CRYSTALLOGRAPHY ONLINE: WORKSHOP ON THE USE AND APPLICATIONS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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ECM31
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CRYSTALLOGRAPHY ONLINE: BILBAO CRYSTALLOGRAPHIC SERVER

SYMMETRY RELATIONS OF SPACE GROUPS

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GROUP-SUBGROUP RELATIONS

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 $|G|/|H|$

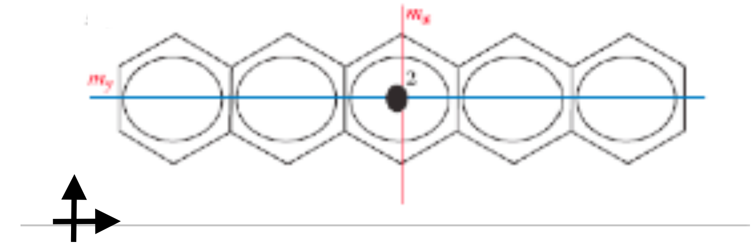
Normal subgroup

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

Example

Subgroups of point groups

Molecule of pentacene



Subgroups of **mm2**

$\{1, 2_z, m_x, m_y\}$

$\{1, 2_z\}$ $\{2_z, m_x\}$ $\{1, m_x\}$

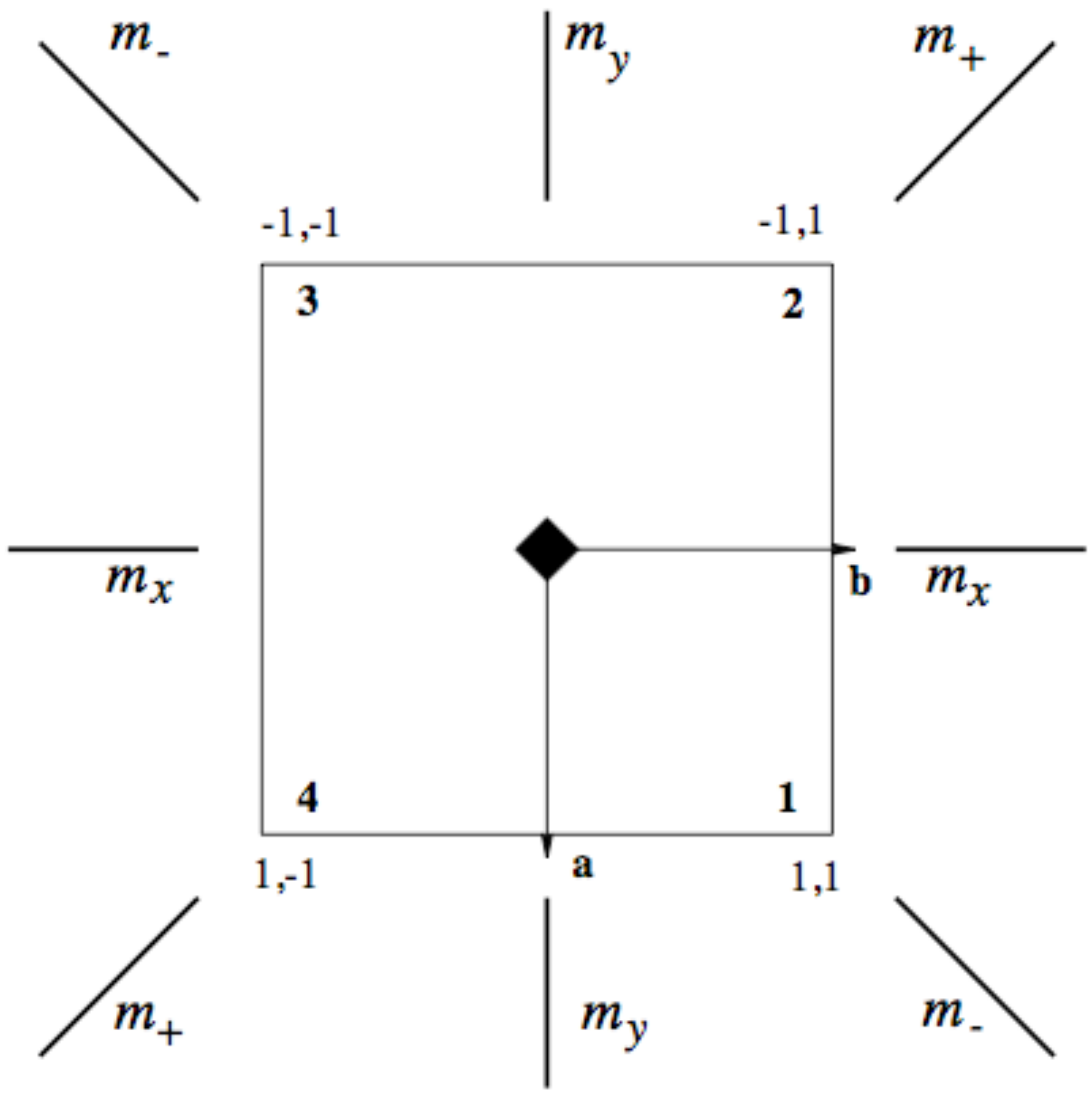
Subgroup graph

				Index
4		**mm2** $= \{1, 2_z, m_x, m_y\}$		1
2	$\{1, 2_z\}$	$\{1, m_x\}$	$\{1, m_y\}$	2
1		$\{1\}$		4

EXERCISES

Problem 2.1

Consider the group of the square and determine its subgroups



	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
1	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
2	2	1	4^{-1}	4	m_y	m_-	m_x	m_+
4	4	4^{-1}	2	1	m_+	m_y	m_-	m_x
4^{-1}	4^{-1}	4	1	2	m_-	m_x	m_+	m_y
m_x	m_x	m_y	m_-	m_+	1	4^{-1}	2	4
m_+	m_+	m_-	m_x	m_y	4	1	4^{-1}	2
m_y	m_y	m_x	m_+	m_-	2	4	1	4^{-1}
m_-	m_-	m_+	m_y	m_x	4^{-1}	2	4	1

Multiplication table of $4mm$

4mm: $\{e\},\{4_z,4_z^{-}\}, \{2_z\},\{m_y,m_x\},\{m_+,m_-\}$

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

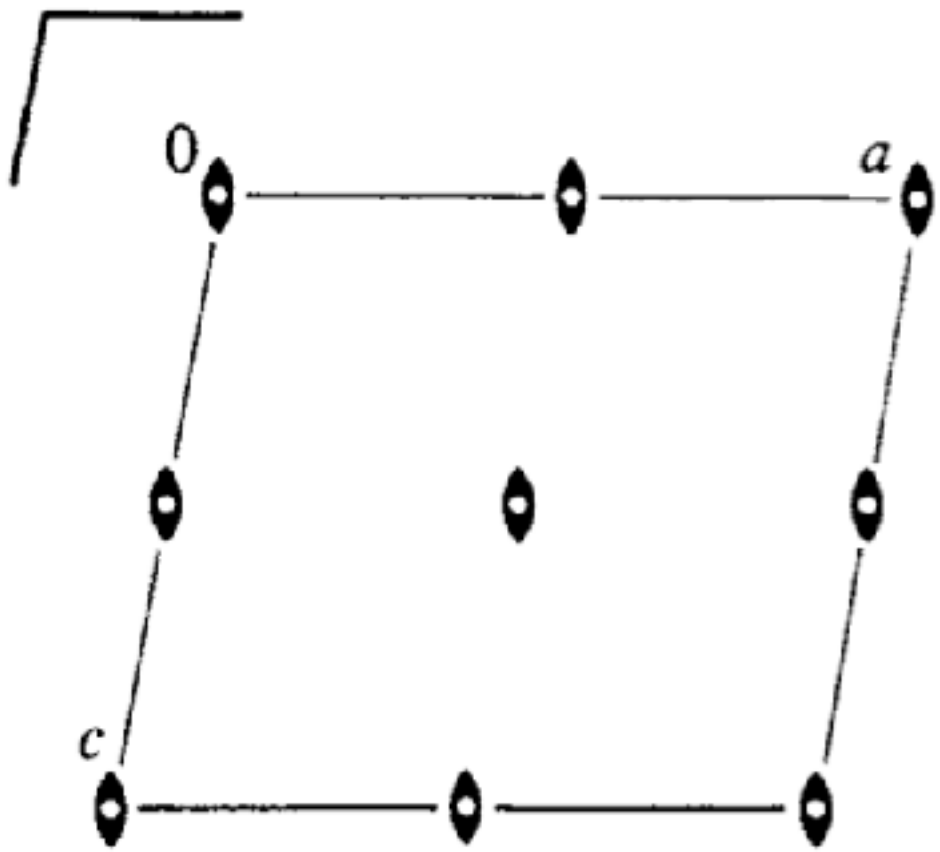
Point group $P_G = \{I, W_2, W_3, \ldots, W_i\}$

Example: P12/m1

Coset decomposition G:T_G

Factor group $G/T_G \simeq P_G$

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



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

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

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

Subgroups of space groups

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:

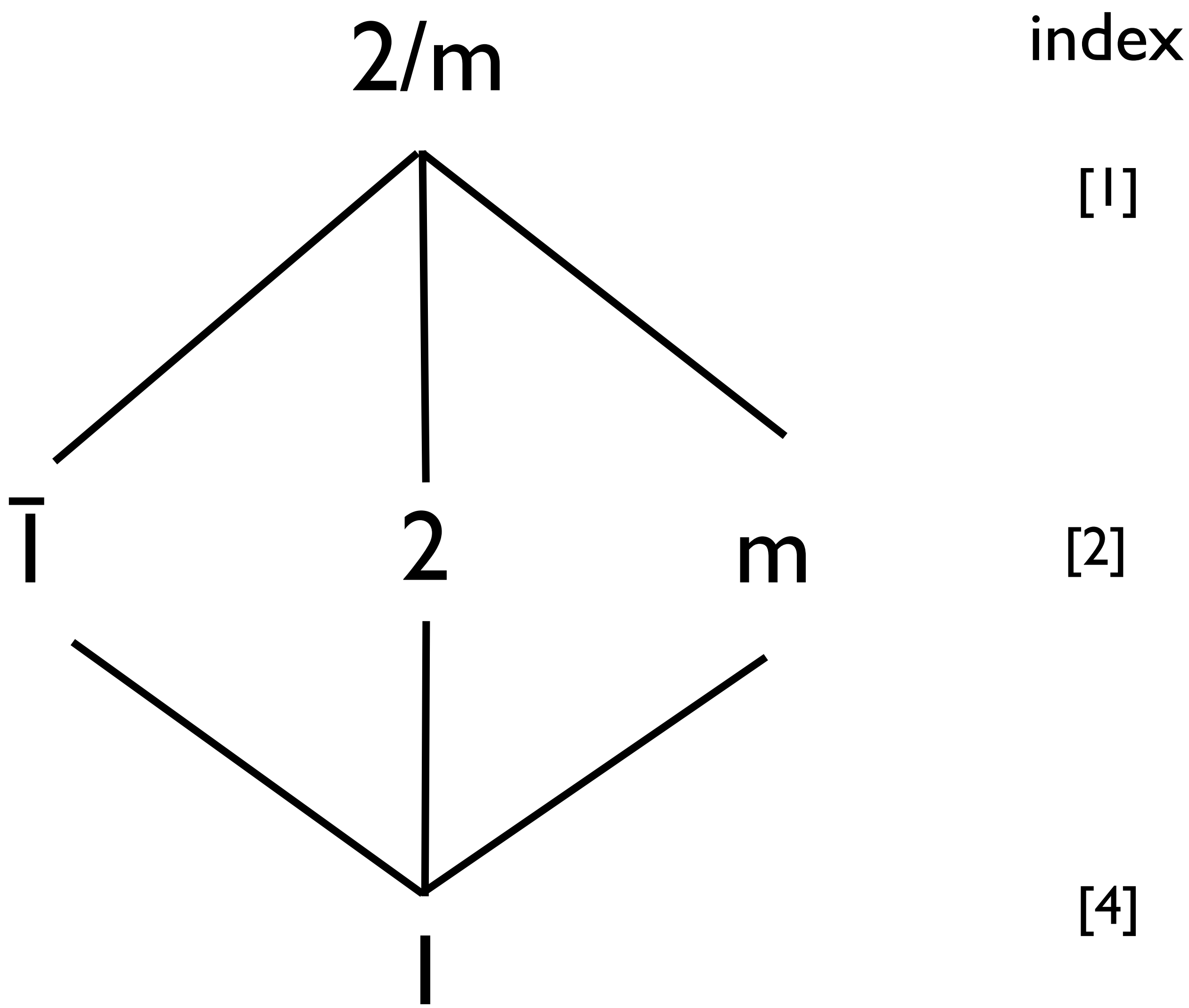
$H_1 = T_G \cup T_G 2$
P121

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

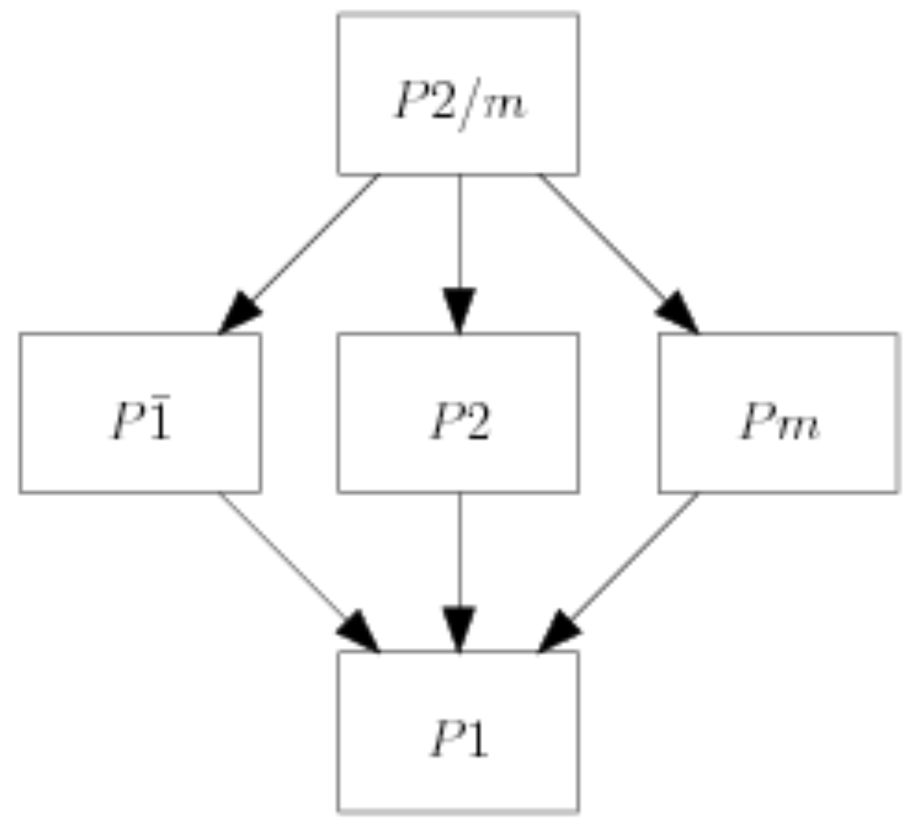
$H_3 = T_G \cup T_G\,m$
Pm

Example: P12/m1

Translationengleche subgroups H<G:



Subgroup diagram of point group 2/m



Translationengleiche subgroups of space group *P*2/m

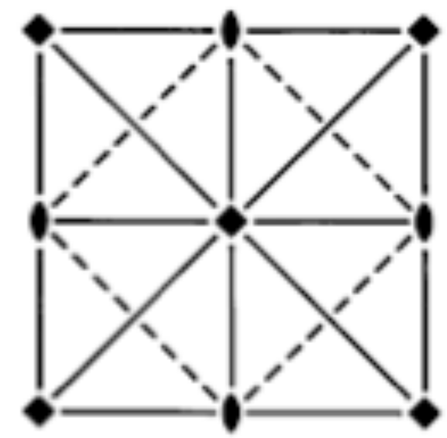
EXERCISES

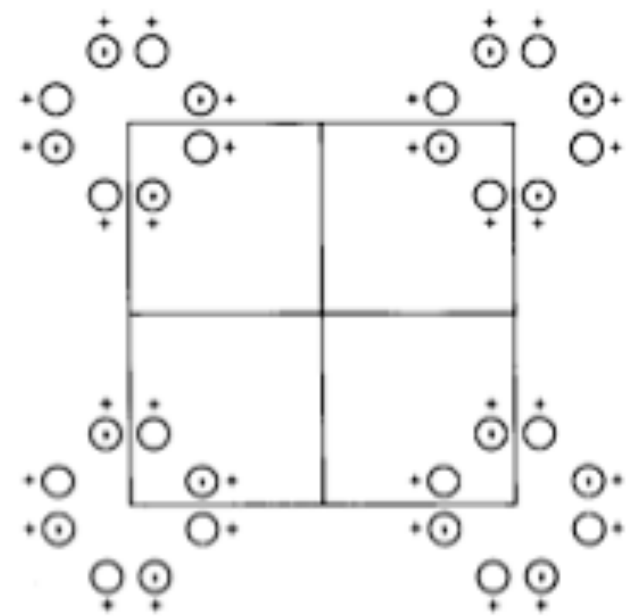
Problem 2.2

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

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 (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

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:

Example: P1

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

Coset decomposition

$P1 = T_e + T_e t_a$

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

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.*

Subgroups of space groups

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

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

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)
...	...

INFINITE number of maximal isomorphic subgroups

International Tables for Crystallography, Vol. A1

eds. H. Wondratschek, U. Mueller

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)	$\langle 2+(2u,0,0)\rangle$ $p>2$; $0\leq q<p$; $0\leq r<p$; $0\leq u<p$ 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)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\leq q<p$; $0\leq u<p$ 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)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

Subgroups of space groups

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:

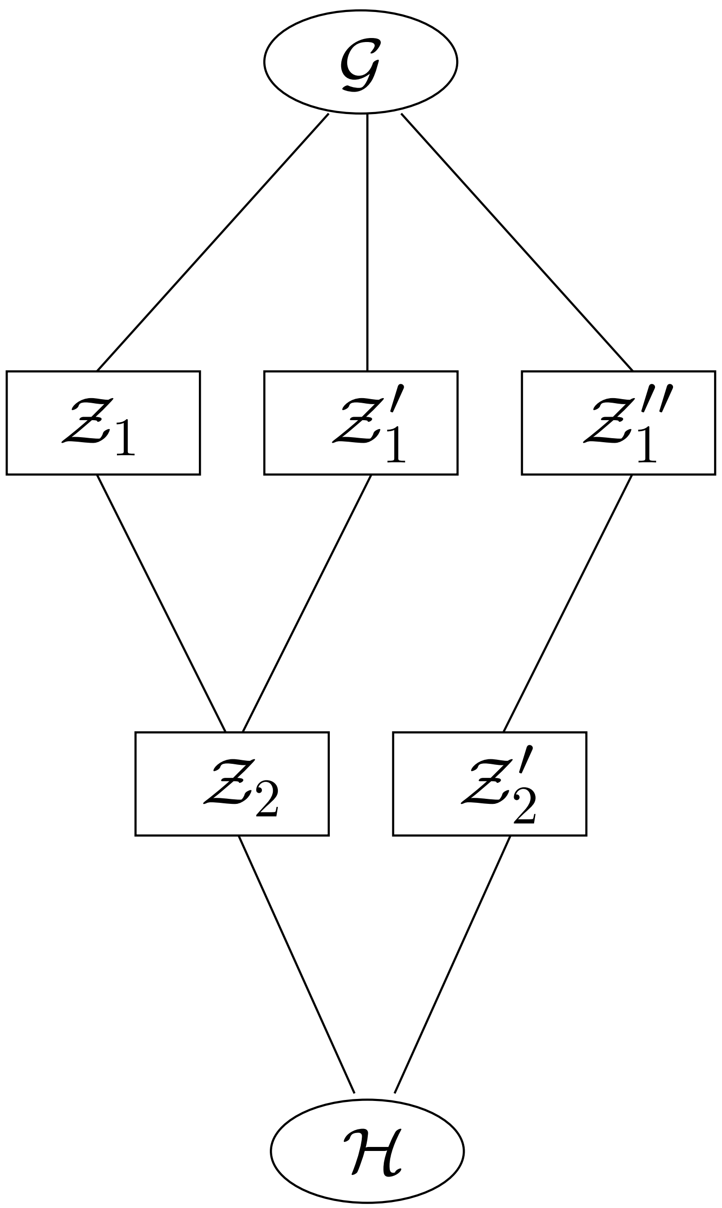
$H_1 = T_i \cup T_i 2$
P2

$H_2 = T_i \cup T_i t_c\, 2$
$P2_1$

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

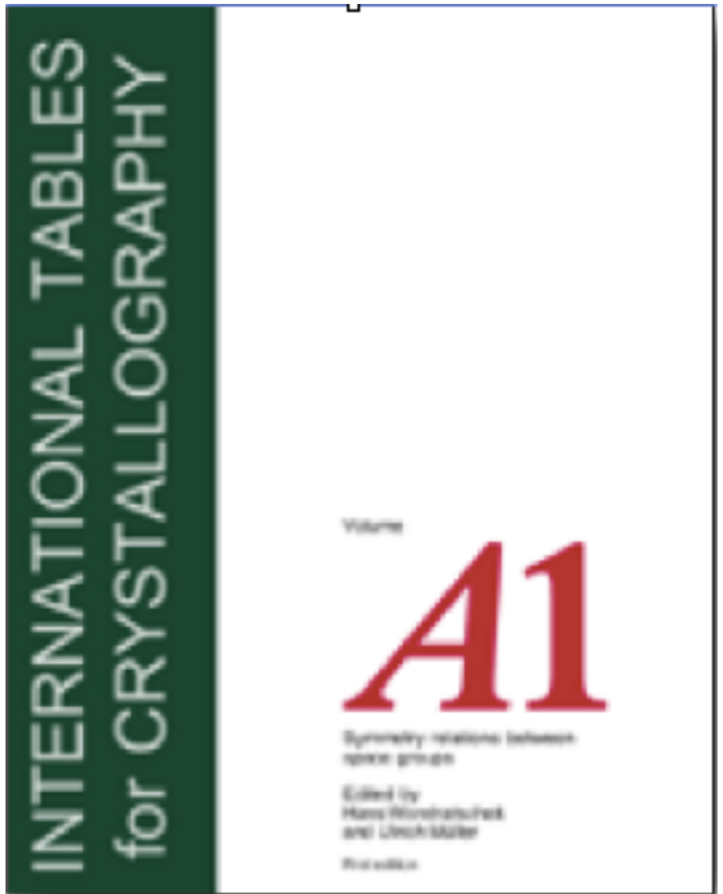
$$G \xrightarrow{i_P} M \xrightarrow{i_L} H$$

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

Corollary

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

GROUP-SUBGROUP RELATIONS OF SPACE GROUPS



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Space-group symmetry

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20-21 August 2

News:

- New Article in Nature
  07/2017: Bradlyn *et al.* "Top
  chemistry" *Nature* (2017). 54
- New program: BANDR
  04/2017: Band representatio
  Band representations of Dou
- New section: Double
  groups
  - New program: D
    04/2017: General pos
    Space Groups
  - New program:
    REPRESENTATIONS DPG

Group-Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
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.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS ⚠	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

International Tables for Crystallography, Vol. A1

eds. H. Wondratschek, U. Mueller

Maximal subgroups of space groups

*P*4*mm* No. 99 *P*4*mm*

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**

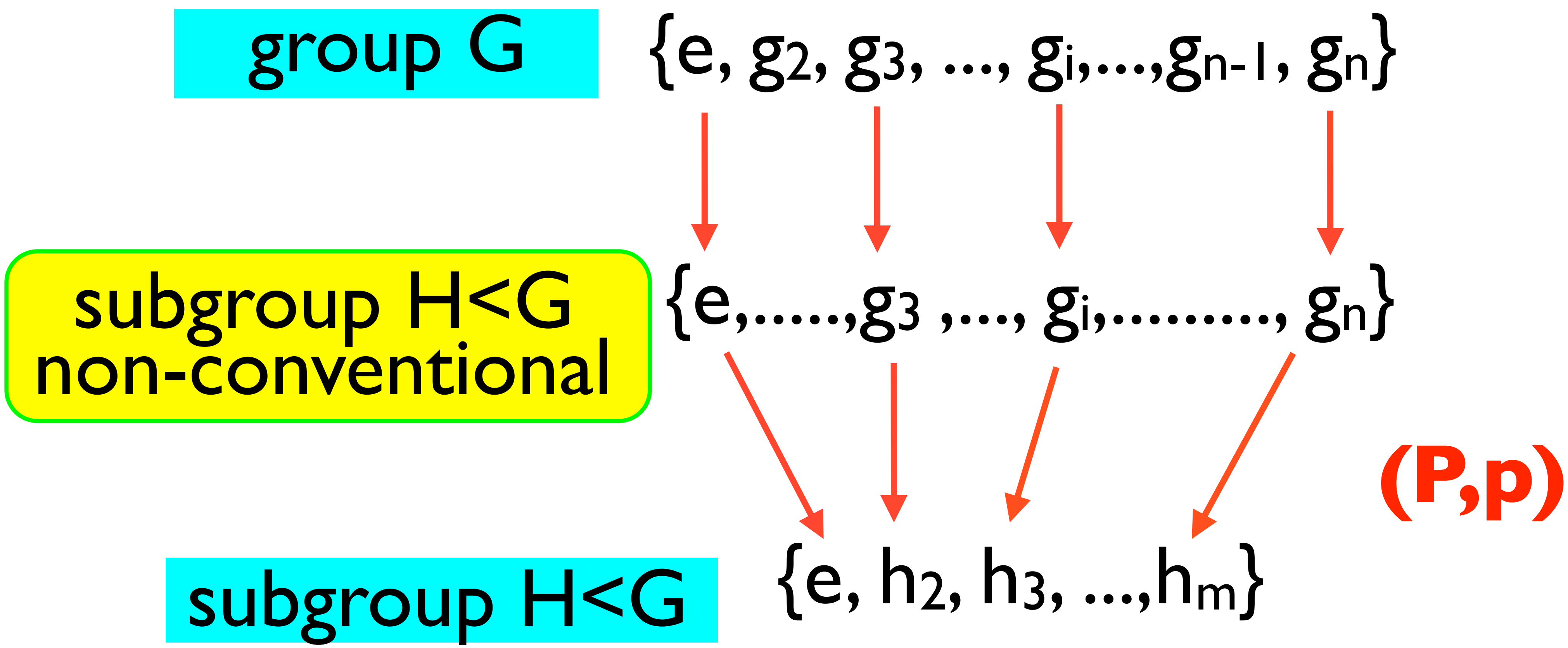
[p] $\mathbf{c}' = p\mathbf{c}$

$P4mm$ (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	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

Transformation matrix: (P,p)



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

Bilbao Crystallographic Server

Problem: SUBGROUPS OF SPACE GROUPS

SUBGROUPGRAPH

Bilbao Crystallographic Server → SUBGROUPGRAPH | Help

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

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

EXERCISES

Problem 2.3

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.

EXERCISES

Problem 2.4

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.

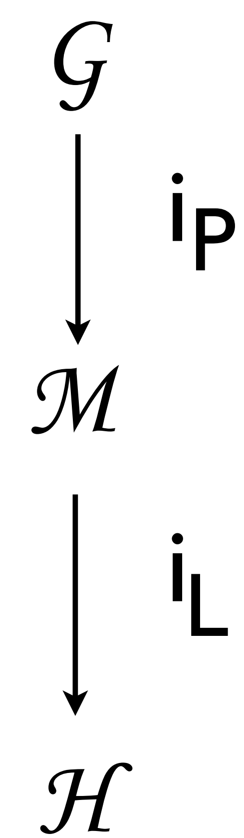
SUBGROUPS CALCULATIONS: HERMANN

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 $\mathcal{G}$

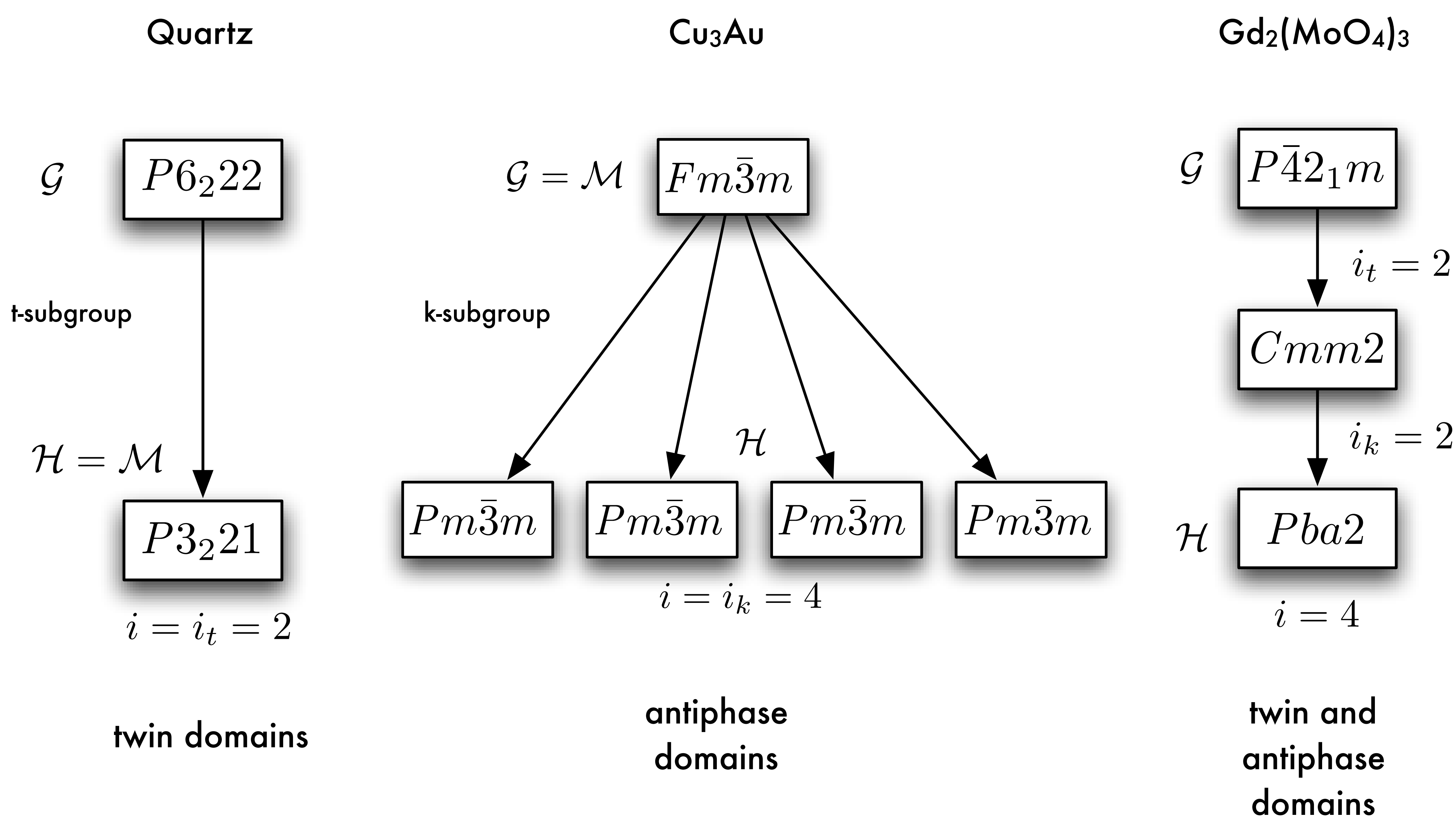
$\mathcal{H}$ is a *k*-subgroup of $\mathcal{M}$



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**



EXAMPLE

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

Lead vanadate $Pb_3(VO_4)_2$

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

$\mathcal{R}\text{-}3m$

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

$\mathcal{C}2/m$

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

$\mathcal{P}2_1/c$

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 $P2_1/c$

$|P_H|=?$

$Z_{H,p}=?$

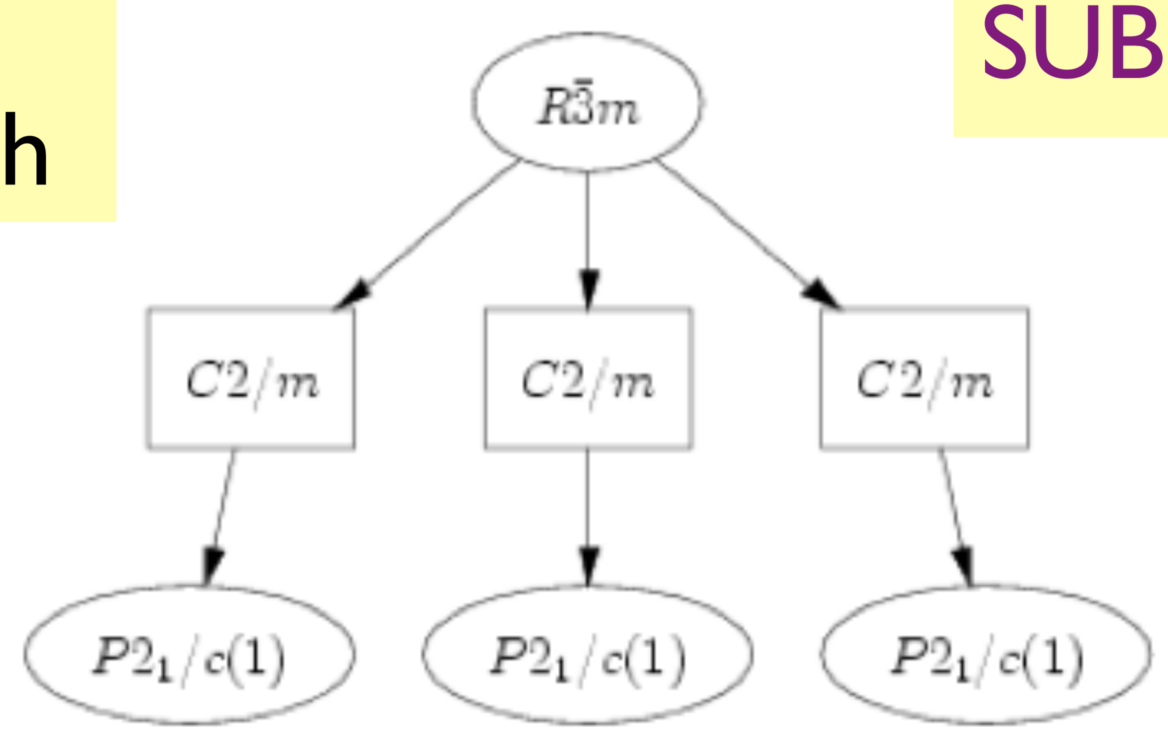
```
14
7.5075 6.0493 9.4814 90. 115.162 90.
7
Pb 1 2a 0 0 0
Pb 2 4e 0.3835 0.5815 0.2879
PV 1 4e 0.2071 0.0143 0.3999
O  1 4e 0.2872 0.2559 0.0159
O  2 4e 0.2598 0.7979 0.0216
O  3 4e 0.3194 0.9784 0.2823
O  4 4e 0.0335 0.5431 0.2091
```

$Pb_3(VO_4)_2$: 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

EXERCISES

Problem 2.5

(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?

GENERAL
AND
SPECIAL WYCKOFF
POSITIONS
SITE-SYMMETRY

Group Actions

Group Actions. A *group action* of a group $\mathcal{G}$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair (g, ω) an object $\omega' = g(\omega)$ of Ω such that the following hold:

(i) applying two group elements g and g' consecutively has the same effect as applying the product $g'g$, *i.e.* $g'(g(\omega)) = (g'g)(\omega)$

(ii) applying the identity element e of $\mathcal{G}$ has no effect on ω, *i.e.* $e(\omega) = \omega$ for all ω in Ω.

Orbit and Stabilizer

The set $\omega^{\mathcal{G}} := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of ω is called the *orbit of ω under $\mathcal{G}$*.

The set $S_{\mathcal{G}}(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object ω is a subgroup of $\mathcal{G}$ called the *stabilizer* of ω in $\mathcal{G}$.

General and special Wyckoff positions

Orbit of a point X_o under G: $G(X_o)=\{(W,w)\ X_o,(W,w)\in G\}$

Multiplicity

Site-symmetry group $S_o=\{(W,w)\}$ of a point X_o

$$(W,w)X_o = X_o$$

$$\left(\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} w \\ w \\ w \end{pmatrix} \right) \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

Multiplicity: $|P|/|S_o|$

General position X_o

$S=\{(I,\mathbf{o})\}\simeq \mathbf{1}$

Multiplicity: $|P|$

Special position X_o

$S>\mathbf{1}=\{(I,\mathbf{o}),...,\}$

Multiplicity: $|P|/|S_o|$

Site-symmetry groups: oriented symbols

General position

(i) coordinate triplets of an image point $\tilde{X}$ of the original point X= $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

-presentation of infinite image points $\tilde{X}$ under the action of (W,w) of G

(ii) short-hand notation of the matrix-column pairs (W,w) of the symmetry operations of G

-presentation of infinite symmetry operations of G

$(W,w) = (I,t_n)(W,w_0),\ 0 \leq w_{i0} < 1$

General Position of Space groups

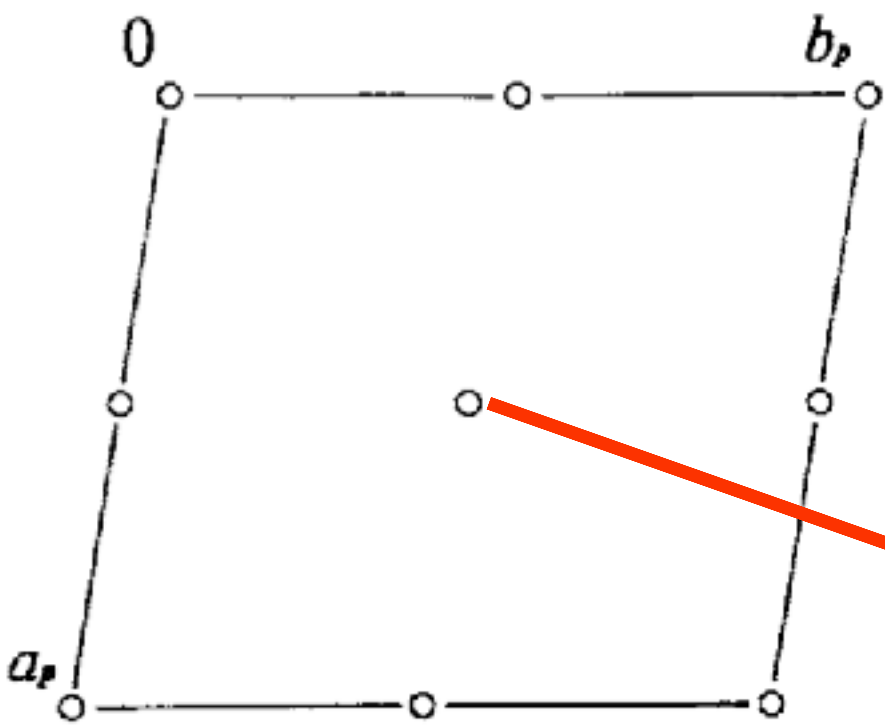
As coordinate triplets of an image point $\tilde{X}$ of the original point $X=\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

General position

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

Example: Calculation of the Site-symmetry groups

Group P-1



$S=\{(W,w), (W,w)X_o = X_o\}$

$$\left(\begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right) \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ 0 \\ -1/2 \end{pmatrix}$$

$S_f=\{(1,0), (-1,101)X_f = X_f\}$

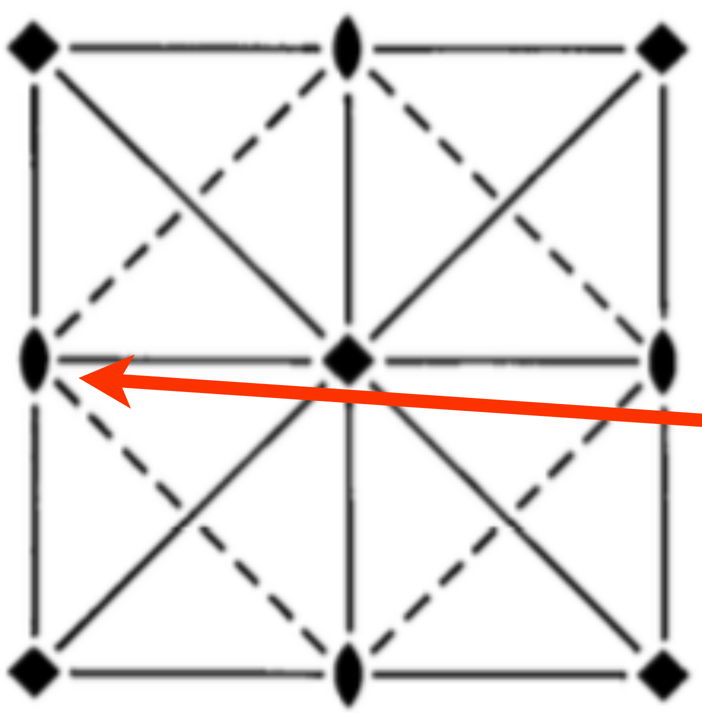
$S_f \simeq \{1, -1\}$ isomorphic

Positions

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

EXERCISES

General and special Wyckoff positions of P4mm



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*	$0,0,z$			

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

Bilbao Crystallographic Server

Problem: Wyckoff positions
Site-symmetry groups
Coordinate transformations

WYCKPOS

Wyckoff Positions

space group

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**.

If you are using this program in the preparation of a paper, please cite it in the following form:

Aroyo, et. al. *Zeitschrift fuer Kristallographie* (2006), 221, 1, 15-27.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Standard basis

Transformation of the basis

ITA settings

ITA-Settings for the Space Group 68

ces must be read by columns. P is the transformation f

$(\mathbf{a}, \mathbf{b}, \mathbf{c})_n = (\mathbf{a}, \mathbf{b}, \mathbf{c})_s P$

ITA number	Setting	P	P^{-1}
68	*C c c e* [origin 1]	a,b,c	a,b,c
68	*A e a a* [origin 1]	c,a,b	b,c,a
68	*B b e b* [origin 1]	b,c,a	c,a,b
68	*C c c e* [origin 2]	a,b,c	a,b,c
68	*A e a a* [origin 2]	c,a,b	b,c,a
68	*B b e b* [origin 2]	b,c,a	c,a,b

$Ccce$	D_{2h}^{22}	mmm	Orthorhombic
No. 68	$C\ 2/c\ 2/c\ 2/e$		Patterson symmetry $Cmmm$

16	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$
8	h	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$
8	g	. . 2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$
8	f	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	
8	e	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	
8	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	
8	c	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	
4	b	2 2 2	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$		
4	a	2 2 2	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$		

Wyckoff Positions of Group 68 (*Ccce*) [origin choice 2]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (1/2,1/2,0) +
16	i	1	(x,y,z) (-x+1/2,-y,z) (-x,y,-z+1/2) (x+1/2,-y,-z+1/2) (-x,-y,-z) (x+1/2,y,-z) (x,-y,z+1/2) (-x+1/2,y,z+1/2)
8	h	..2	(1/4,0,z) (3/4,0,-z+1/2) (3/4,0,-z) (1/4,0,z+1/2)
8	g	..2	(0,1/4,z) (0,1/4,-z+1/2) (0,3/4,-z) (0,3/4,z+1/2)
8	f	.2.	(0,y,1/4) (1/2,-y,1/4) (0,-y,3/4) (1/2,y,3/4)
8	e	2..	(x,1/4,1/4) (-x+1/2,3/4,1/4) (-x,3/4,3/4) (x+1/2,1/4,3/4)
8	d	-1	(0,0,0) (1/2,0,0) (0,0,1/2) (1/2,0,1/2)
8	c	-1	(1/4,3/4,0) (1/4,1/4,0) (3/4,3/4,1/2) (3/4,1/4,1/2)
4	b	222	(0,1/4,3/4) (0,3/4,1/4)
4	a	222	(0,1/4,1/4) (0,3/4,3/4)

Space Group : 68 (*Ccce*) [origin choice 2
Point : (0,1/4,1/4)
Wyckoff Position : 4a

Site Symmetry Group 222

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	
-x,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4
-x,-y+1/2,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,1/4,z
x,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 x,1/4,1/4

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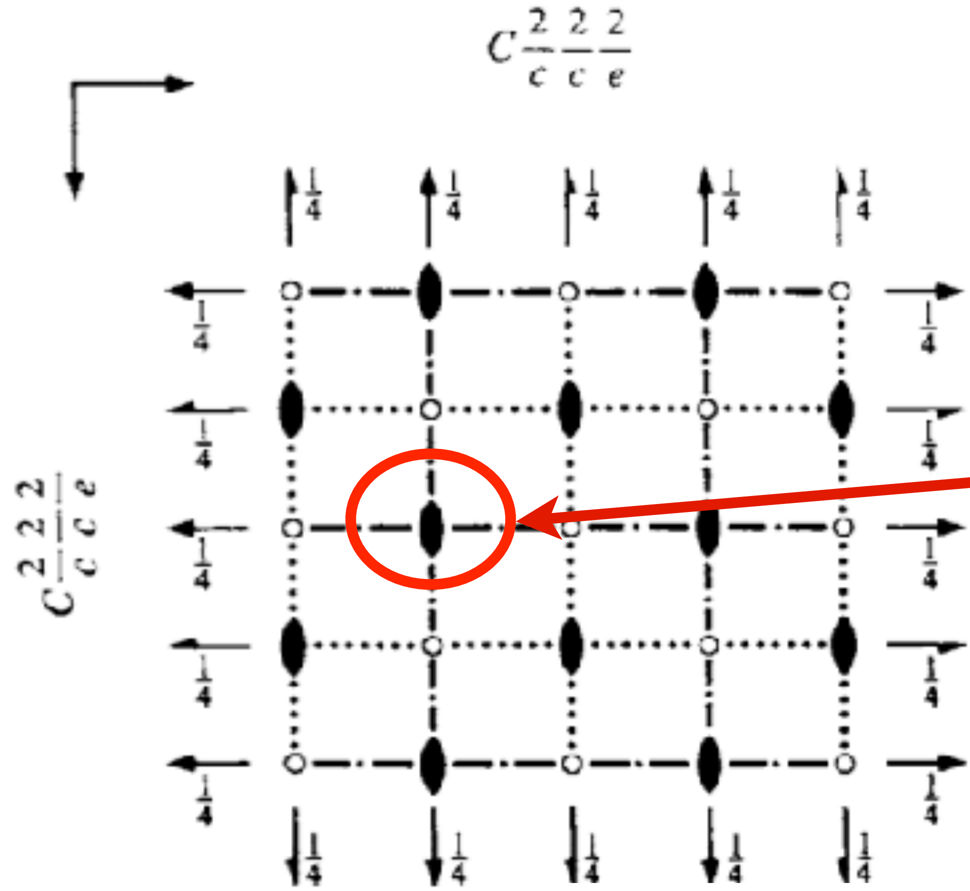
Example WYCKPOS: Wyckoff Positions Ccce (68)



2 1/2,y,1/4

2 x,1/4,1/4

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)
Variable parameters (x,y,z) are also accepted

x = 1/2 y = 1/4 z = 1/4

Show

Space Group : 68 (*Ccce*) [origin choice 2]
Point : (1/2,1/4,1/4)
Wyckoff Position : 4b

Site Symmetry Group 222

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
-x+1,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 1/2,y,1/4
-x+1,-y+1/2,z	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/2,1/4,z
x,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 x,1/4,1/4

EXERCISES

Problem 2.6

Consider the special Wyckoff positions of the the space group *P4mm*.

Determine the site-symmetry groups of Wyckoff positions *1a* and *1b*. Compare the results with the listed ITA data

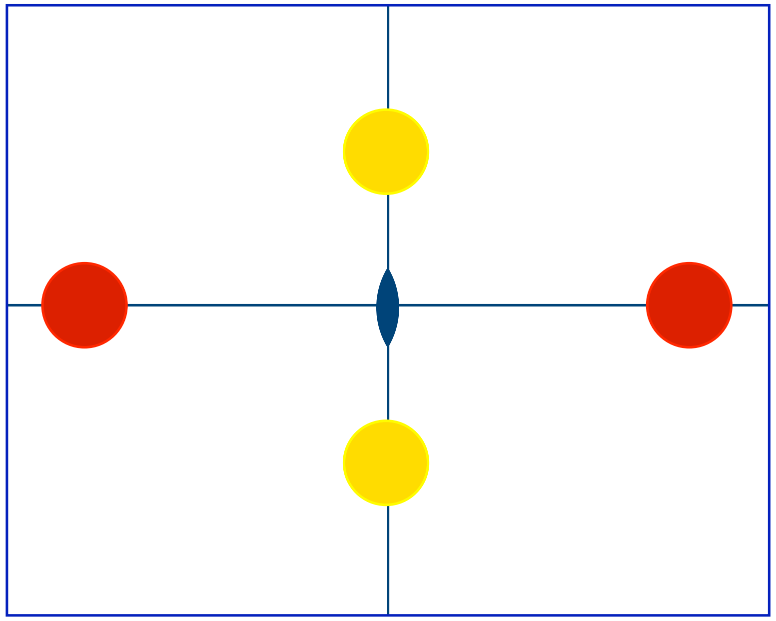
The coordinate triplets (x,1/2,z) and (1/2,x,z), belong to Wyckoff position *4f*. Compare their site-symmetry groups.

Compare your results with the results of the program WYCKPOS.

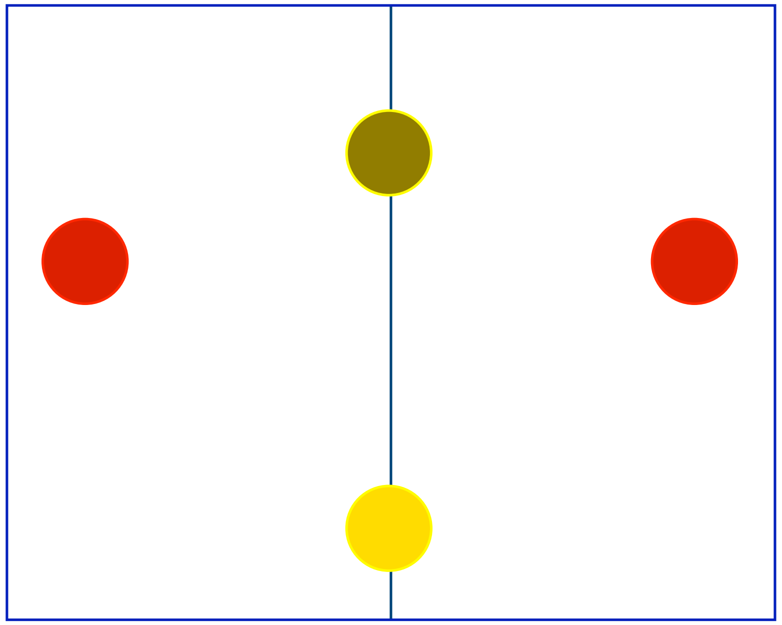
RELATIONS BETWEEN WYCKOFF POSITIONS

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

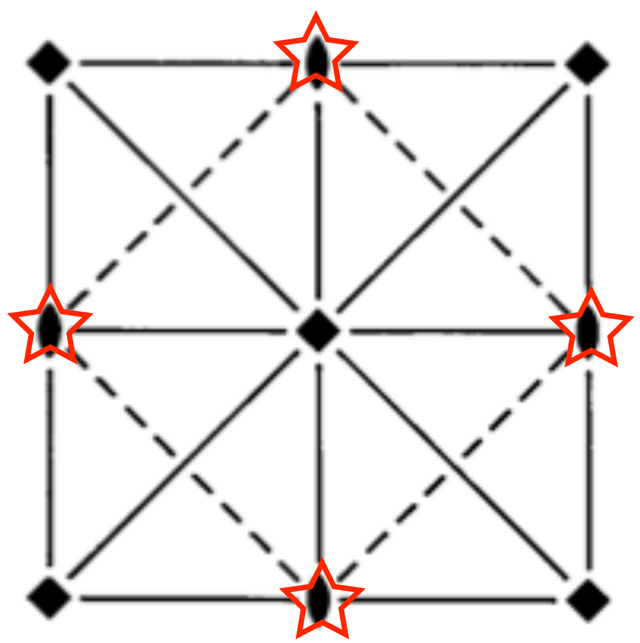
EXAMPLE

Group-subgroup pair

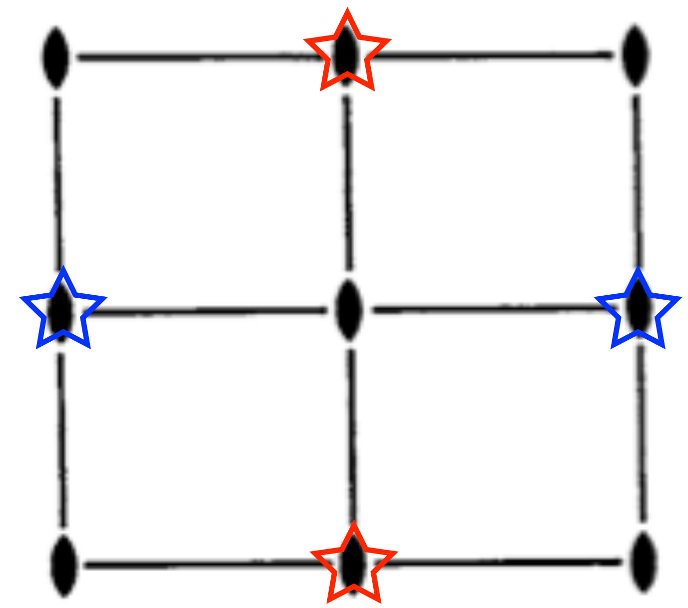
P4mm>*Pmm2*, [i]=2

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

P4mm



Pmm2



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

No. 99 $P4mm$

	Axes	Coordinates	Wyckoff positions 1a	1b	2c	4d	4e	4f	8g
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

WYCKSPLIT

Wyckoff Positions Splitting

Conventional Settings

Non conventional Settings

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup or choose it	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)	1 1 0 -1 1 0 0 0 1
origin shift:	0 0 0

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)

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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)

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

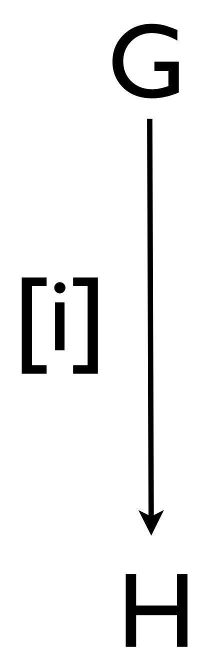
ITA1 data:

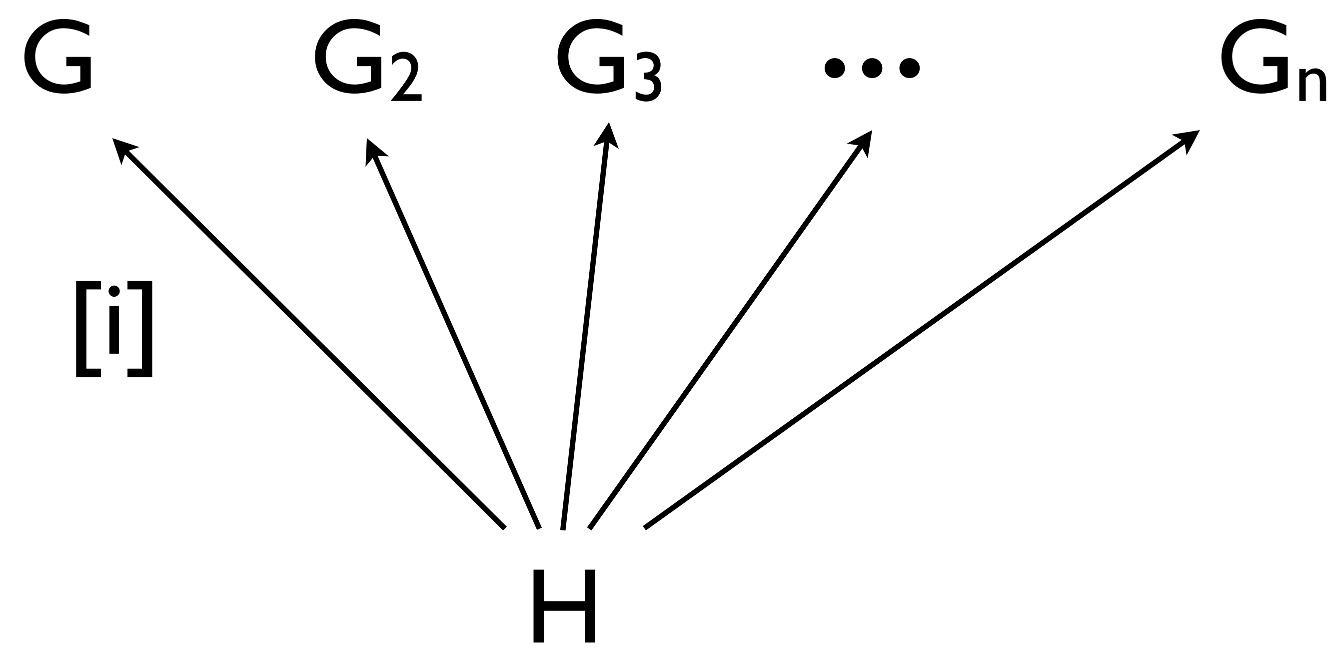
minimal non-isomorphic *k*- and *t*-supergroups types

The Supergroup Problem

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

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



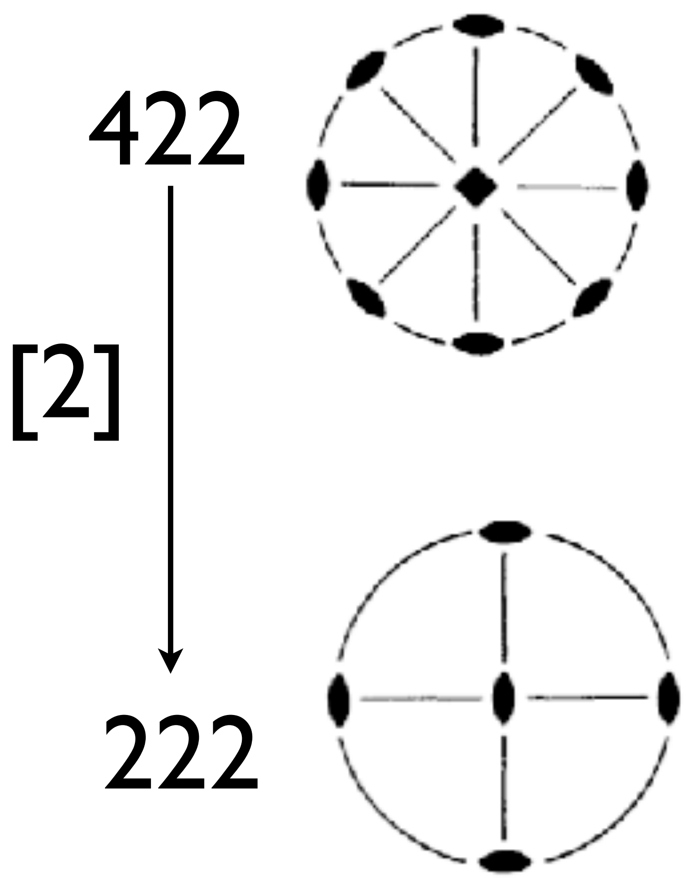


all G_k>H contain H as subgroup

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

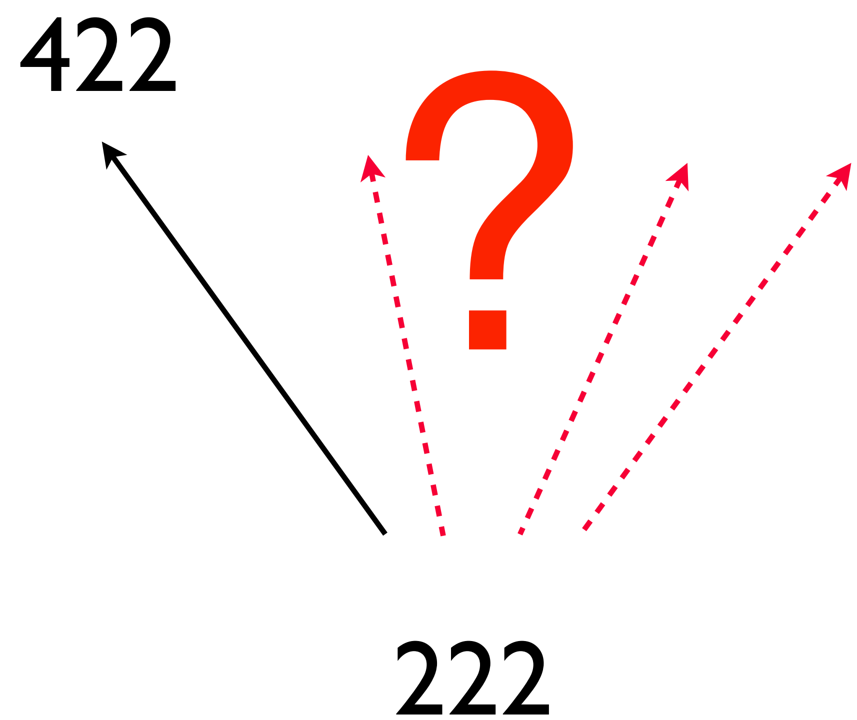
Example: Supergroup problem

Group-subgroup pair 422>222



How many are the subgroups 222 of 422?

Supergroups 422 of the group 222

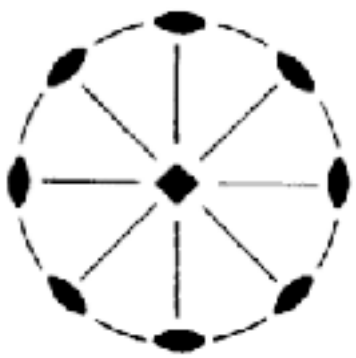


How many are the supergroups 422 of 222?

Example: Supergroup problem

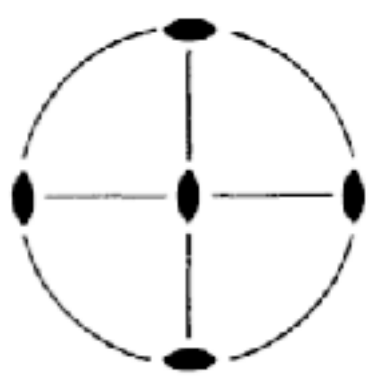
Group-subgroup pair 422>222

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

$$4_z22 = 222 + 4_z222$$

$$4_y22 = 222 + 4_y222$$

$$4_x22 = 222 + 4_x222$$

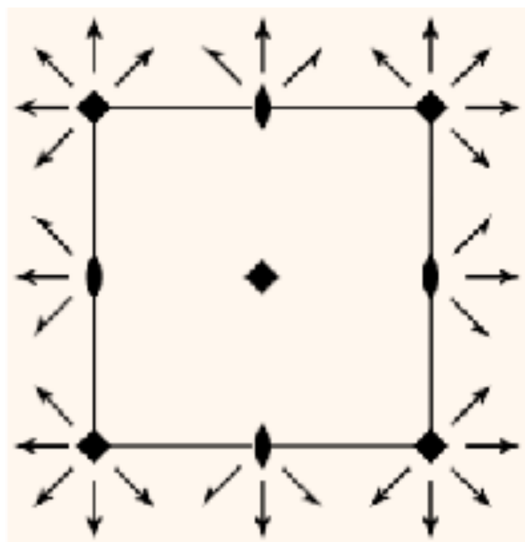
Example: Supergroup problem

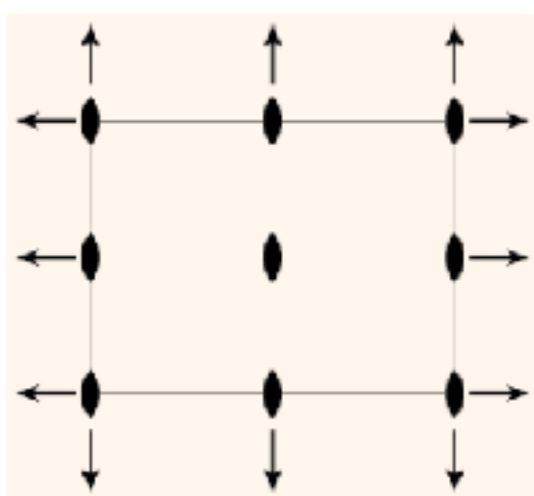
Group-subgroup pair P422>P222

P422

[2]

P222





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

Supergroups P422 of the group P222

$P4_z22$ $P4_x22$ $P4_y22$

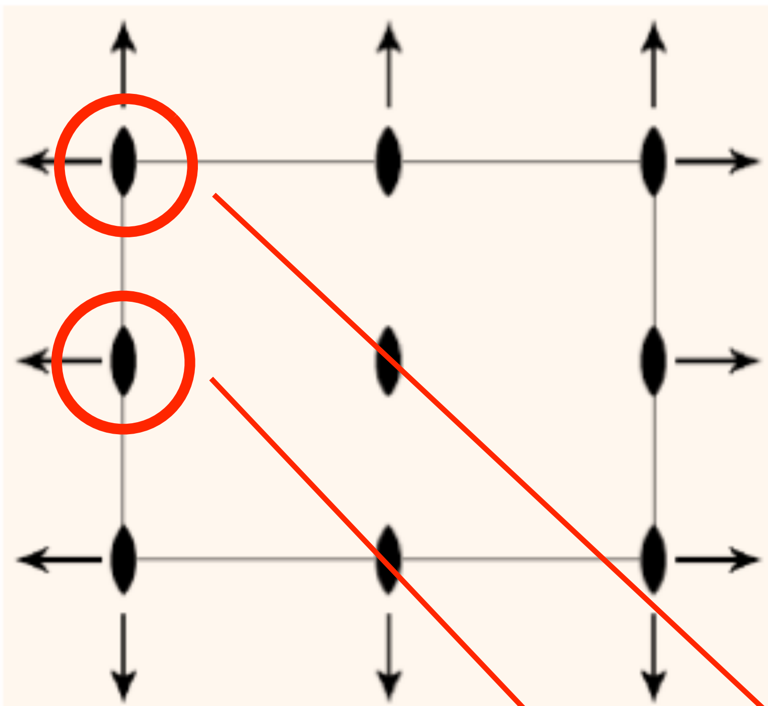
[2]

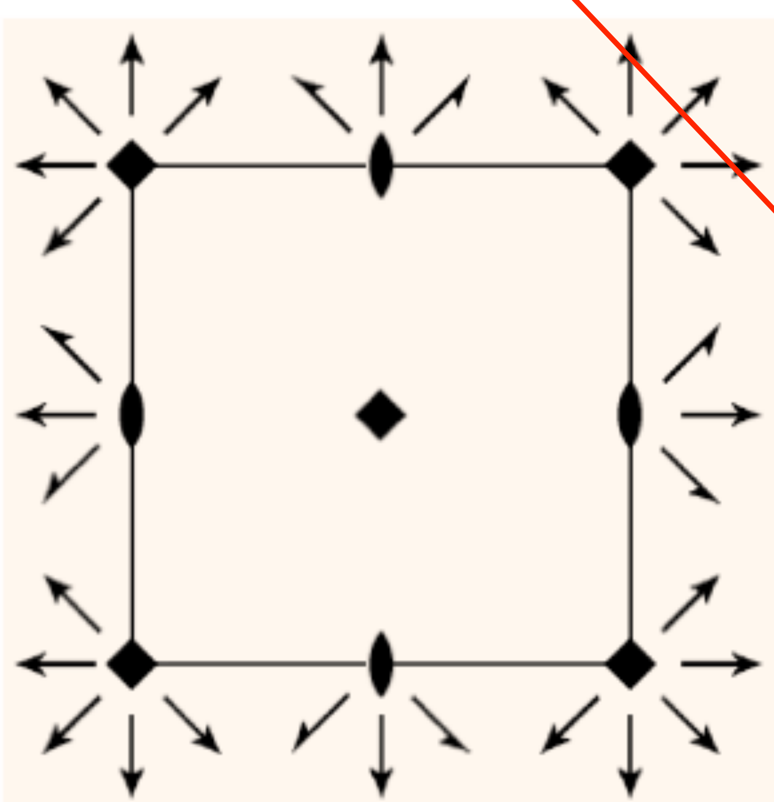
P222

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

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**

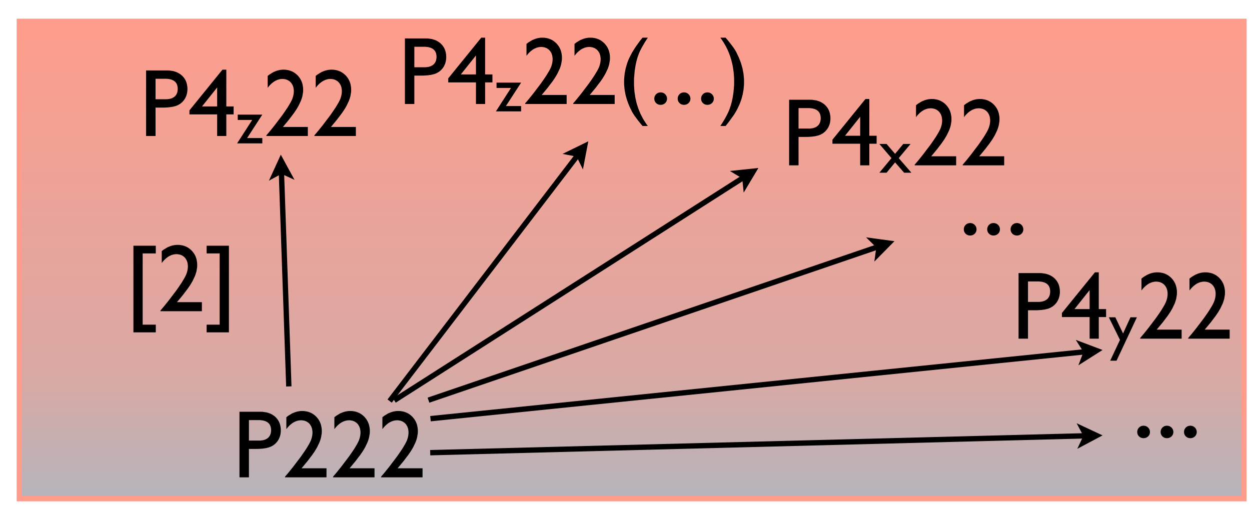
[2] *A*222 (21, *C*222); [2] *B*222 (21, *C*222); [2] *C*222 (21); [2] *I*222 (23)

- **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

supergroup

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

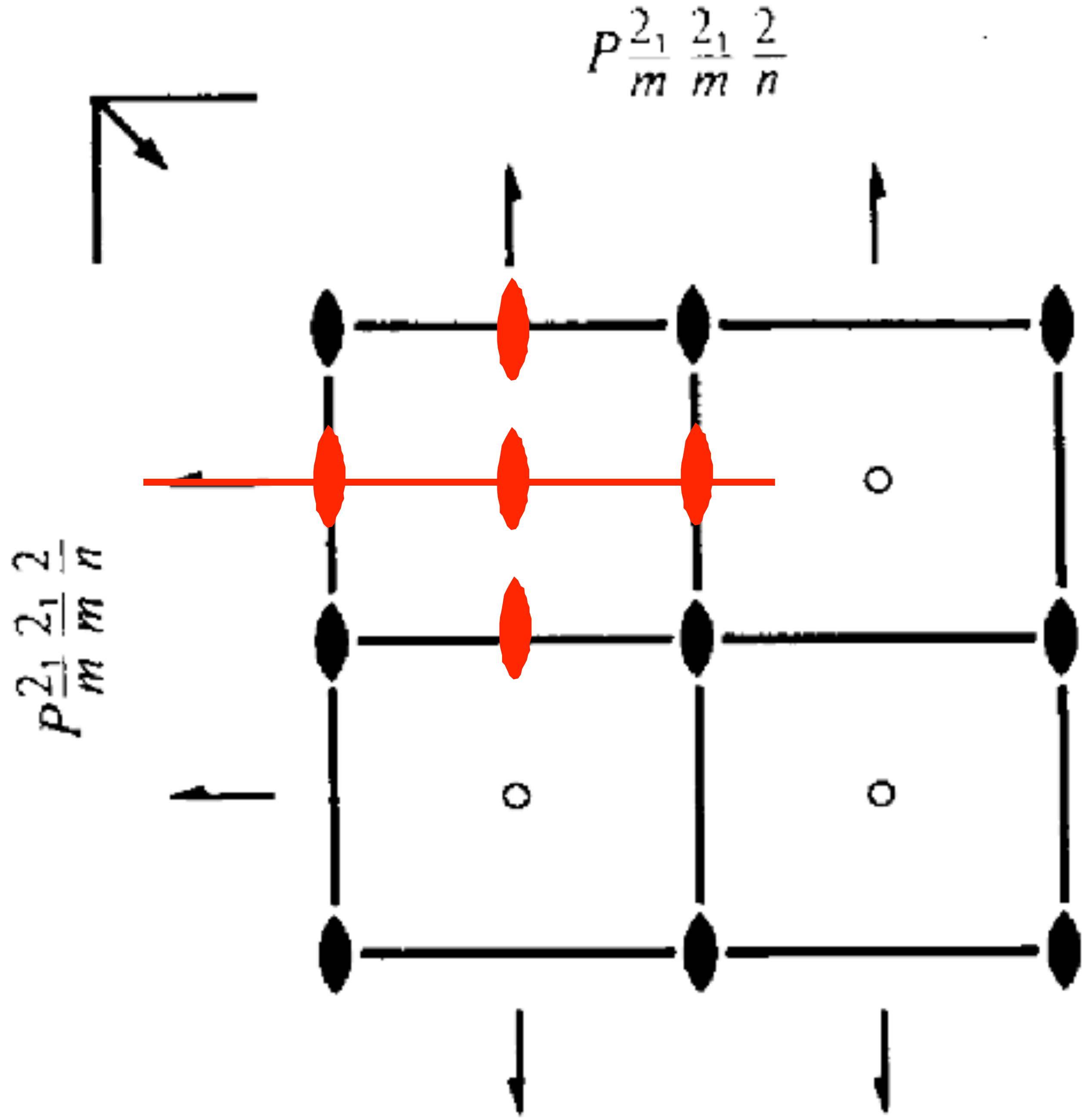
Supergroups (of index 2) isomorphic to the group 89 (*P*422) of the group 16 (*P*222)

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

NORMALIZERS
OF
SPACE GROUPS

Normalizers of space groups

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



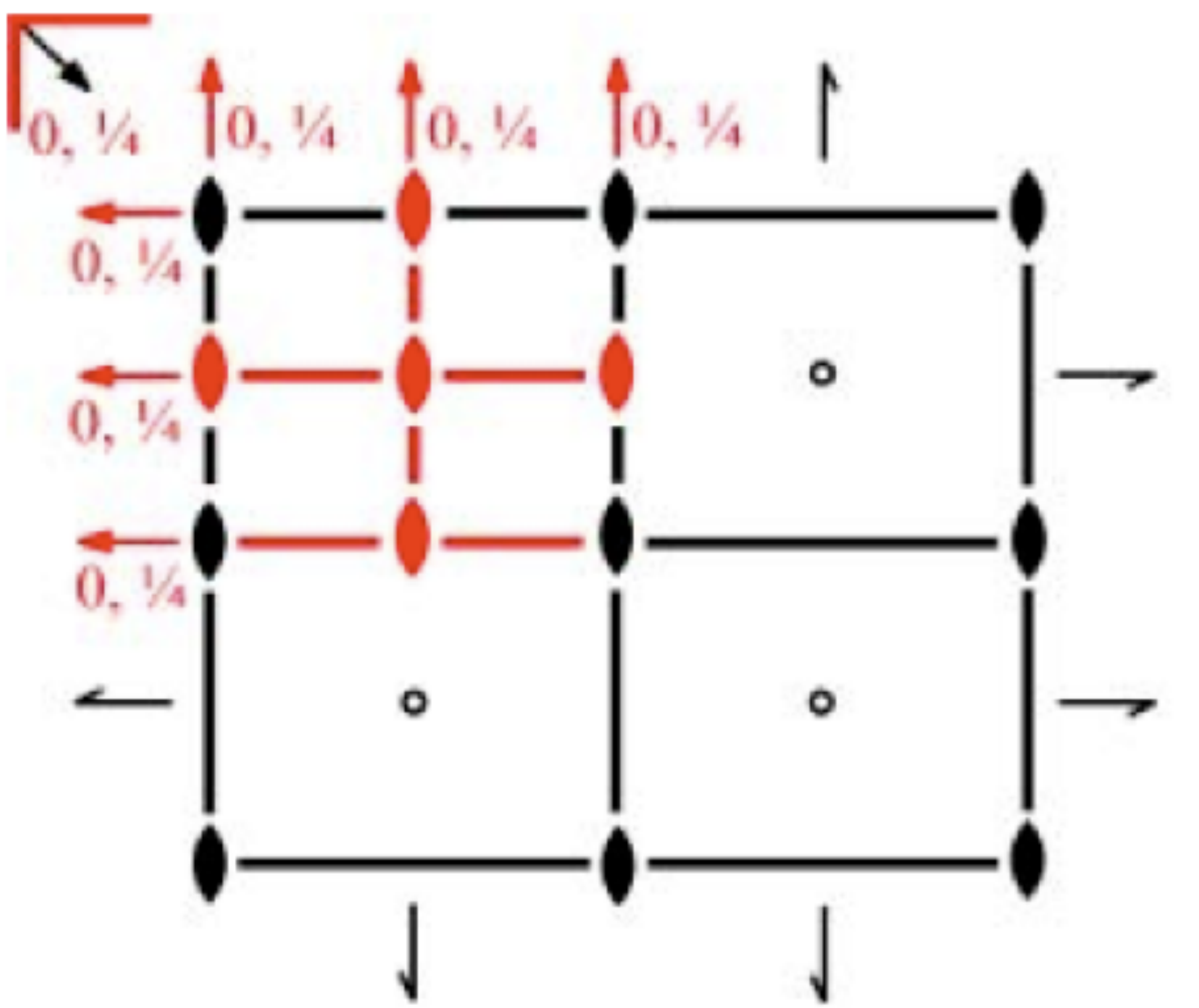
Example: Pmmn

the symmetry of symmetry

Normalizers of space groups

Normalizers N(G) : $g^{-1}\{G\}g = \{G\}$ $\left\{ \begin{array}{l} \text{Euclidean} \\ \text{Affine} \end{array} \right.$

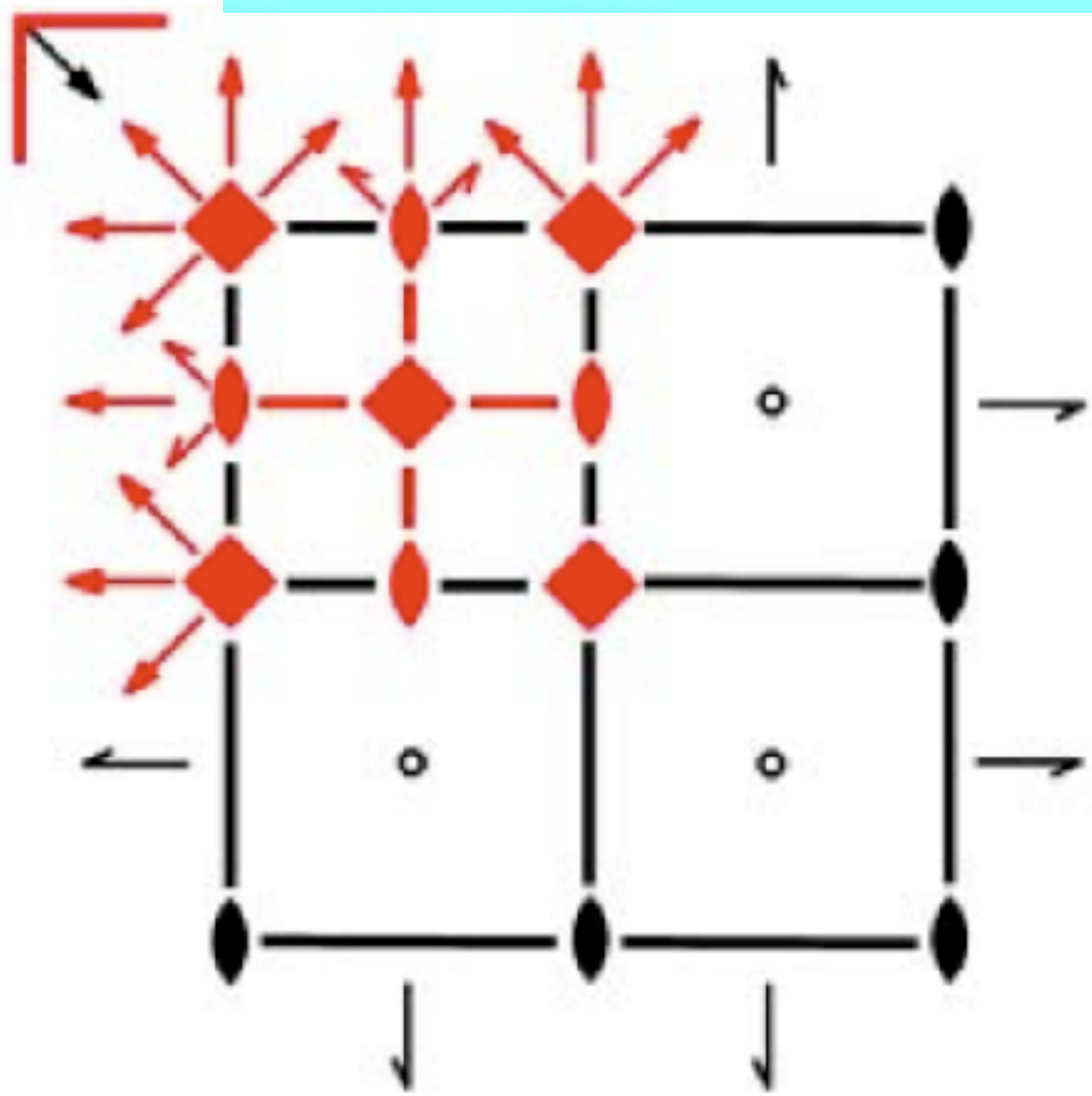
the symmetry
of symmetry



Space group: Pmmn (a,b,c)

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

Normalizers for specialized metrics



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

Bilbao Crystallographic Server

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: ○

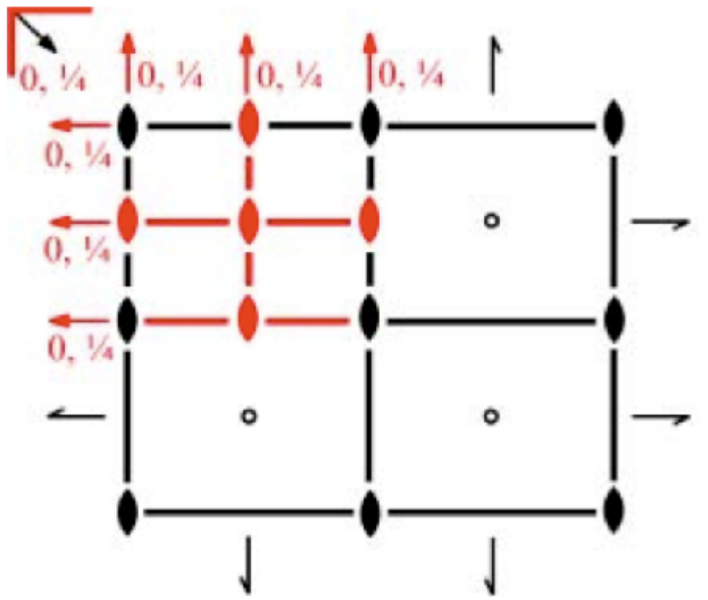
Enhanced Euclidean normalizer (specialized metrics)

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 ip=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*