CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

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SYMMETRY RELATIONS BETWEEN SPACE GROUPS

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MAXIMAL SUBGROUPS OF SPACE GROUPS

I. MAXIMAL TRANSLATIONENGLEICHE SUBGROUPS

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

Let $H_1<G$, $H_2<G$

then, $H_1 \sim H_2$, if $\exists\, g \in G$: $g^{-1}H_1g = H_2$

SPACE GROUPS

Space group G:

The set of all symmetry operations (isometries) of a **crystal pattern**

Translation subgroup T:
T ◁ G

The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups P_G:

The factor group of the space group G with respect to the translation subgroup T: $P_G \cong G/H$

$$(\boldsymbol{W},\boldsymbol{w}) \longrightarrow \boldsymbol{W} \quad P_G=\{\boldsymbol{W} \mid (\boldsymbol{W},\boldsymbol{w}) \in G\}$$

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

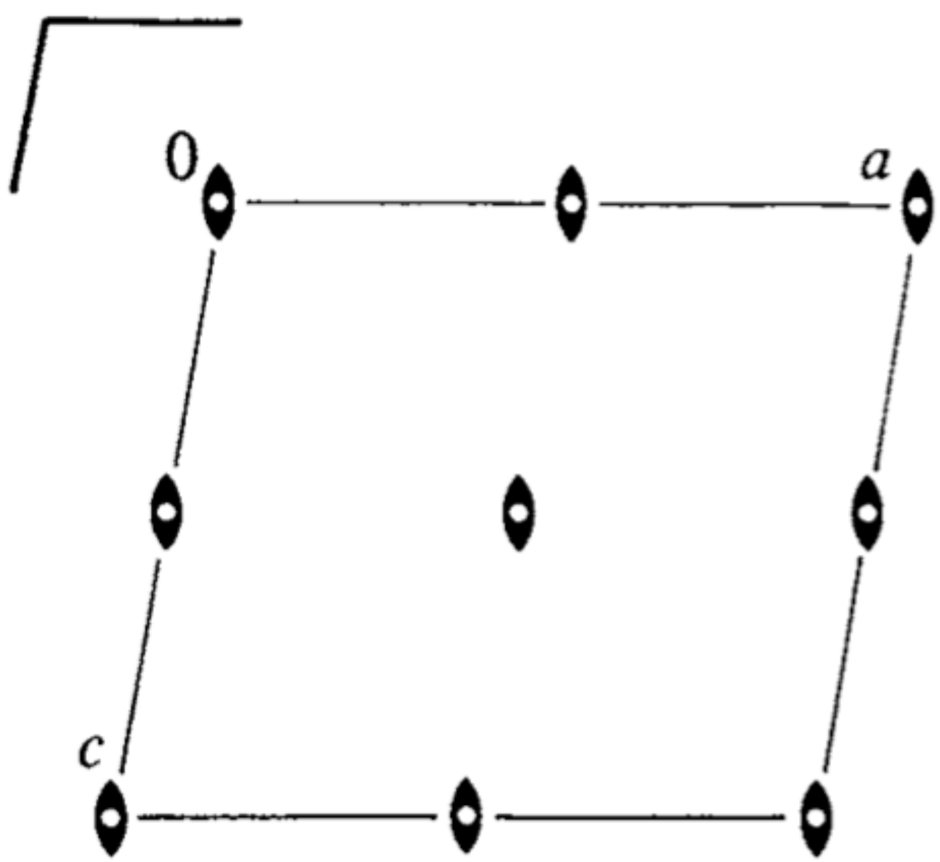
Point group $P_G = \{I, W_2, W_3, \ldots, W_i\}$

Example: P12/m1

Coset decomposition G:T_G

Factor group $G/T_G \simeq P_G$

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



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

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

Translationengleiche subgroups $H<G$: *t*-subgroups

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

Example: P12/m1

Coset decomposition $G:T_G$

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:

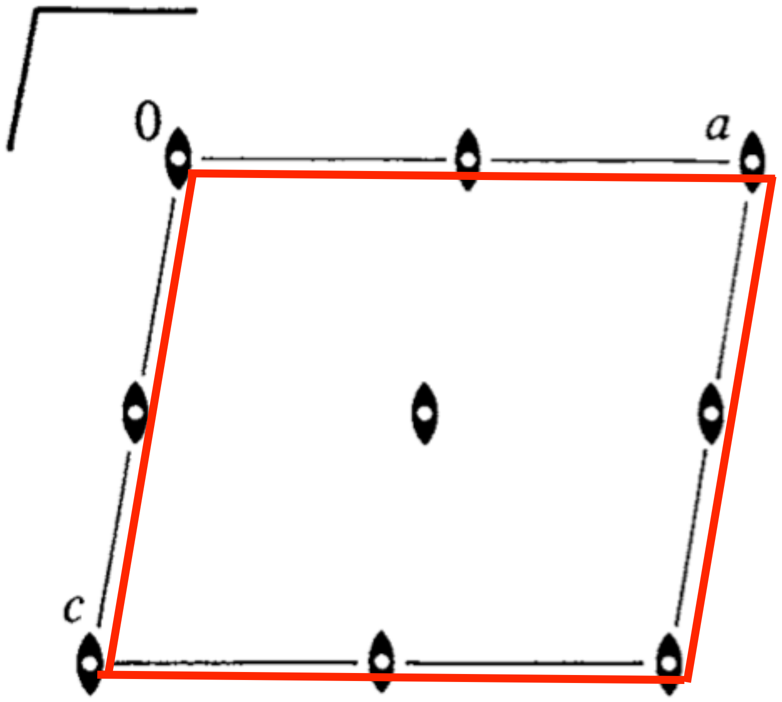
$H_1 = T_G \cup T_G\,2$
P121

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

$H_3 = T_G \cup T_G\,m$
Pm

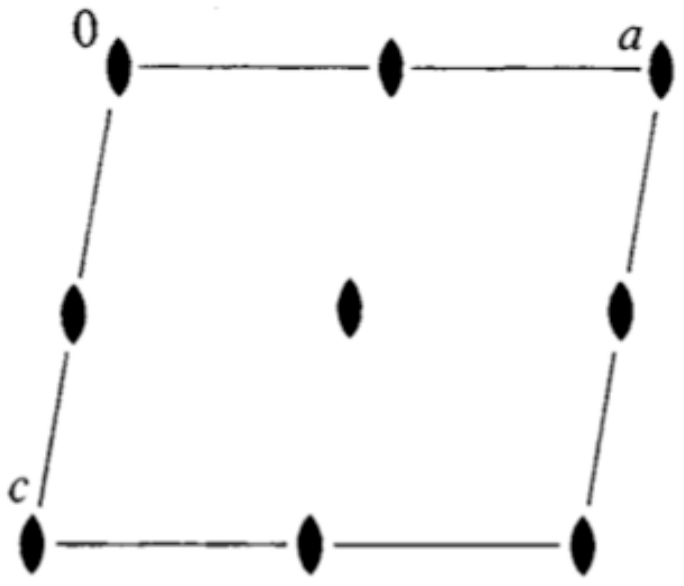
Example: P12/m1

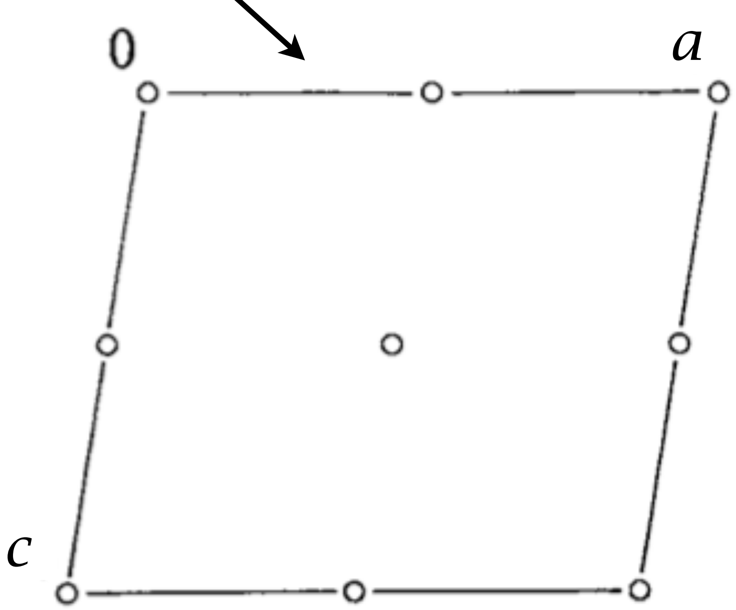
Translationengleche subgroups H<G:



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

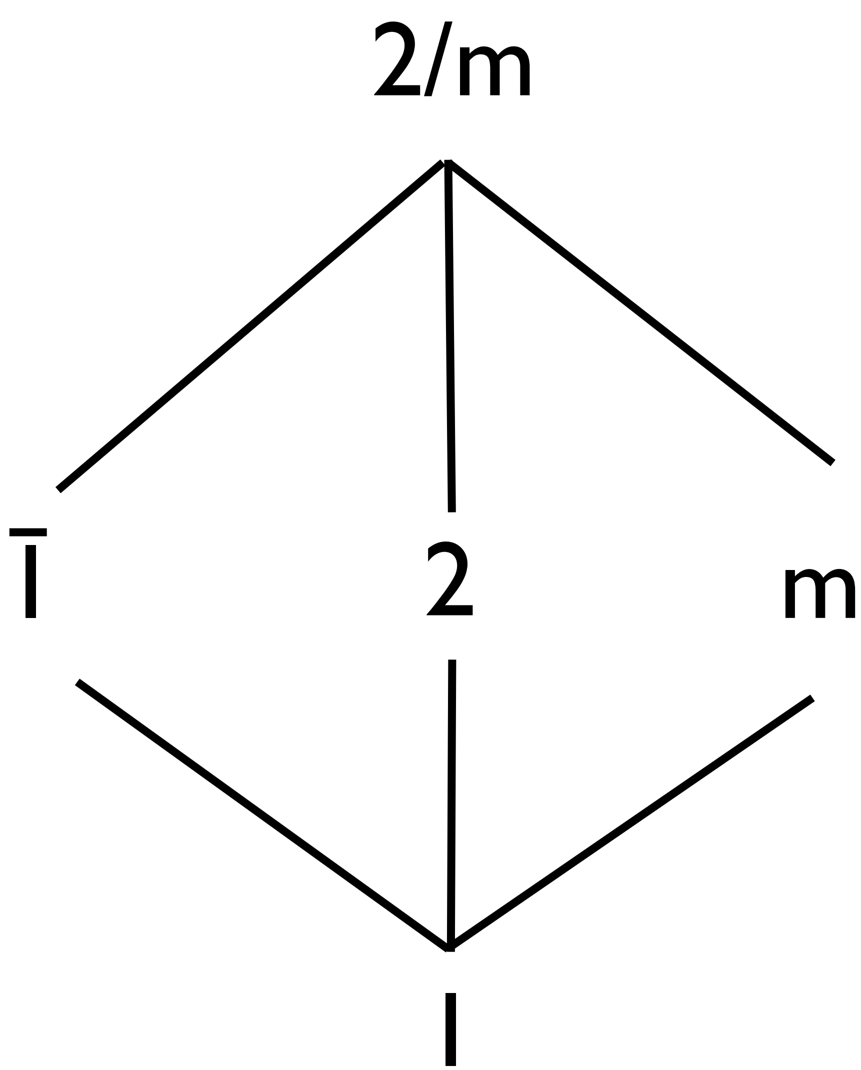
$P121 = T_G \cup T_G 2$





Example: P12/m1

Translationengleiche subgroups H<G:



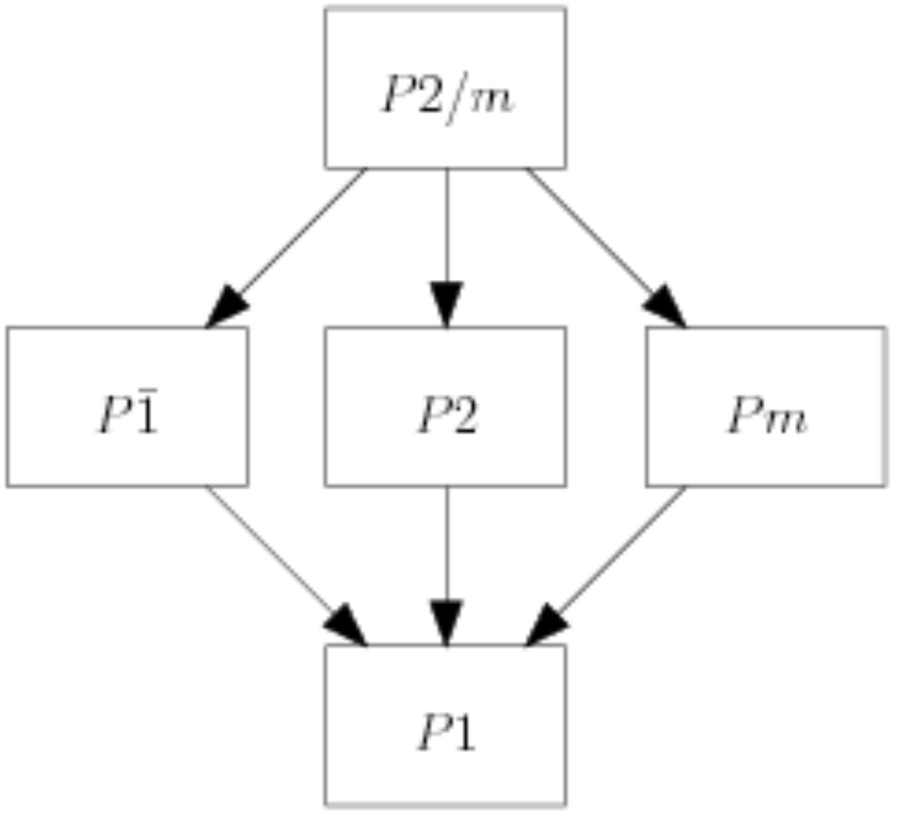
index

[1]

[2]

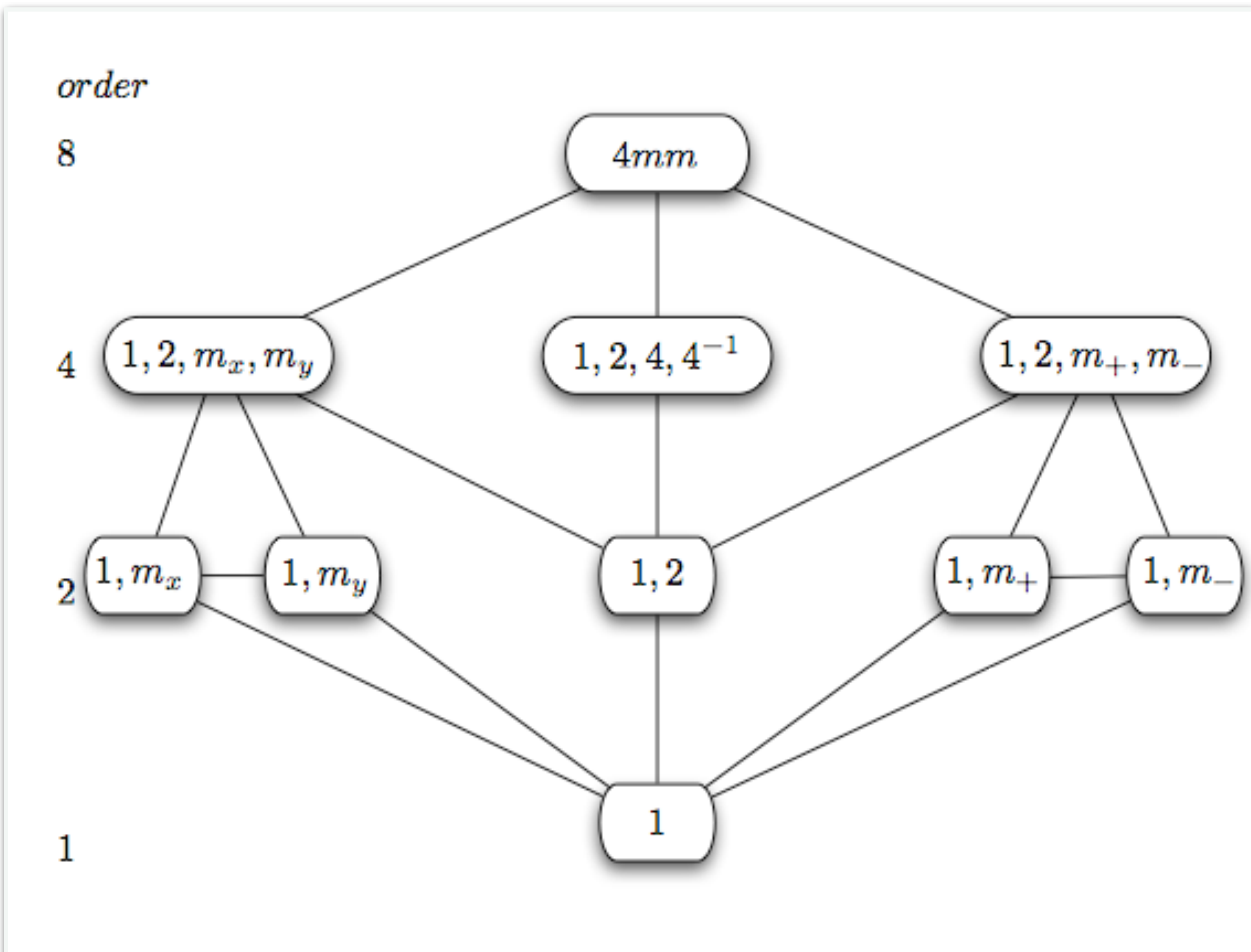
[4]

Subgroup diagram of point group 2/m



Translationengleiche subgroups of space group *P*2/m

Construct the diagram of the *t*-subgroups of *P4mm* using the 'analogy' with the subgroup diagram of 4*mm*



Transformation matrix: (P,p)

group G $\{e, g_2, g_3, \ldots, g_i, \ldots, g_{n-1}, g_n\}$

subgroup H<G non-conventional $\{e, \ldots\ldots, g_3, \ldots, g_i, \ldots\ldots\ldots, g_n\}$

(P,p)

subgroup H<G $\{e, h_2, h_3, \ldots, h_m\}$

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

International Tables for Crystallography, Vol. A1

eds. H. Wondratschek, U. Mueller

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	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

EXERCISES

Problem 1.6.3.4 (a)

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).

Problem 1.6.3.4 (b)

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

$P1 = T = T_H \cup T_H\, t_a(a,0,0)$

P1=T

(I,0)
(I, a)
(I, 2a)
(I, 3a)
(I, 4a)
(I, 5a)
...
(I, t_j)
...

$t_a(a,0,0)$

(I,0)
(I, 2a)
(I, 4a)
...
(I,2*n*a)
...

isomorphic *k*-subgroup:

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

$T_H\, t_a(a,0,0)$

(I, a)
~~(I, 3a)~~
~~(I, 5a)~~
~~...~~
(I,(2*n*+1)a)
...

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

INFINITE number of maximal isomorphic subgroups

Klassengleiche subgroups H<G: ***k***-subgroups

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

Example: P12/m1

Coset decomposition $G:T_G$

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

Klassengleiche subgroup

P2/m>P2/m(2**b**)
isomorphic

$P2/m(2b)=T_{2b}P_G$

non-isomorphic ***k***-subgroups:

P2/m>P2$_1$/m(2**b**)

$P2_1/m(2\mathbf{b}) = T_{2\mathbf{b}} \cup T_{2\mathbf{b}}t_b 2 \cup T_{2\mathbf{b}}\bar{1} \cup T_{2\mathbf{b}}t_b m$

$t_b=(0,1,0)$

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

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

Example: C2

Coset decomposition

$C2 = T_c + T_c2$

$(T_i + T_i t_c)$

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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- **Series of maximal isomorphic subgroups**

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

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

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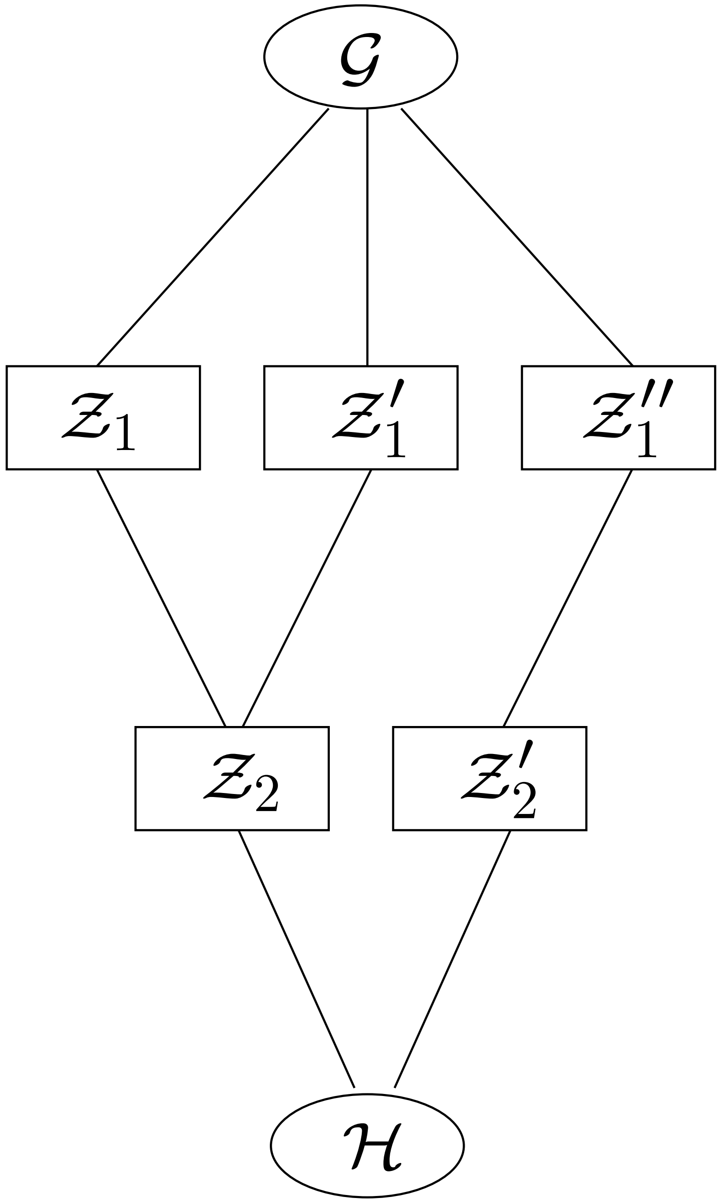
GENERAL SUBGROUPS OF SPACE GROUPS

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

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

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

EXERCISES

Problem 1.6.3.3

Richness of group-subgroup relations of space groups

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 ?

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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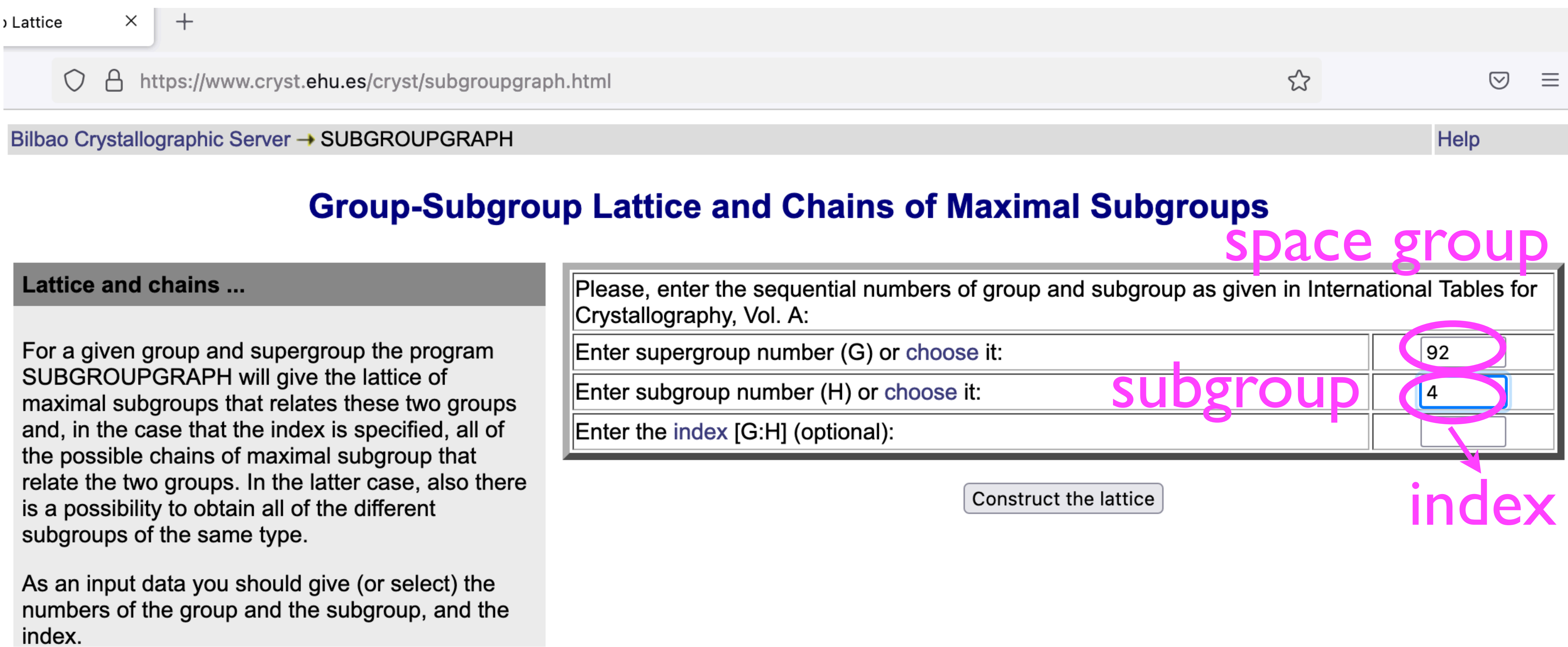
Problem: SUBGROUPS OF SPACE GROUPS

SUBGROUPGRAPH



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

Subgroups of Space groups

$G \overset{[i]}{>} H$

G

$\downarrow i_P$ *t*-subgroup

M

$\downarrow i_L$ *k*-subgroup

H

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

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

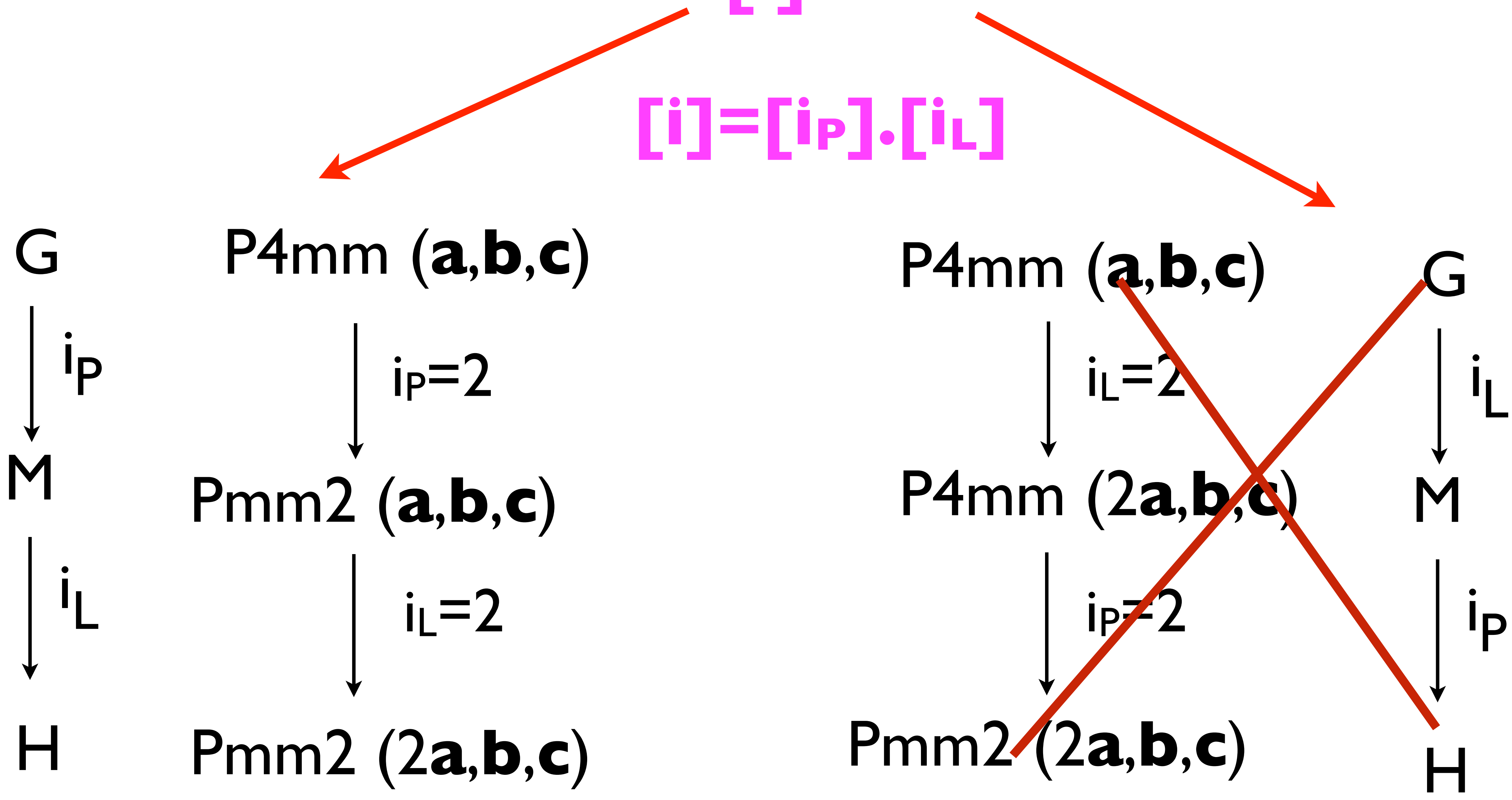
isomorphic to the point group P_G of G

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

Example: P4mm (**a**,**b**,**c**) > Pmm2 (2**a**,**b**,**c**)

$[i]=4$

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



PROBLEM:

Domain-structure analysis (initial steps)

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

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

When a **crystal homogeneous** in the parent (prototypic, high-symmetry) phase undergoes a phase transition into a low- symmetry phase (ferroic, if the point-group symmetry, is lowered) then this **daughter** phase is almost always formed as a **non-homogeneous** structure consisting of **homogeneous regions** called **domains**

Domain

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

Different domains can exhibit different **tensor properties**, different **diffraction patterns** and can differ in other physical properties.

optical observation of domain structure

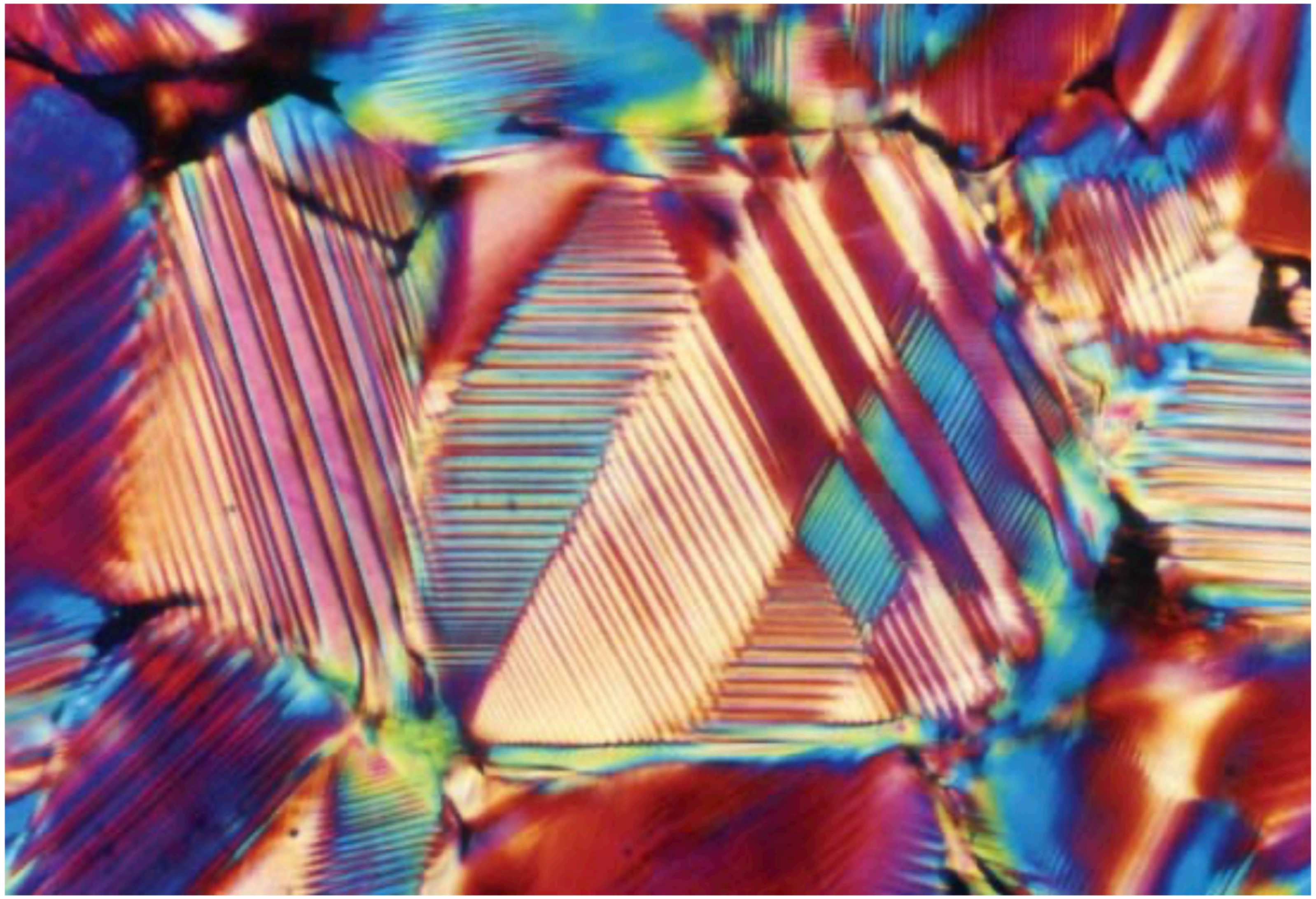


Fig. 3.4.1.1. Domain structure of tetragonal barium titanate ($BaTiO_3$). A thin section of barium titanate ceramic observed at room temperature in a polarized-light microscope (transmitted light, crossed polarizers). Courtesy of U. Täffner, Max-Planck-Institut für Metallforschung, Stuttgart. Different colours correspond to different ferroelastic domain states, connected areas of the same colour are ferroelastic domains and sharp boundaries between these areas are domain walls. Areas of continuously changing colour correspond to gradually changing thickness of wedge-shaped domains. An average distance between parallel ferroelastic domain walls is of the order of 1–10 μm.

Phase transitions domain structures

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

Domains

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*.

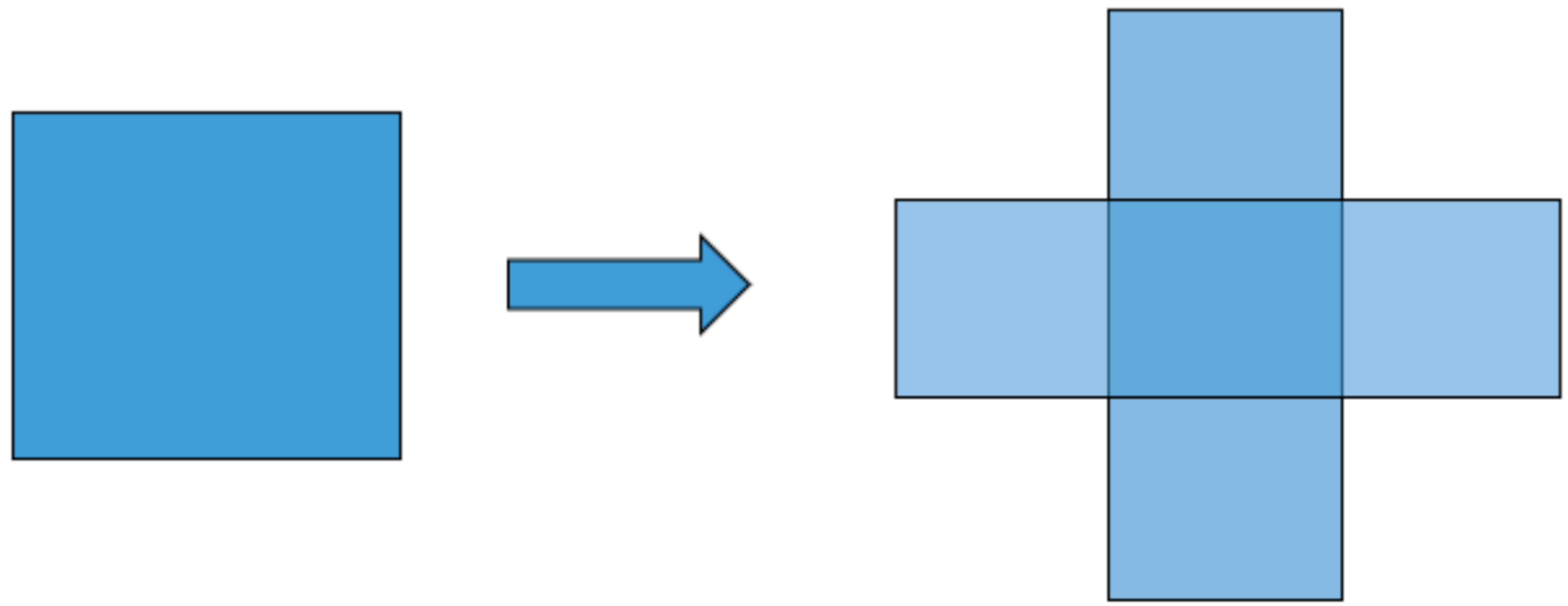
Two domains belong to the same *domain state* if their crystal patterns are identical, *i.e.* if they occupy different regions of space that are part of the *same* crystal pattern.

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.

Symmetry Reduction

initial phase

daughter phase



symmetry of
a square

symmetry of
a rectangle

two possible
orientations

Domain-structure analysis

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 $\mathcal{M}$

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

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

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

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

```
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
```

Low-symmetry phase $P2_1/c$

$|P_H|=?$

$Z_{H,p}=?$

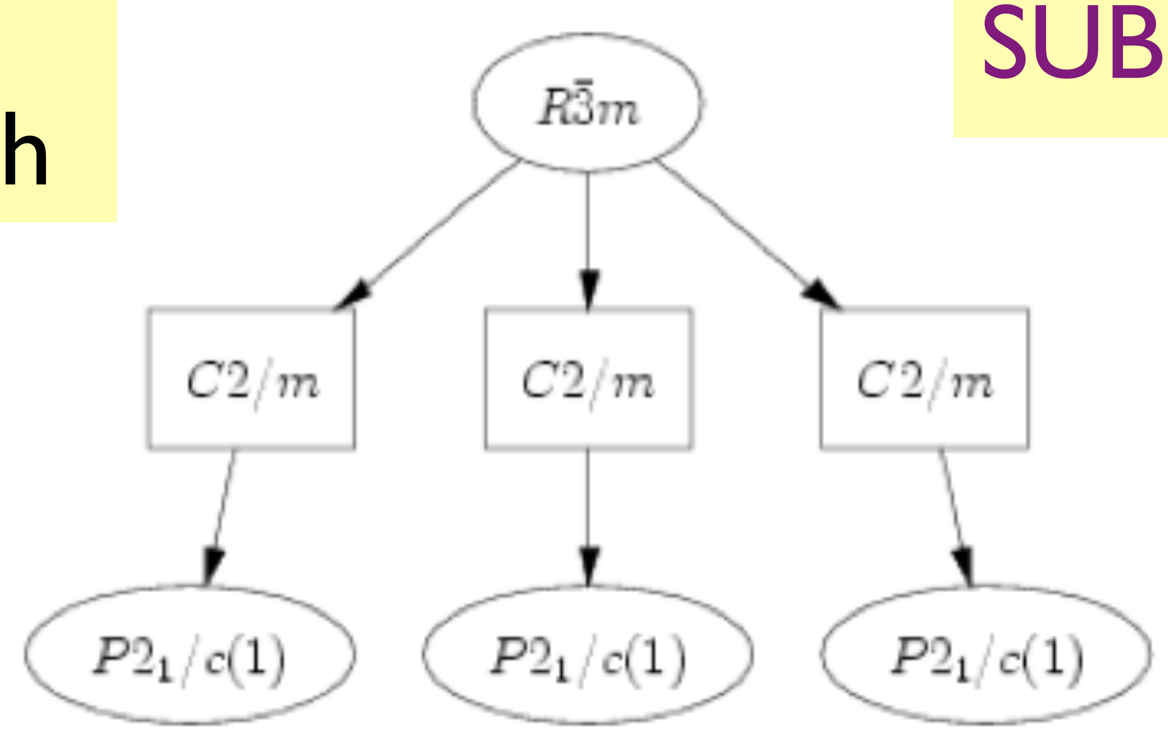
```
14
7.5075 6.0493 9.4814 90. 115.162 90.
7
Pb 1 2a 0 0 0
Pb 2 4e 0.3835 0.5815 0.2879
PV 1 4e 0.2071 0.0143 0.3999
O  1 4e 0.2872 0.2559 0.0159
O  2 4e 0.2598 0.7979 0.0216
O  3 4e 0.3194 0.9784 0.2823
O  4 4e 0.0335 0.5431 0.2091
```

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

Group-Subgroup Lattice

Maximal-subgroup graph

SUBGROUPGRAPH

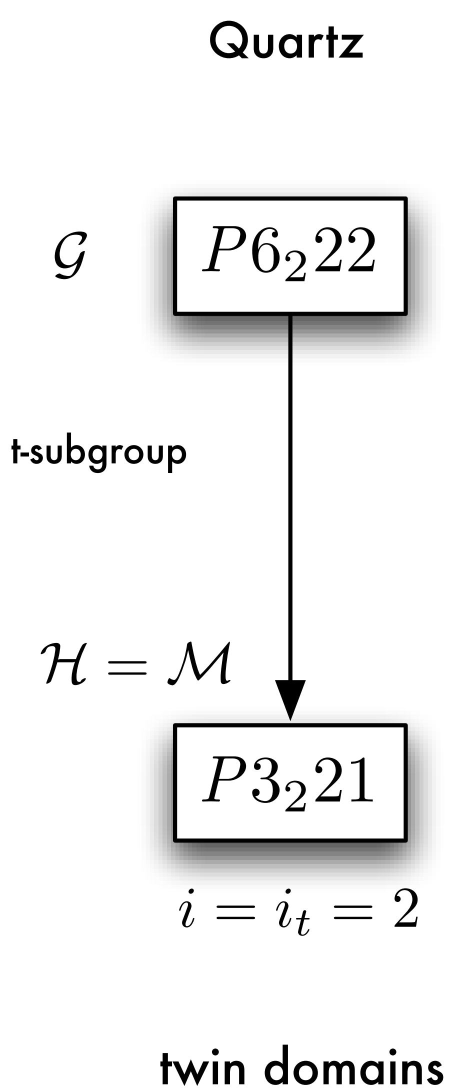


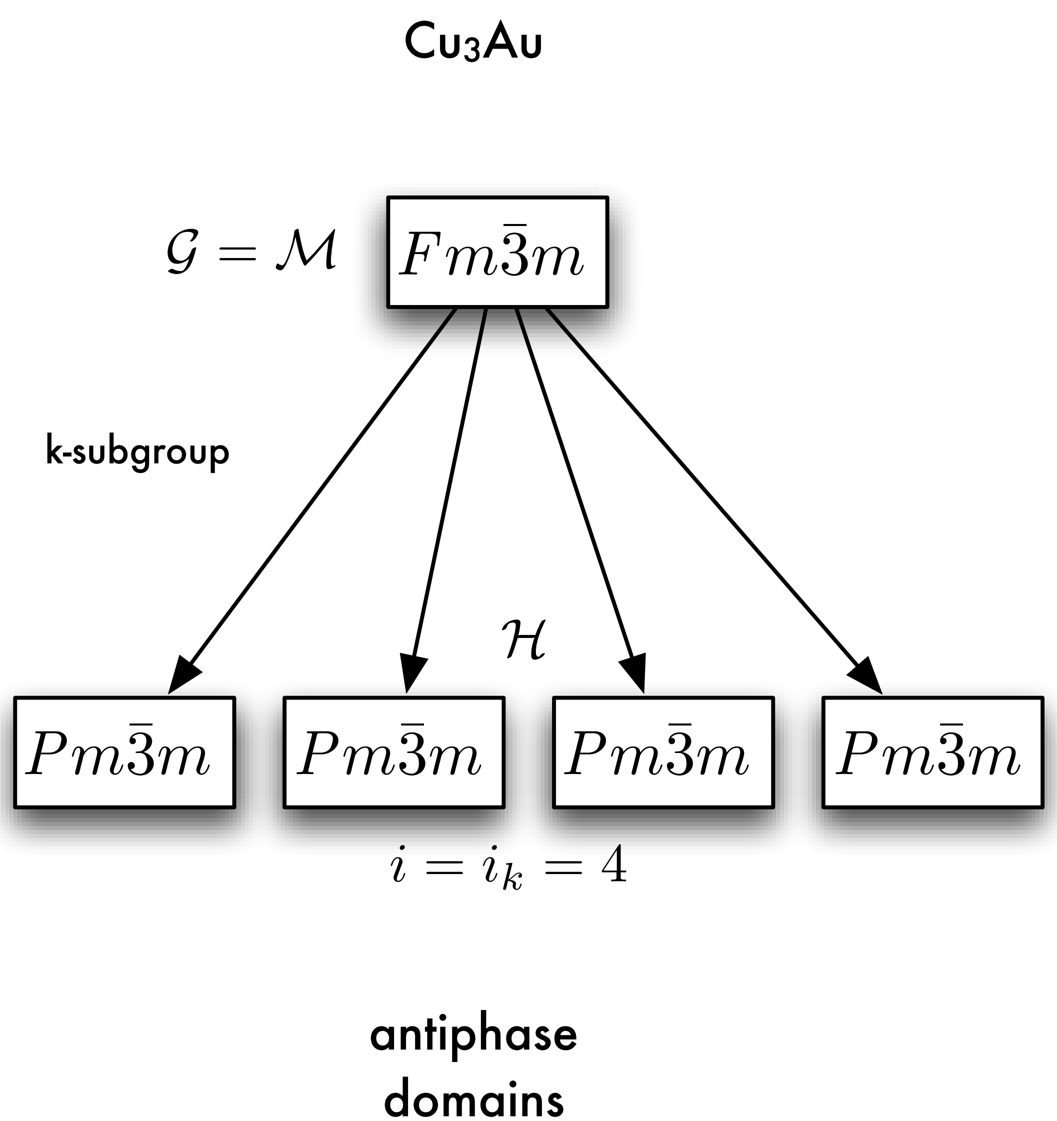
number of domain states= index [i] = [i_P].[i_L]=6

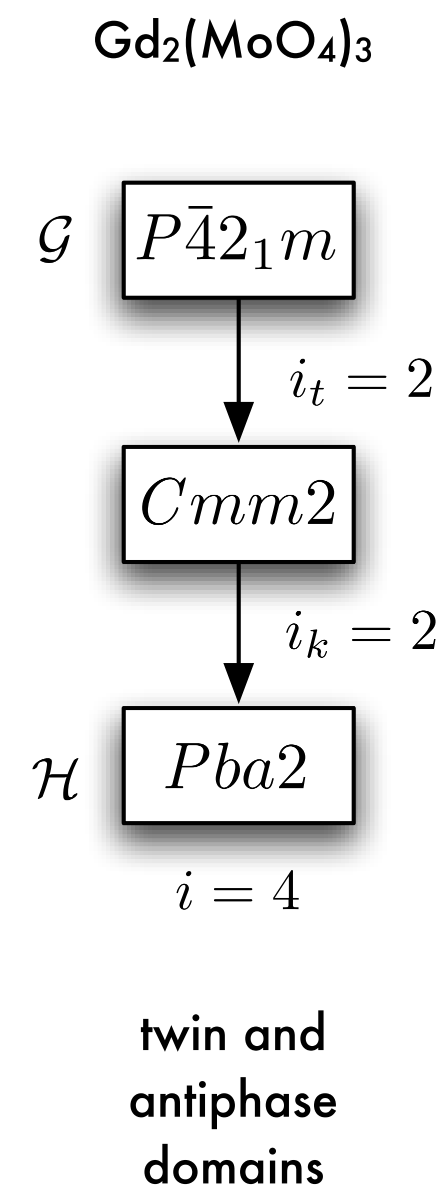
number of ferroelastic domain states: i_P = 12:4=3

number of different subgroups $P2_1/c$: 3

Problem: CLASSIFICATION OF DOMAINS **HERMANN**







EXERCISES

Problem 1.6.3.5

(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?

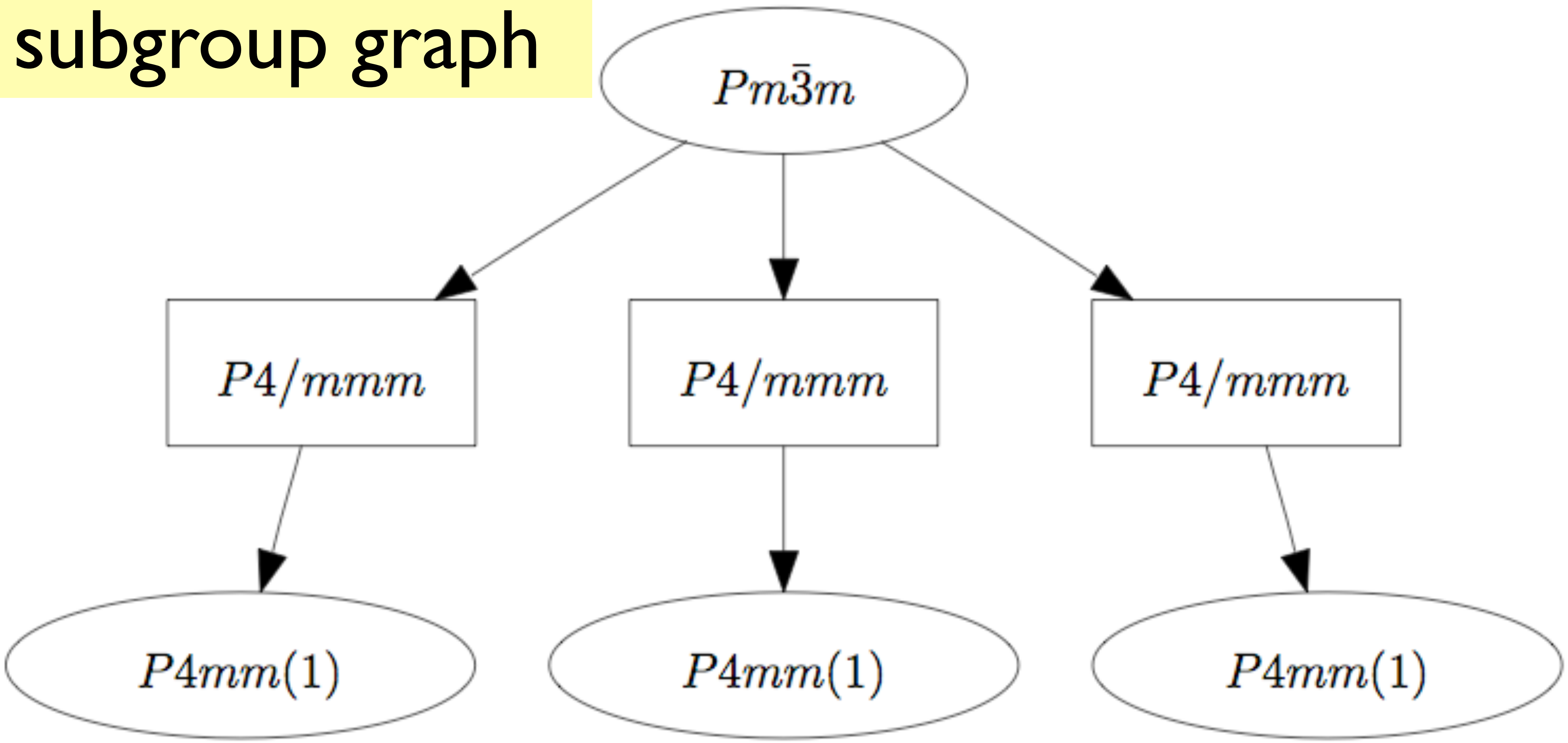
EXERCISE

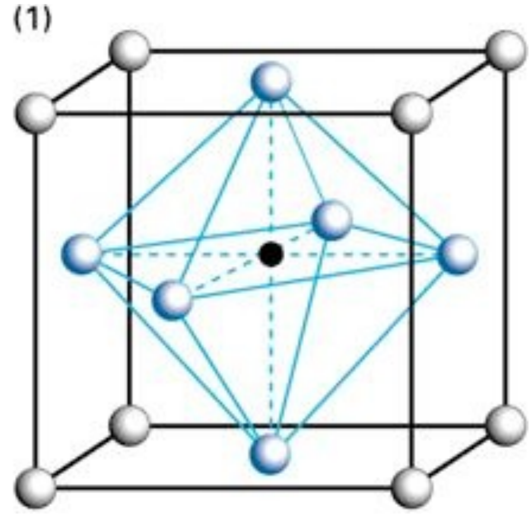
Problem 1.6.3.6

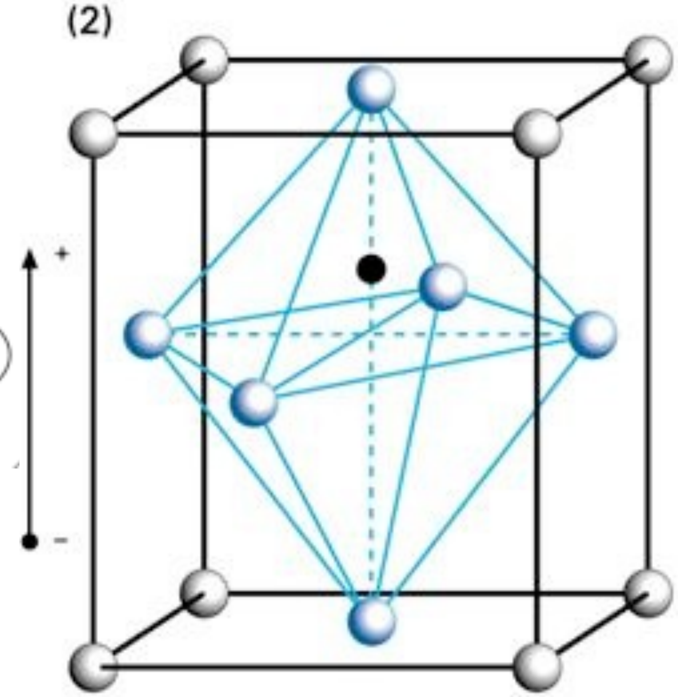
At high temperatures, $BiTiO_3$ has the cubic perovskite structure, space group Pm-3m (No. 221). Upon cooling, it distorts to three *slightly* deformed structures, all three being ferroelectric, with space groups P4mm (No.99), Amm2 (No.38) and R3m (No.160). Can we expect twinned crystals of the low symmetry forms? If so, how many and what kind of domain states could occur?

$BaTiO_3$: Ferroelectric Domains in P4mm phase

Maximal-subgroup graph







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

number of ferroelectric domain states: 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 ⦿ 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: $P_i = q_i P$

P_1	P_2	P_3	P_4	P_5	P_6
0	0	V	-V	0	0
0	0	0	0	V	-V
V	-V	0	0	0	0

Problem 1.6.3.7

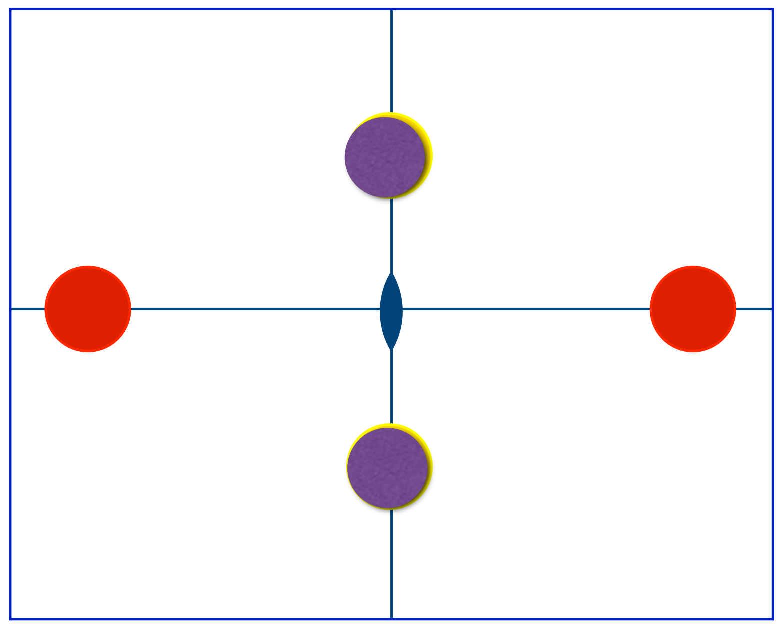
$SrTiO_3$ has the cubic perovskite structure, space group *Pm-3m*. Upon cooling below 105K, the coordination octahedra are mutually rotated and the space group is reduced to *I4/mcm*; *c* is doubled and the conventional unit cell is increased by a factor of four.

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.

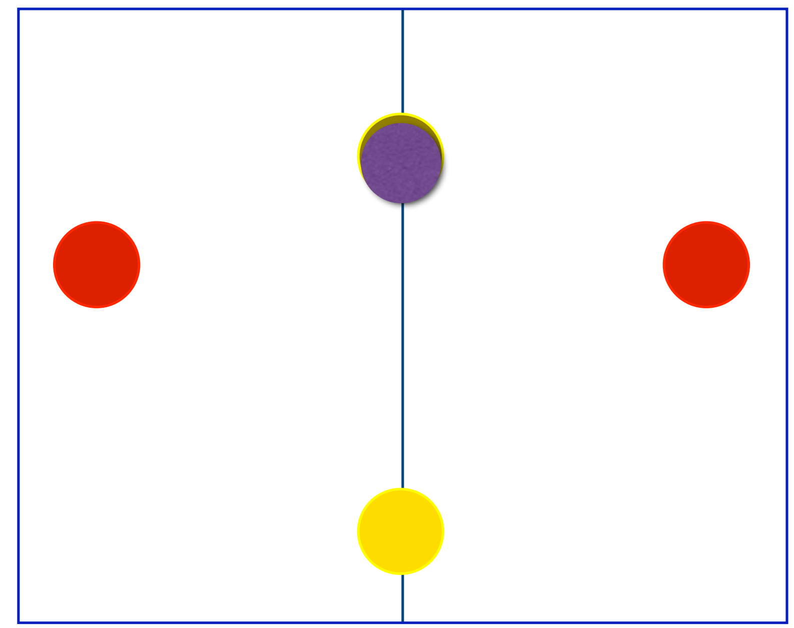
RELATIONS BETWEEN WYCKOFF POSITIONS

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 (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (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 *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	m m 2	$\frac{1}{2},\frac{1}{2},z$			
1	c	m m 2	$\frac{1}{2},0,z$			
1	b	m m 2	$0,\frac{1}{2},z$			
1	a	m m 2	$0,0,z$			

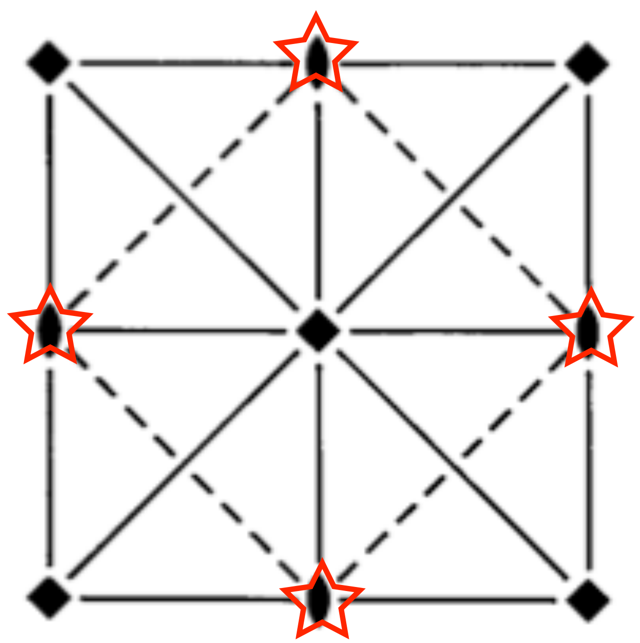
EXAMPLE

Group-subgroup pair

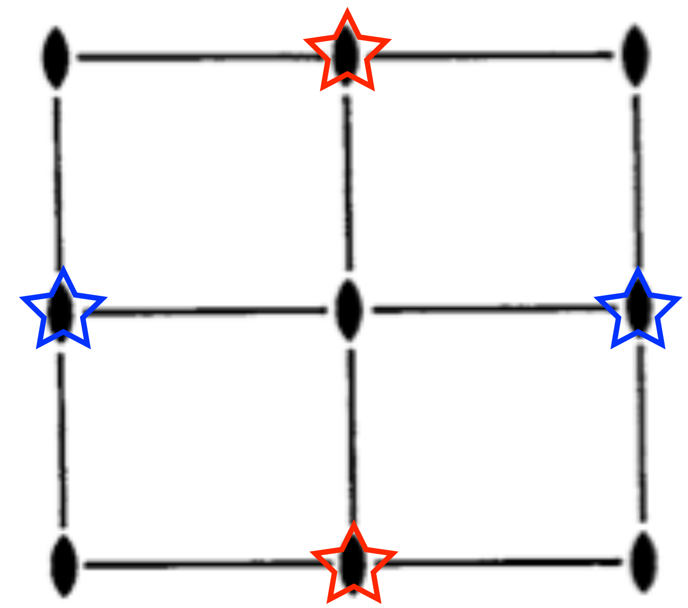
*P*4*mm*>*Pmm*2, [i]=2

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 $P4mm$

	Axes	Coordinates	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
Enter subgroup or choose it	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:	1 1 0 -1 1 0 0 0 1
origin shift:	0 0 0

group

subgroup

Transformation matrix (P,p)

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 1.6.3.8

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

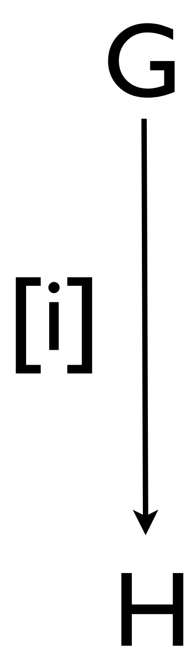
ITA1 data:

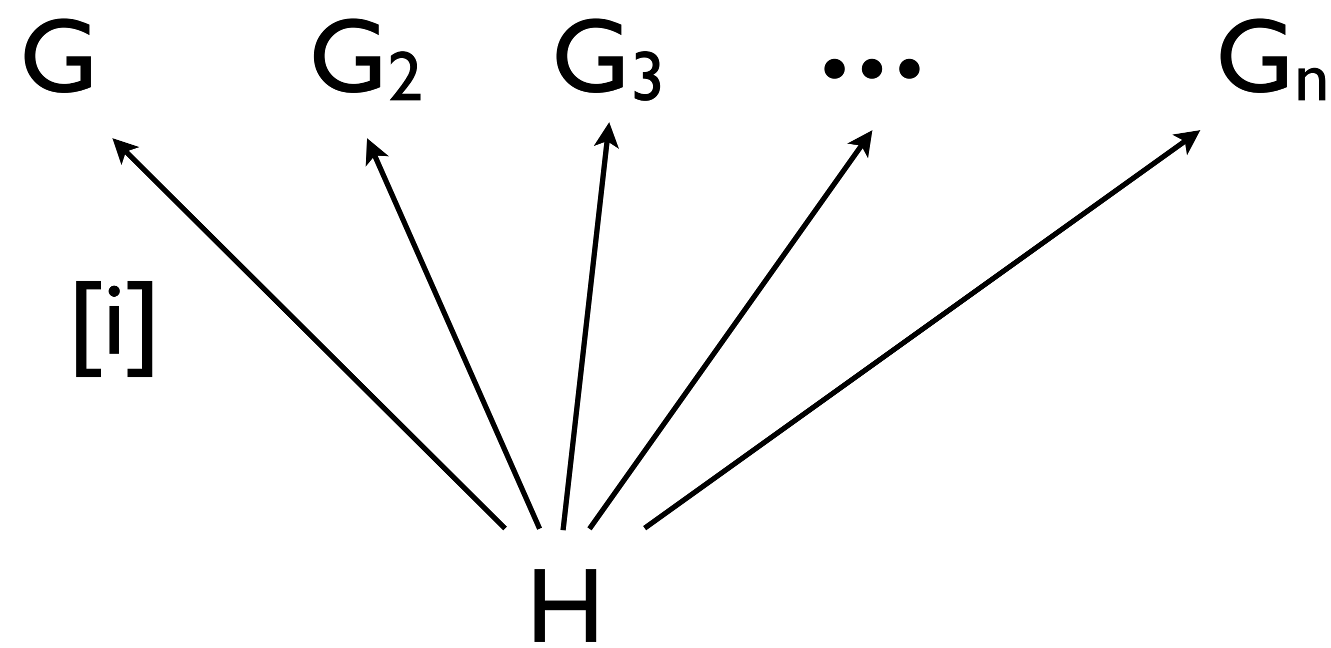
minimal non-isomorphic *k*- and *t*-supergroups types

The Supergroup Problem

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

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



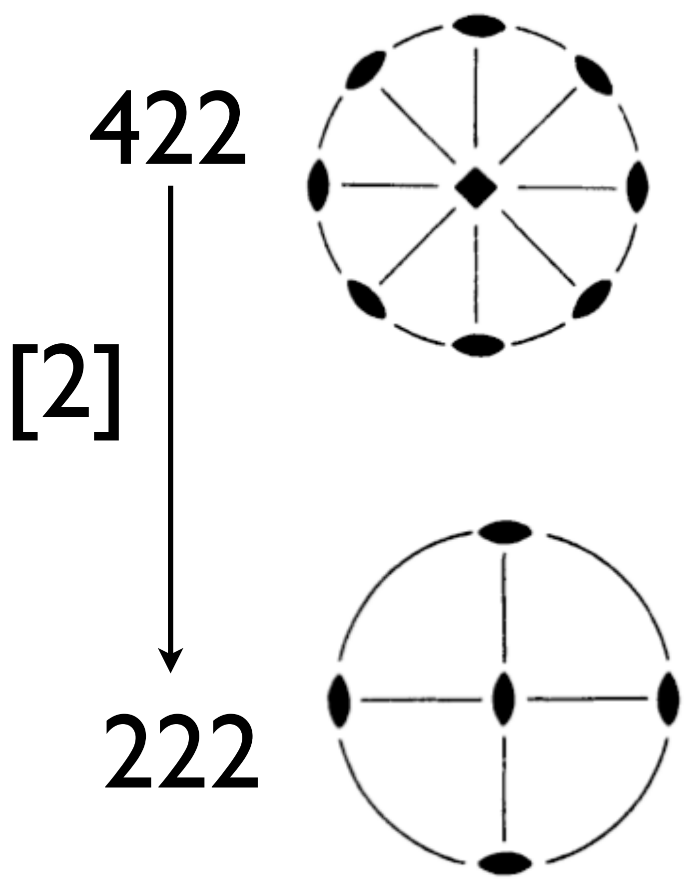


all $G_k>H$ contain H as subgroup

$$G_k=H+Hg_2+...+Hg_{ik}$$

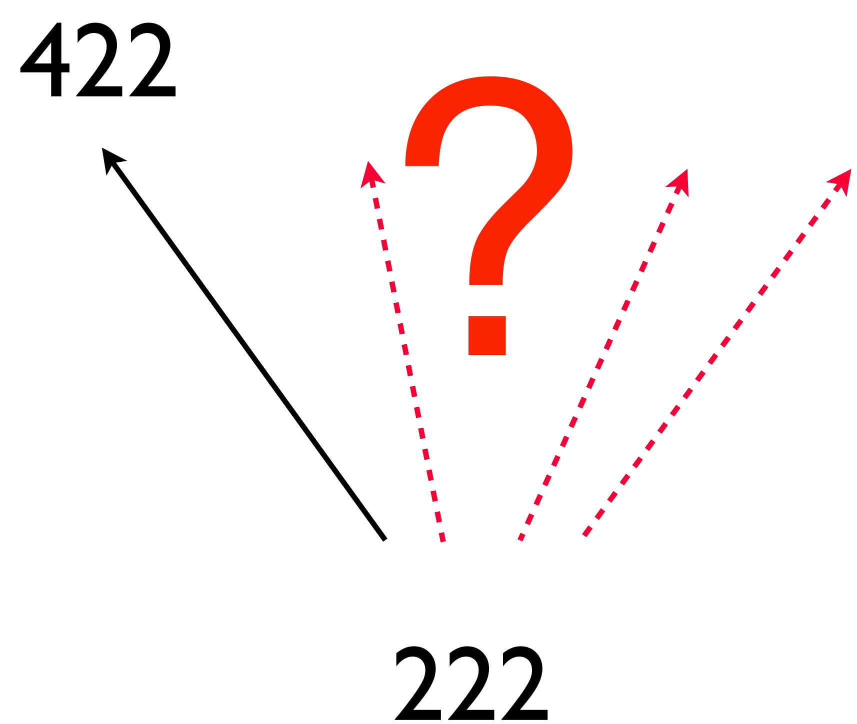
Example: Supergroup problem

Group-subgroup pair 422>222



How many are the subgroups 222 of 422?

Supergroups 422 of the group 222

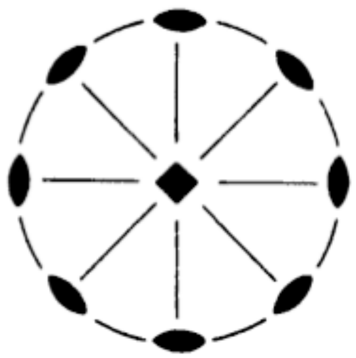


How many are the supergroups 422 of 222?

Example: Supergroup problem

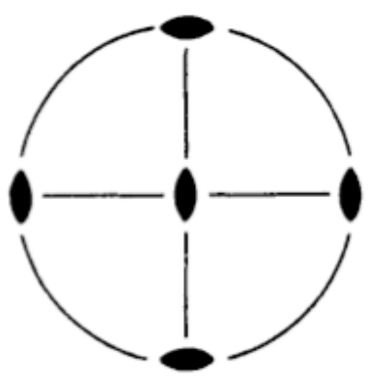
Group-subgroup pair 422>222

422



[2]

$2_z2_x2_y$ $\quad$ $2_z2_+2_-$



$$4_z22 = 2_z2_x2_y + 4_z(2_z2_x2_y)$$

$$4_z22 = 2_z2_+2_- + 4_z(2_z2_+2_-)$$

Supergroups 422 of the group 222

4_z22 $\quad$ 4_x22 $\quad$ 4_y22

[2]

222

$$4_z22=222+4_z222$$

$$4_y22=222+4_y222$$

$$4_x22=222+4_x222$$

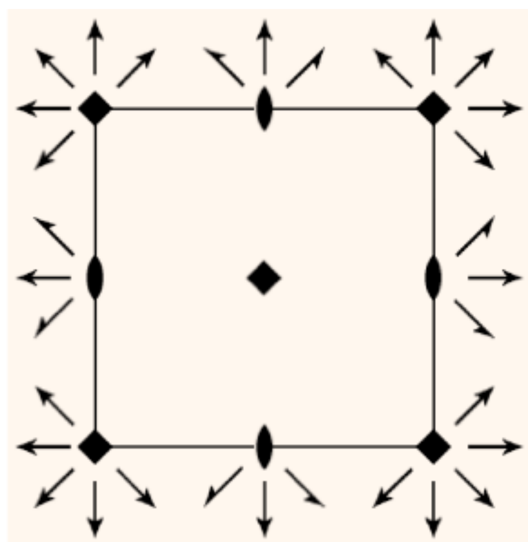
Example: Supergroup problem

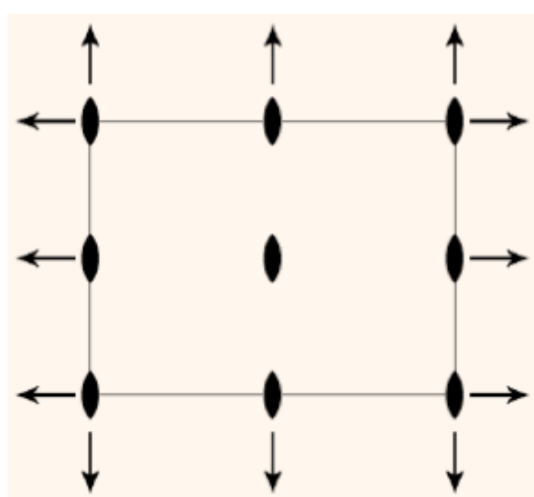
Group-subgroup pair P422>P222

P422

[2]

P222





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

Supergroups P422 of the group P222

$P4_z22$ $P4_x22$ $P4_y22$

[2]

P222

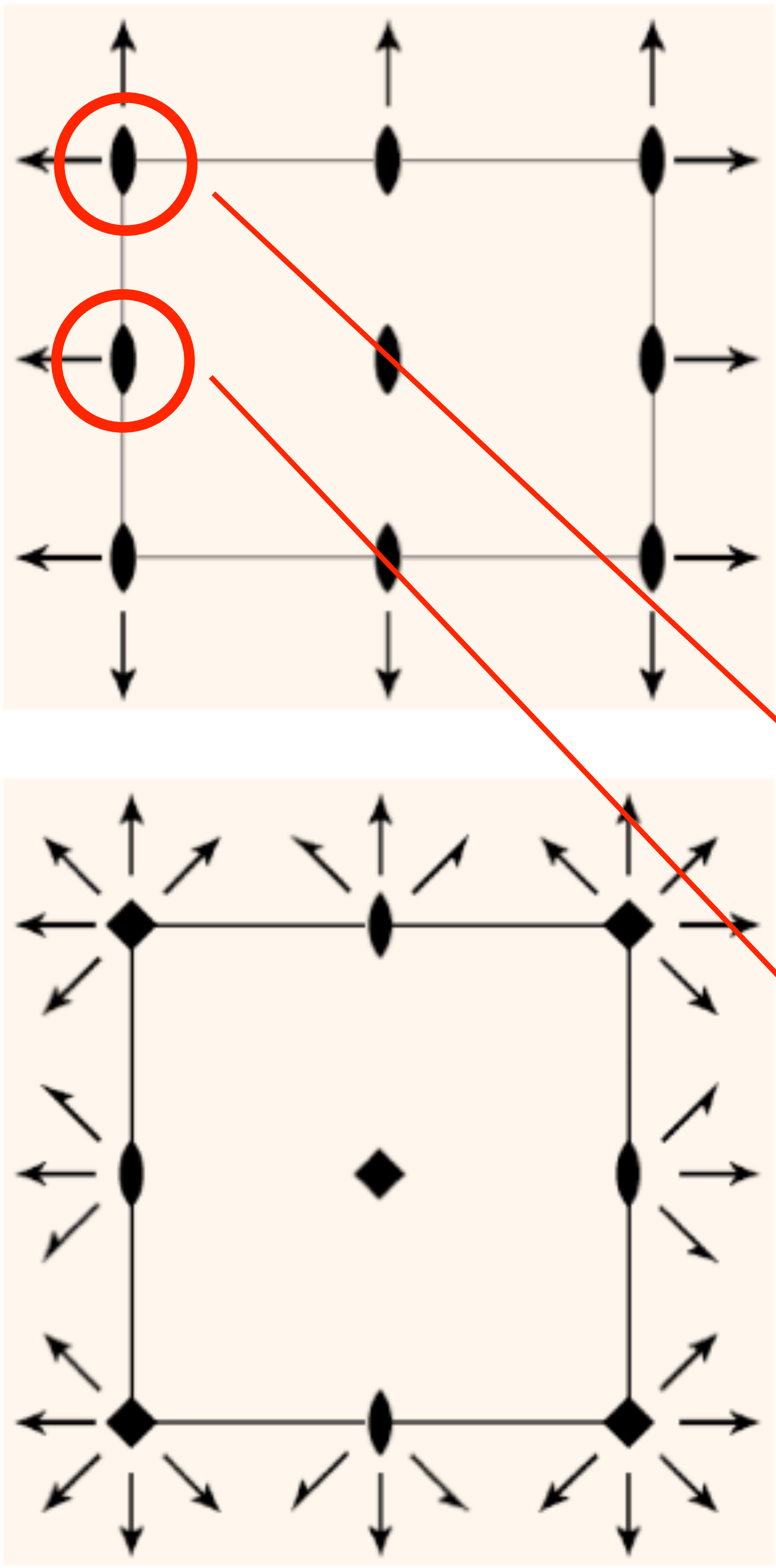
$P4_z22 = 222 + (222)(4_z,0)$

$P4_x22 = 222 + (222)(4_x,0)$

$P4_y22 = 222 + (222)(4_y,0)$

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**

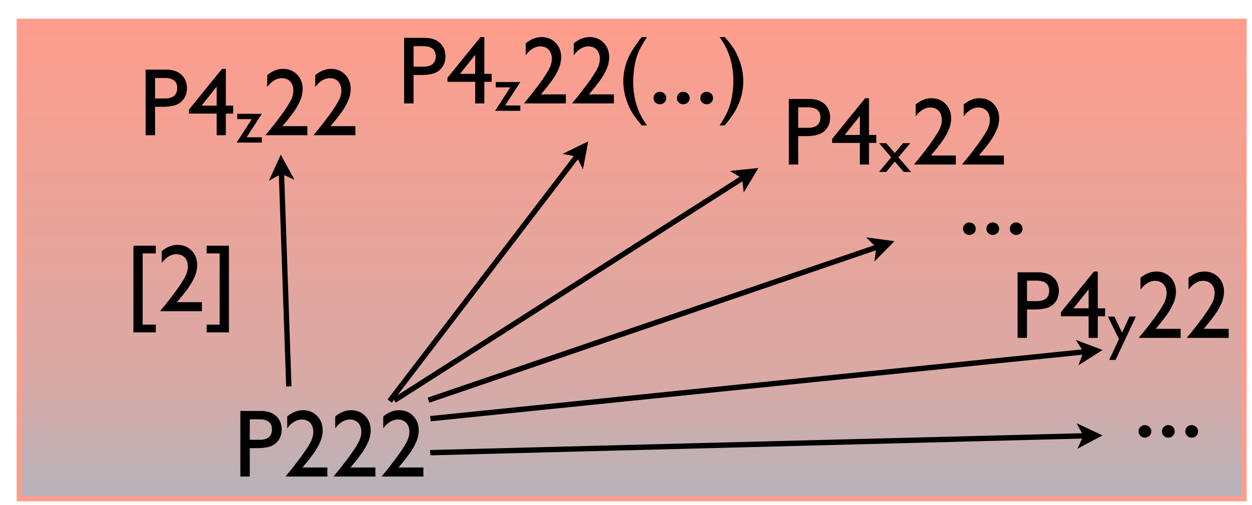
[2] *A*222 (21, *C*222); [2] *B*222 (21, *C*222); [2] *C*222 (21); [2] *I*222 (23)

- **Decreased unit cell** none

Incomplete data

Space-group type only

No transformation matrix



Bilbao Crystallographic Server

Problem: SUPERGROUPS OF SPACE GROUPS

SUPERGROUPS MINSUP

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

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

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

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 1.6.3.9

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?

GENERATION OF SPACE GROUPS

Generation of space groups

Crystallographic groups are **solvable** groups

Composition series: $P1 \triangleleft Z_2 \triangleleft Z_3 \triangleleft \ldots \triangleleft G$

index 2 or 3

Set of generators of a group is a set of group elements such that each element of the group can be obtained as an ordered product of the generators

$$W = (g_h)^{k_h} * (g_{h-1})^{k_{h-1}} * \ldots * (g_2)^{k_2} * g_1$$

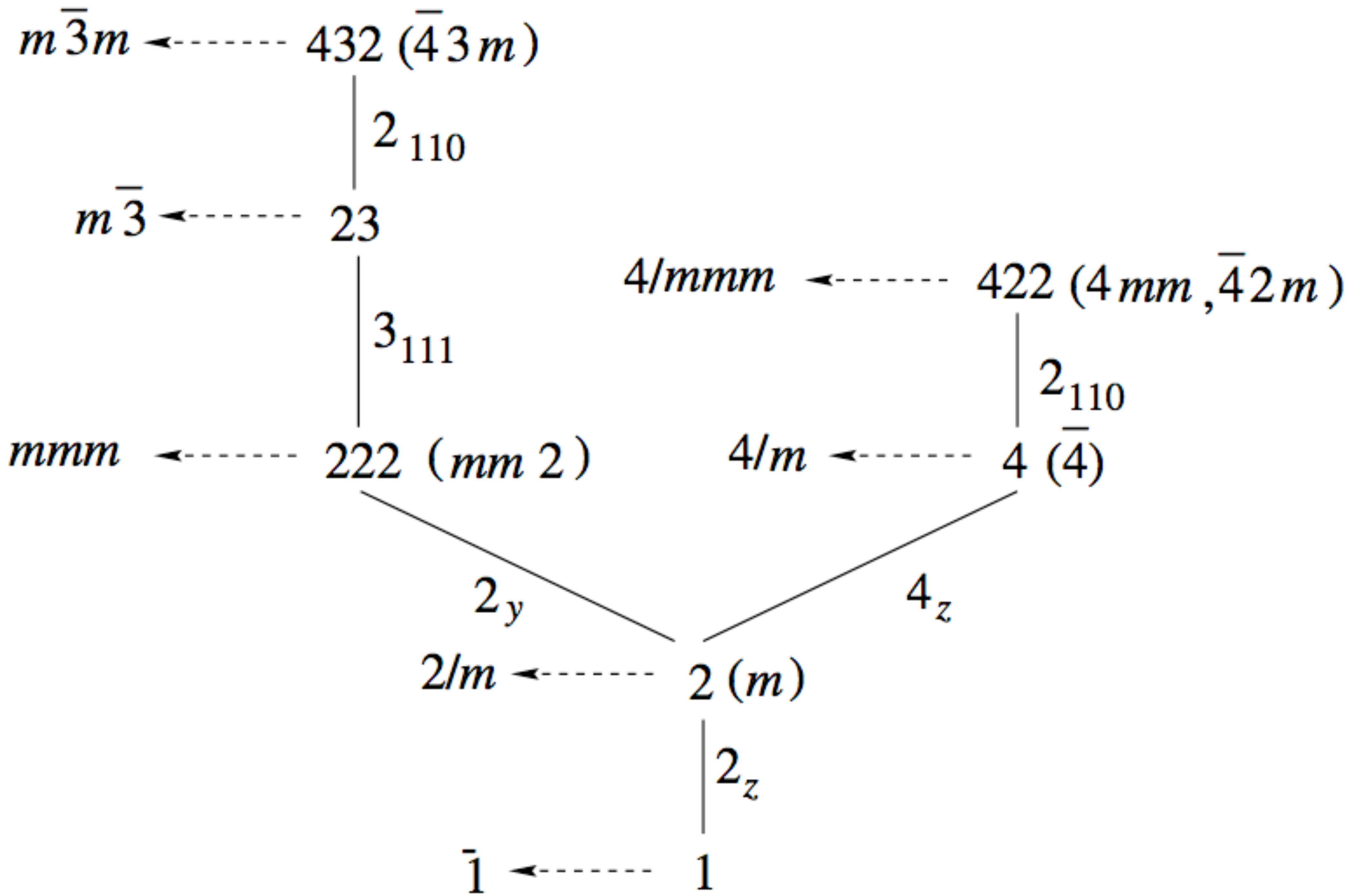
g_1 - identity

g_2, g_3, g_4 - primitive translations

g_5, g_6 - centring translations

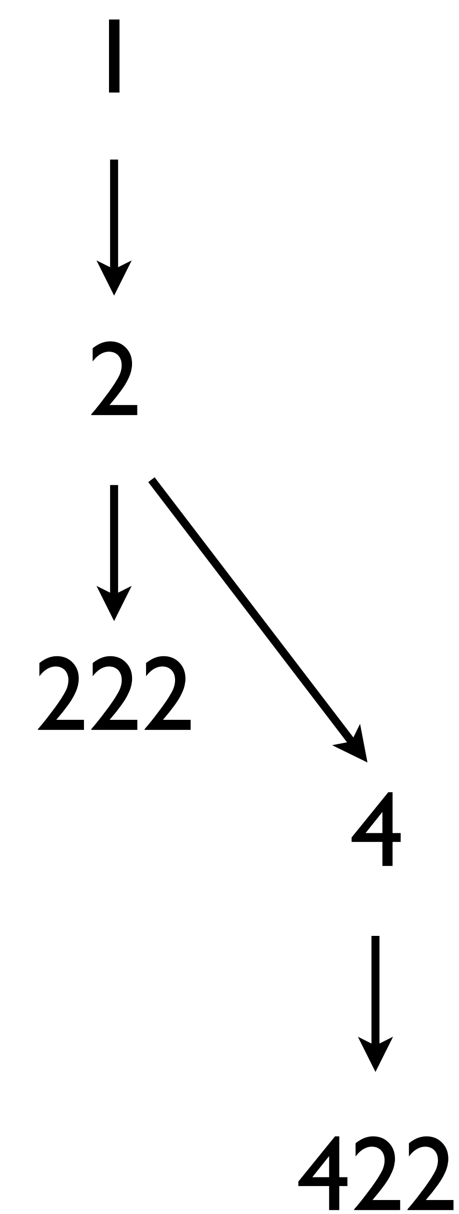
$g_7, g_8, \ldots,$ - generate the rest of elements

Generation of sub-cubic point groups

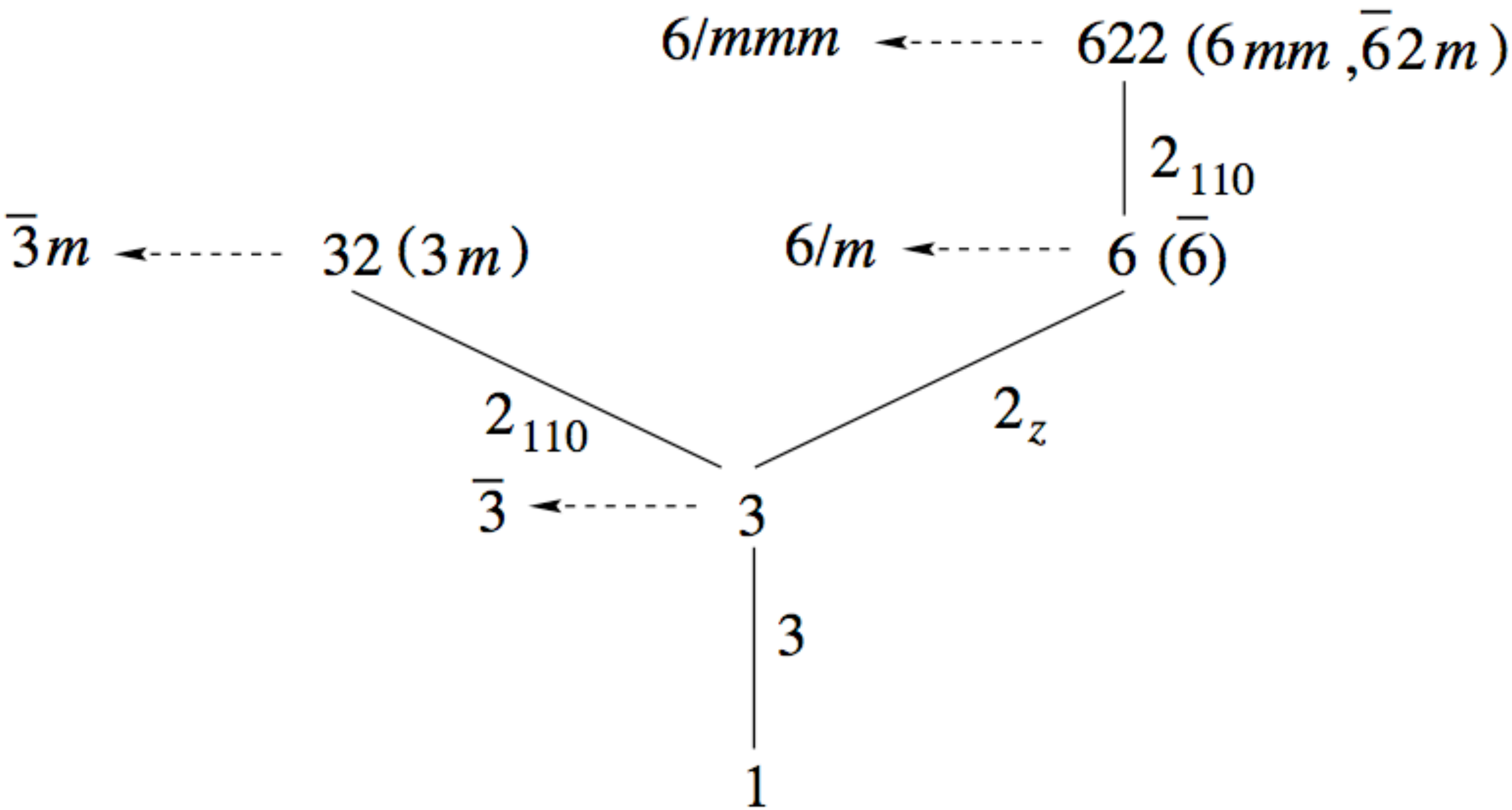


Generation of orthorhombic and tetragonal groups

Hermann–Mauguin symbol of crystal class	Generators G_i (sequence left to right)
1 $\bar{1}$	1 $\bar{1}$
2 m $2/m$	2 m $2, \bar{1}$
222 $mm2$ mmm	$2_z, 2_y$ $2_z, m_y$ $2_z, 2_y, \bar{1}$
4 $\bar{4}$ $4/m$ 422 $4mm$ $\bar{4}2m$ $\bar{4}m2$ $4/mmm$	$2_z, 4$ $2_z, \bar{4}$ $2_z, 4, \bar{1}$ $2_z, 4, 2_y$ $2_z, 4, m_y$ $2_z, \bar{4}, 2_y$ $2_z, \bar{4}, m_y$ $2_z, 4, 2_y, \bar{1}$

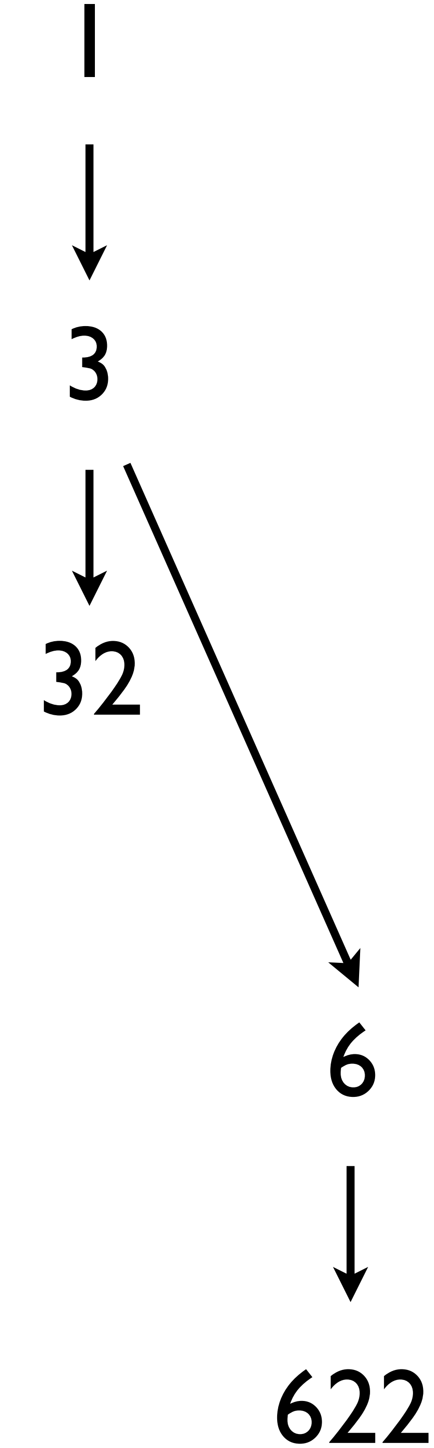


Generation of sub-hexagonal point groups



Generation of trigonal and hexagonal groups

3	3
$\bar{3}$	$3, \bar{1}$
321	$3, 2_{110}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}$)
312	$3, 2_{1\bar{1}0}$
$3m1$	$3, m_{110}$
(rhombohedral coordinates	$3_{111}, m_{10\bar{1}}$)
$31m$	$3, m_{1\bar{1}0}$
$\bar{3}m1$	$3, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}, \bar{1}$)
$\bar{3}1m$	$3, 2_{1\bar{1}0}, \bar{1}$
6	$3, 2_z$
$\bar{6}$	$3, m_z$
$6/m$	$3, 2_z, \bar{1}$
622	$3, 2_z, 2_{110}$
$6mm$	$3, 2_z, m_{110}$
$\bar{6}m2$	$3, m_z, m_{110}$
$\bar{6}2m$	$3, m_z, 2_{110}$
$6/mmm$	$3, 2_z, 2_{110}, \bar{1}$



EXERCISES

Problem 1.6.3.10 (A)

Generate the space group C2mm using the selected generators

Compare the results of your calculation with the coordinate triplets listed under General position of the ITA data of C2mm

EXERCISES

Problem 1.6.3.10 (B)

Generate the space group ***P4mm*** using the selected generators.

Compare the results of your calculation with the coordinate triplets listed under General position of the ITA data of ***P4mm***

Hint: Construct the composition series for the space group ***P4mm*** in analogy with the composition series of ***4mm***

$$\mathbf{1} \overset{2_z}{\underset{[2]}{\triangleleft}} \mathbf{2} \overset{4_z}{\underset{[2]}{\triangleleft}} \mathbf{4} \overset{m_x}{\underset{[2]}{\triangleleft}} \mathbf{4mm}$$