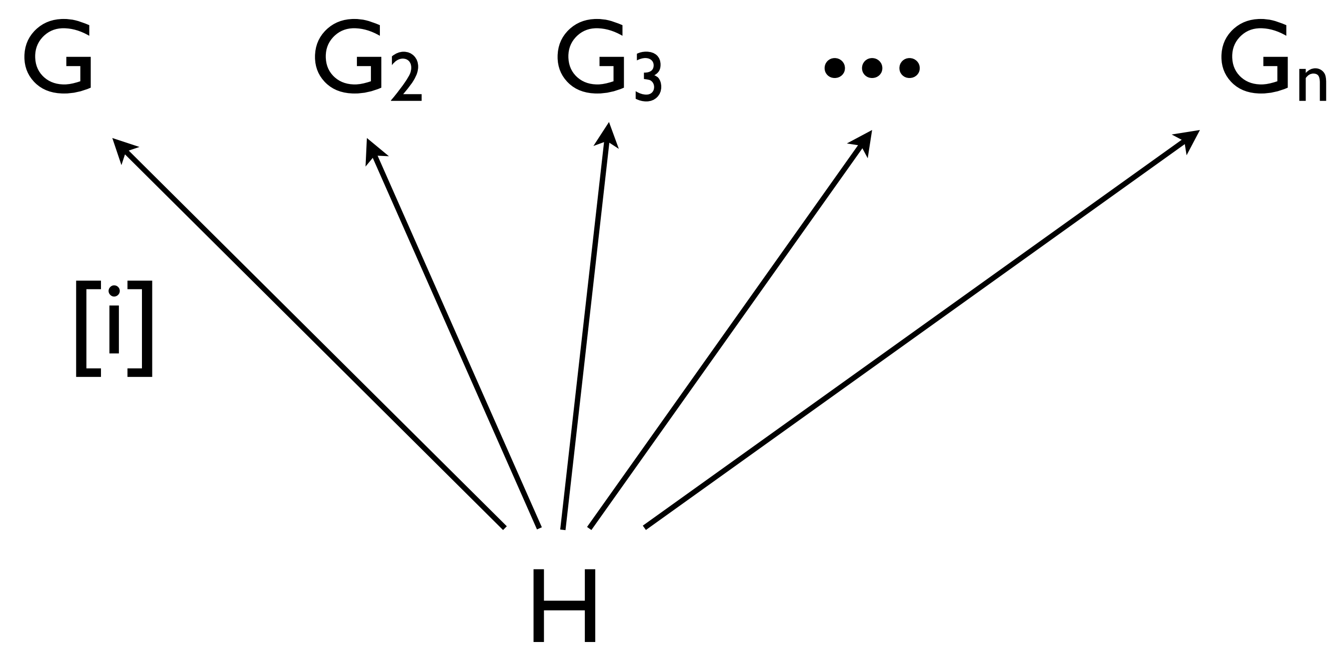
minimal non-isomorphic *k*- and *t*-supergroups types

The Supergroup Problem

Given a group-subgroup pair G>H of index [i]

Determine: all G_k>H of index [i], $G_i \simeq G$





all G_k>H contain H as subgroup

$G_k = H + Hg_2 + \ldots + Hg_{ik}$

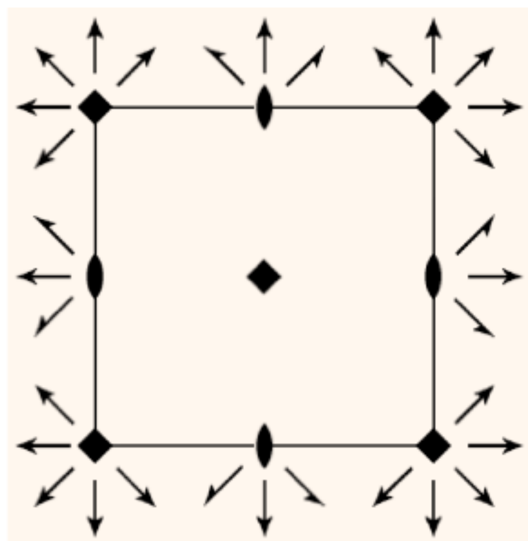
Example: Supergroup problem

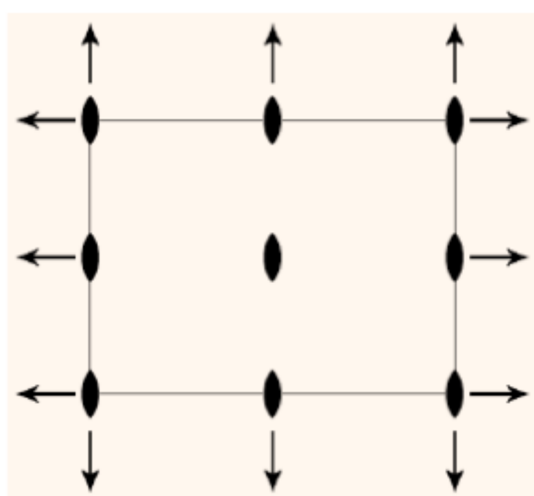
Group-subgroup pair P422>P222

P422

[2]

P222





$$P422 = 222 + (222)(4,0)$$

Supergroups P422 of the group P222

$P4_z22$ $P4_x22$ $P4_y22$

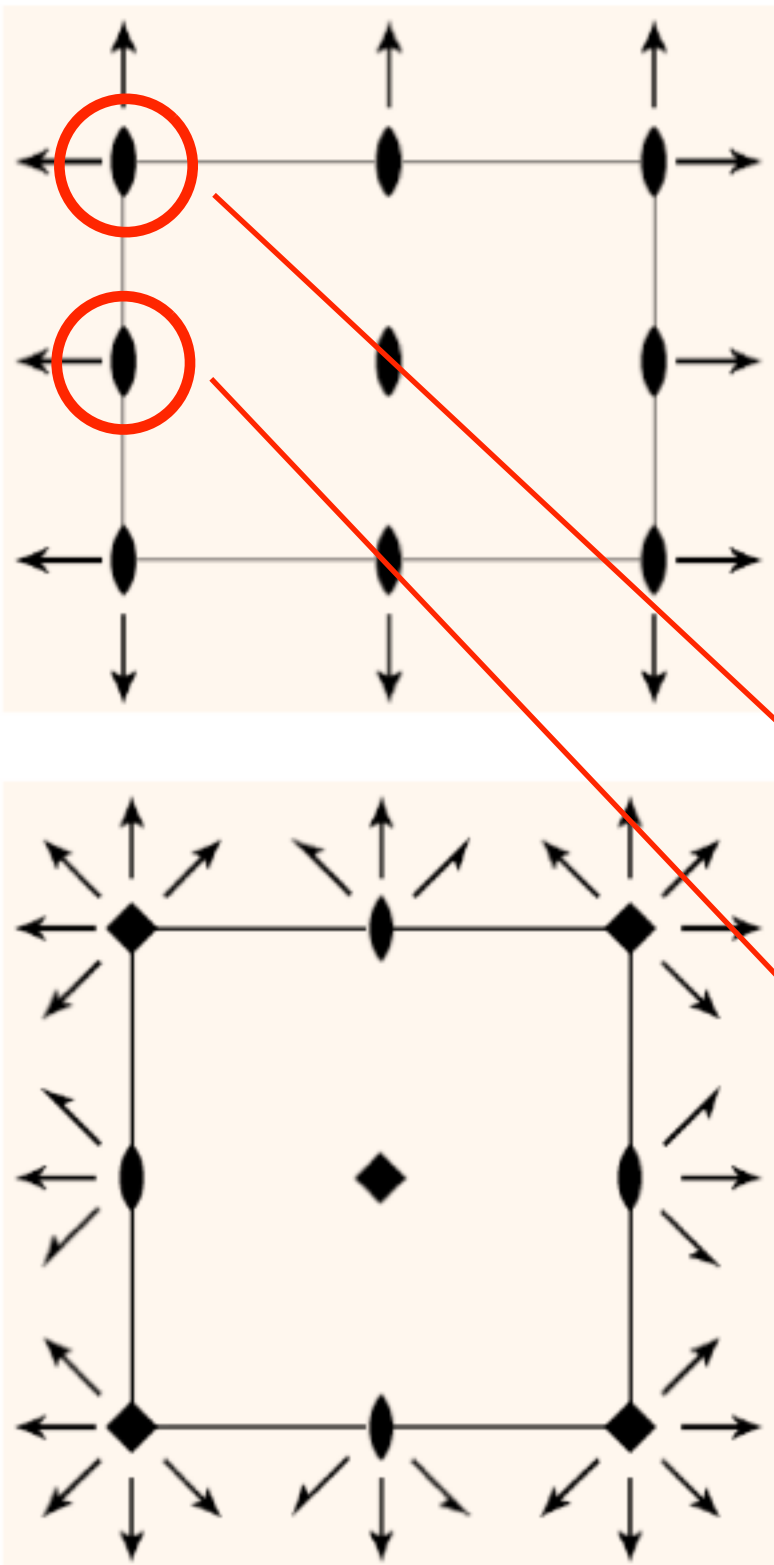
[2]

P222

$$P4_z22 = 222 + (222)(4_z,0)$$
$$P4_x22 = 222 + (222)(4_x,0)$$
$$P4_y22 = 222 + (222)(4_y,0)$$

Are there more supergroups P422 of P222?

Example: Supergroups P422 of P222



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

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

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

	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	$(0,\frac{1}{2},0)$	$(0,\frac{1}{2},\frac{1}{2})$	$(P422)'_3$

International Tables for Crystallography, Vol. A1

eds. H. Wondratschek, U. Mueller

Minimal Supergroup Data

***P*222** No. 16 ***P*222**

I Minimal *translationengleiche* supergroups

[2] *Pmmm* (47); [2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *P*422 (89); [2] $P4_222$ (93); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2m$ (111); [3] *P*23 (195)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

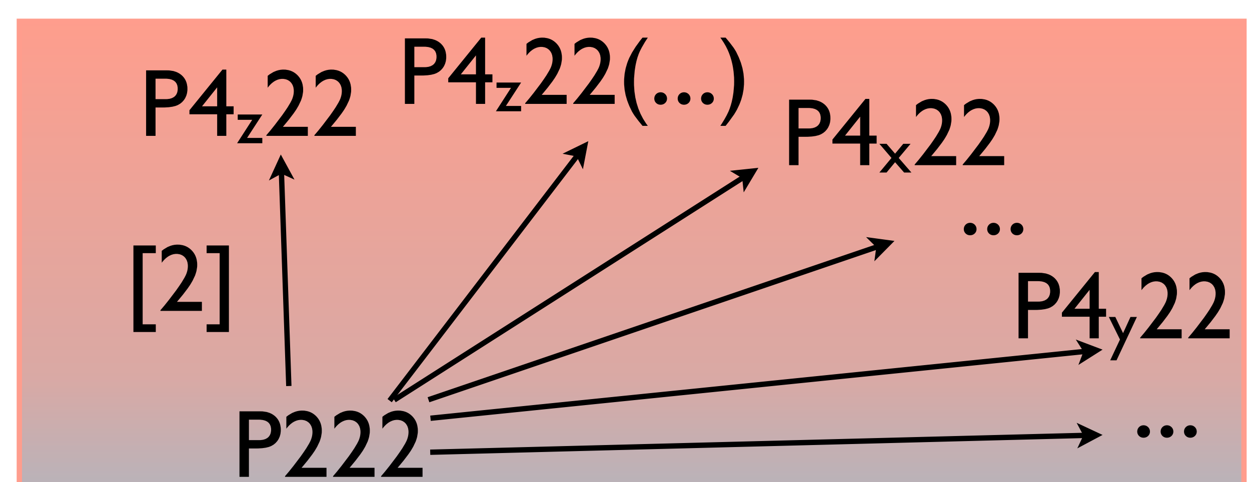
[2] *A*222 (21, *C*222); [2] *B*222 (21, *C*222); [2] *C*222 (21); [2] *I*222 (23)

- **Decreased unit cell** none

Incomplete data

Space-group type only

No transformation matrix



Problem: SUPERGROUPS OF SPACE GROUPS

SUPERGROUPS MINSUP

Click here to see the list with all minimal supergroups of a given space group(MINSUP)

supergroup

Please, enter the sequential numbers of group and supergroup as given in the *International Tables for Crystallography*, Vol. A:	
Enter supergroup number (G) or choose it:	89
Enter group number (H) or choose it:	16
Enter the index [G:H]	2

space group

index

By default the Euclidean normalizers are used. If you want to use other normalizer, please check it from the list below:

Group normalizer

Euclidean normalizer

Subgroup normalizer

Euclidean normalizer

Find the Supergroups

Subgroup normalizer

Euclidean normalizer

- Euclidean normalizer
- affine normalizer
- user defined normalizer

option normalizers

Output Supergroups

Supergroups (of index 2) isomorphic to the group 89 (*P*422) of the group 16 (*P*222)

No	Transformation matrix	Coset representatives	Wyckoff Splitting	More...
1	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	(x, y, z) (-y, x, z)	[WP splitting]	Full cosets
2	[1 0 0] [1/2] [0 1 0] [0] [0 0 1] [0]	(x, y, z) (-y-1/2, x+1/2, z)	[WP splitting]	Full cosets

Problem 2.33

Consider the group--supergroup pair $H < G$ with $H = P222$, No. 16, and the supergroup $G = P422$, No. 89, of index [i]=2. Using the program MINSUP determine all supergroups P422 of P222 of index [i]=2.

How does the result depend on the normalizer of the supergroup and/or that of the subgroup?

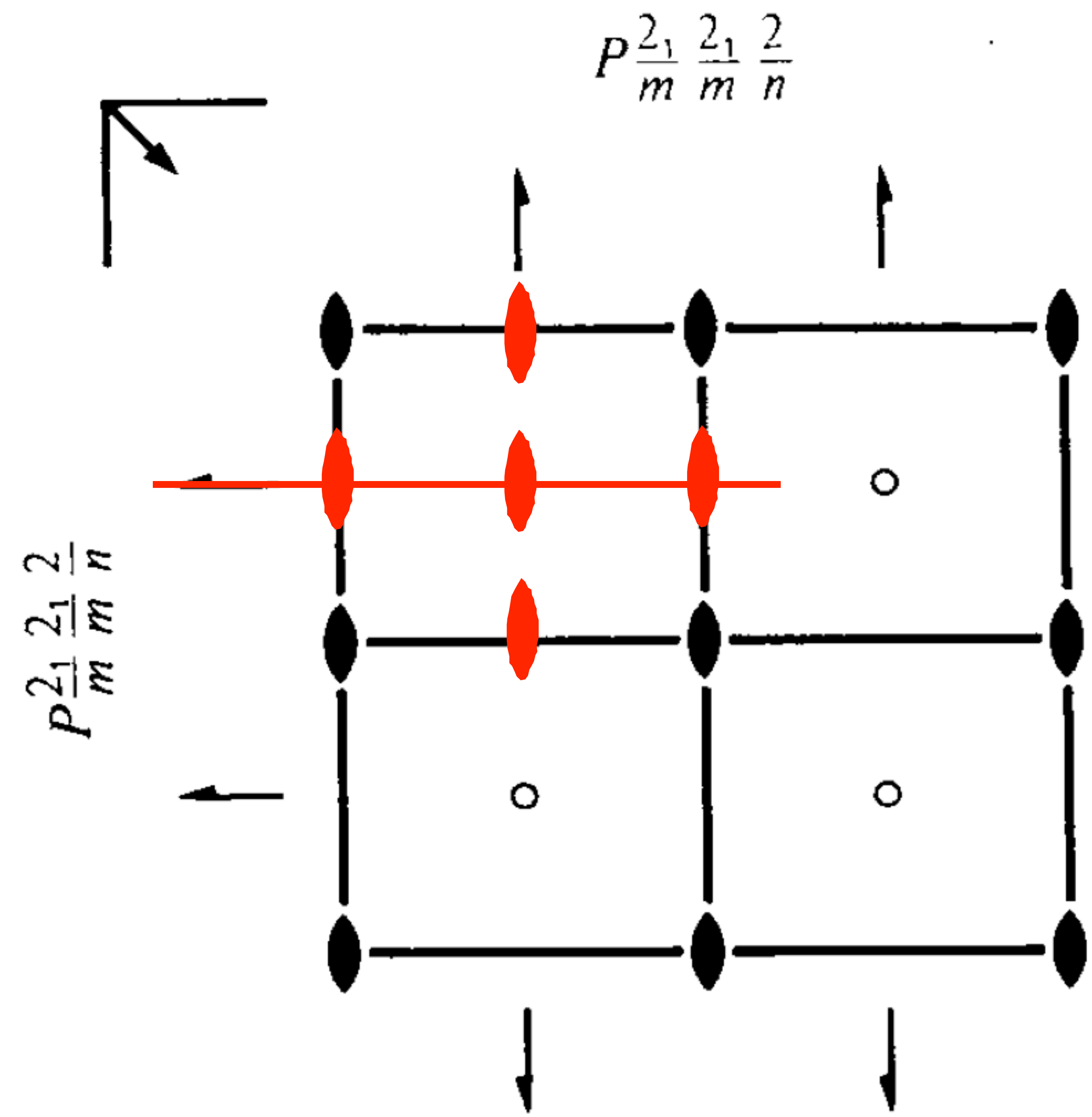
NORMALIZERS
OF
SPACE GROUPS

Normalizers of space groups

Normalizers N(G) : $g^{-1}\{G\}g = \{G\}$ $\begin{cases} \text{Euclidean} \\ \text{Affine} \end{cases}$

Example: Pmmn

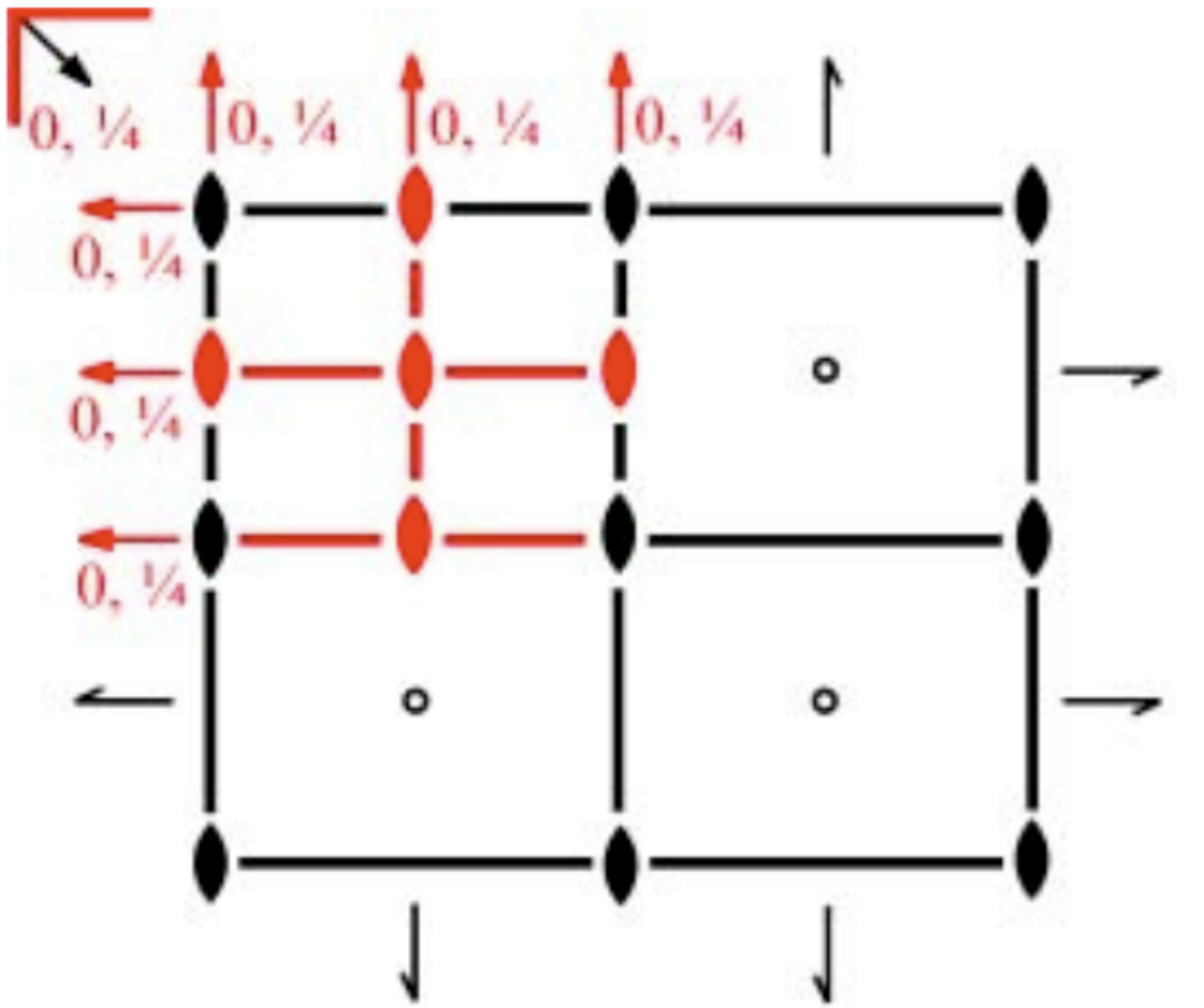
the symmetry of symmetry



Normalizers of space groups

Normalizers N(G) : $g^{-1}\{G\}g = \{G\}$ $\begin{cases}\text{Euclidean}\\ \text{Affine}\end{cases}$

the symmetry
of symmetry

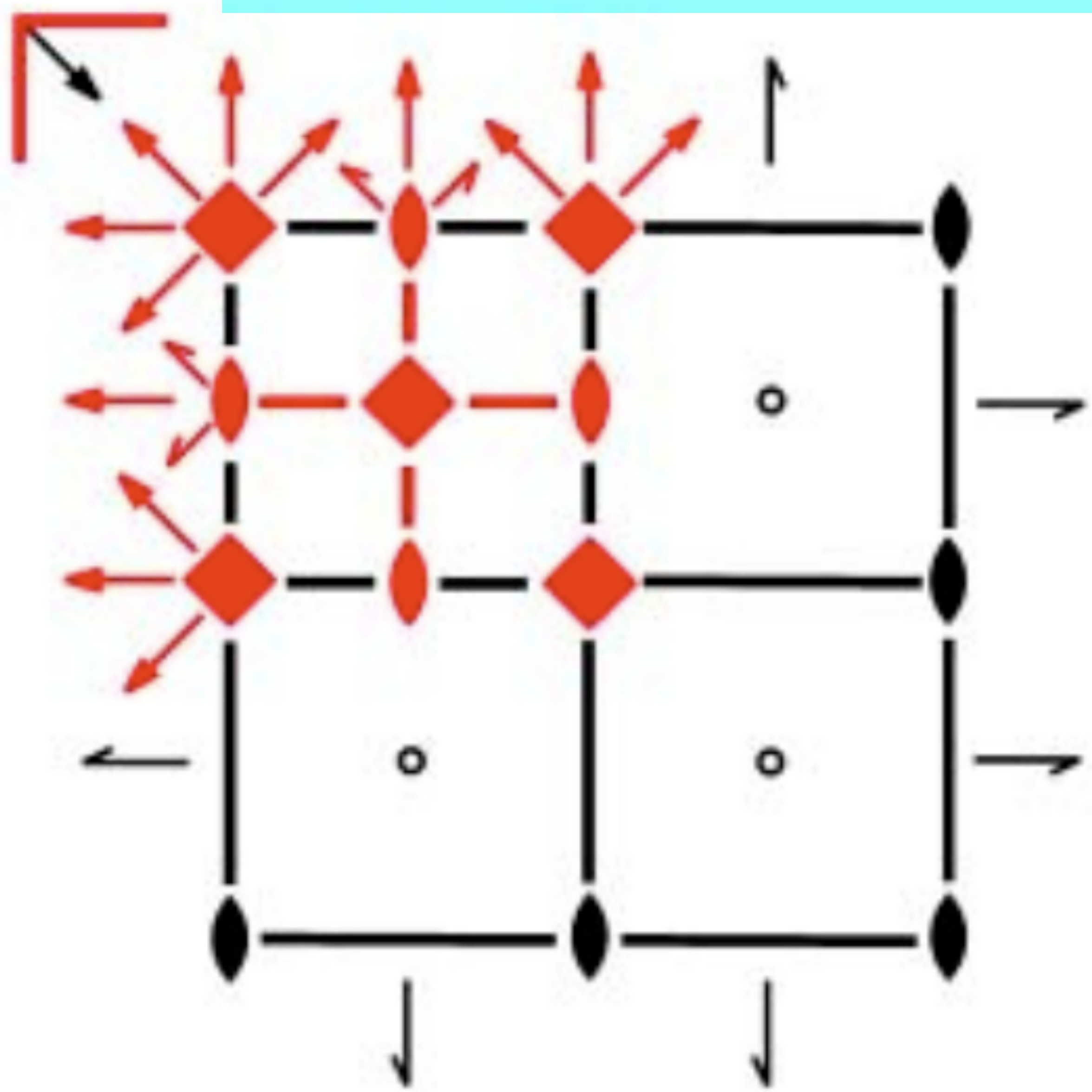


Space group: Pmmn (a,b,c)

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

International Tables for Crystallography, Vol. A, Chapter 15

Normalizers of space groups

E. Koch and W. Fischer

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$	
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors
55	*Pbam*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
		$a = b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
56	*Pccn*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
		$a = b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
57	*Pbcm*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
58	*Pnnm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
		$a = b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
59	*Pmmn* (both origins)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$
		$a = b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$

Example: Pmmn

Problem: Normalizers of space groups NORMALIZER

Normalizers of Space Groups

How to select the group
The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link [**choose it**].

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A [choose] 59

Choose:
- Euclidean (general metric): ○
- Enhaced Euclidean (specialized metric): ⊙
- Affine: ○

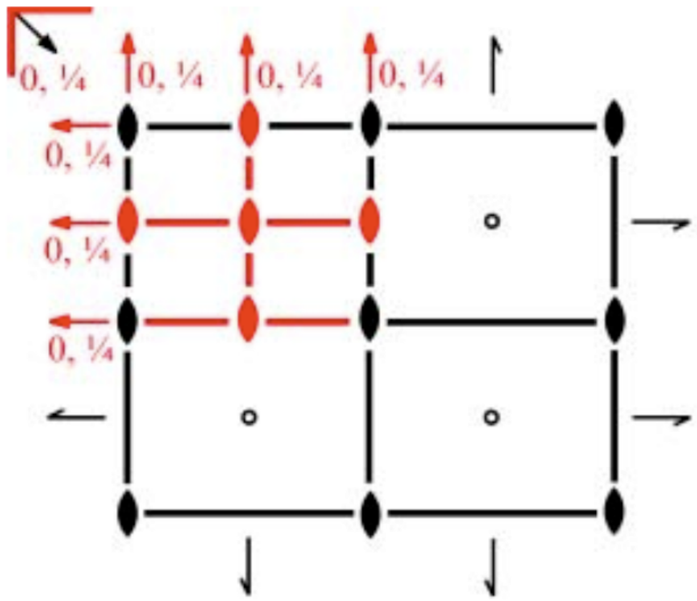
Enhanced Euclidean normalizer (specialized metrics)

Space group:	59
Lattice parameters:	4 4 5 90 90 90

[Show]

Example NORMALIZER: Space group *Pnnm* (59)

Euclidean normalizer (general metric) of *Pmmn* (No. 59)



Space group:	*Pmmn* (59)
Lattice type:	oP
Cell parameters:	4 4 5 90 90 90
Angular tolerance:	0.15 degrees

Euclidean normalizer of *Pmmn* (a,b,c): *Pmmm* (1/2a,1/2b,1/2c).

Index of *Pmmn* in *Pmmm* (**1/2a,1/2b,1/2c**): 8 with **i**$_L$=8 and **i**$_P$=1.

Additional generators of *Pmmm* (**1/2a,1/2b,1/2c**) with respect to *Pmmn*.

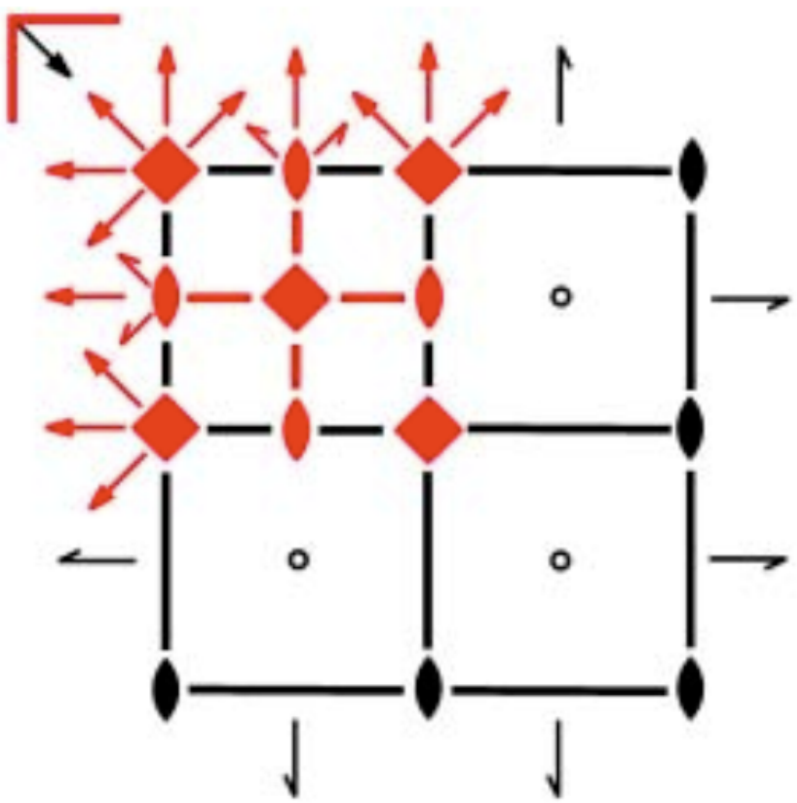
x+1/2,y,z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	*t* (1/2,0,0)
x,y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	*t* (0,1/2,0)
x,y,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	*t* (0,0,1/2)

Cosets representatives
x,y,z x+1/2,y,z x,y+1/2,z x+1/2,y+1/2,z x,y,z+1/2 x+1/2,y,z+1/2 x,y+1/2,z+1/2 x+1/2,y+1/2,z+1/2

The cosets representatives of the Euclidean normalizer *Pmmm* (**1/2a,1/2b,1/2c**) with respect to *Pmmn*

Example NORMALIZER: Space group *Pnnm* (59)

Enhanced Euclidean normalizer (specialized metric) of *Pmmn* (No. 59)



Space group:	*Pmmn* (59)
Lattice type:	oP
Cell parameters:	4 4 5 90 90 90
Angular tolerance:	0.15 degrees

Index of *Pmmn* in *P4/mmm* (**1/2a, 1/2b, 1/2c**): 16 with **i**$_L$=8 and **i**$_P$=2.

Coset representatives of the enhanced Euclidean normalizer *P4/mmm* (**1/2a, 1/2b, 1/2c**)

Coset representatives	More...
x,y,z y,x,z	Full cosets

Cosets 1	Cosets 2
(x,y,z)	(y,x,z)
(-x,-y,z)	(-y,-x,z)
(-x,y,-z)	(y,-x,-z)
(x,-y,-z)	(-y,x,-z)
(-x,-y,-z)	(-y,-x,-z)
(x,y,-z)	(y,x,-z)
(x,-y,z)	(-y,x,z)
(-x,y,z)	(y,-x,z)

Symmetry-equivalent Wyckoff positions   Wyckoff Sets

Cosets representatives of the Affine Normalizer with respect to the Space Group 59 (*Pmmn*) [origin choice 2]

Transformation of the Wyckoff Positions of Space Group 59 (*Pmmn*) [origin choice 2] under Affine Normalizer (*P4/mmm*) **1/2a,1/2b,1/2c**

Index: 16

No. #	Coset Representative		Transformed WP
1	x,y,z	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	a b c d e f g
2	x+1/2,y,z	[1 0 0] [1/2] [0 1 0] [0] [0 0 1] [0]	b a c d e f g
3	x,y+1/2,z	[1 0 0] [0] [0 1 0] [1/2] [0 0 1] [0]	b a c d e f g
4	x,y,z+1/2	[1 0 0] [0] [0 1 0] [0] [0 0 1] [1/2]	a b d c e f g
5	x+1/2,y+1/2,z	[1 0 0] [1/2] [0 1 0] [1/2] [0 0 1] [0]	a b c d e f g

a ⟷ b

Symmetry-equivalent Wyckoff positions — Wyckoff Sets

59	***Pmmn***			
2	*a*	*mm*2	*	*Pmmn a*
2	*b*			
4	*c*	$\bar{1}$		*Pmmm a*
4	*d*			
4	*e*	*m*..	*	*Pmmn e*
4	*f*	.*m*.		
8	*g*	1	*	*Pmmn g*

International Tables for Crystallography, Vol. A
Fischer and Koch, Chapter 14.

Table 14.2.3.2
(selection)

Wyckoff Sets of Space Group 59 (*Pmmn*) [origin choice 2]

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

Letter	Mult	SS	Rep.	Equivalent Positions
g	8	1	(x, y, z)	g
f	4	.m.	(x, 1/4 , z)	ef
e	4	m..	(1/4 , y, z)	ef
d	4	-1	(0, 0, 1/2)	cd
c	4	-1	(0, 0, 0)	cd
b	2	mm2	(1/4 , 3/4 , z)	ab
a	2	mm2	(1/4 , 1/4 , z)	ab

Bilbao Crystallographic Server

Problem 2.36

Using the computer tool NORMALIZER determine the Euclidean normalizer of the group *P*222 (general metric) and the Euclidean normalizers of enhanced symmetry for the cases of specialized metric of *P*222. Compare your results with the data used in Problem 2.25 of the I*T*A Exercises.

Determine the assignment of Wyckoff positions into Wyckoff sets with respect to the different Euclidean normalizers of *P*222 (for general and specialized metrics) and comment on the differences, if any.