Summer School on Mathematical Crystallography

3-7 June 2019, Nancy (France)

International Union of CrystallographyCommision on Mathematical and Theoretical Crystallography

IUCr MaThCryst CRM^2 Cristallographie, Résonance Magnétique et Modélisations AFC C2MP métropole GrandNancy

SYMMETRY RELATIONS OF SPACE GROUPS

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Group-Subgroup Relation of Space Groups

Subgroups of space groups

Supergroups of space groups

Normalizers of space groups

Wyckoff-position splitting

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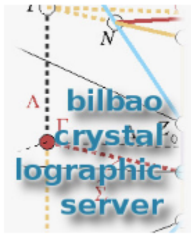

Bilbao Crystallographic Server in forthcoming schools and workshops

News:

- **New Article in Acta Cryst. A** 05/2019: Gallego *et al.* "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server." *Acta Cryst.* (2019) **A75**, 438-447.
- **New Article in Nature** 03/2019: Vergniory *et al.* "A complete catalogue of high-quality topological materials" *Nature* (2019). **566**, 480-485.
- **Updated versions of TENSOR and MTENSOR** 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..

Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

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Space-group symmetry

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)

Point-group symmetry

Plane-group symmetry

Double point and space groups

News:

- *Nature* (2019). 566, 480-485.
- Updated versions of TENSOR and MTENSOR 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..

Subgroups: Some basic results

Subgroup H < G

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

Proper subgroup

H is a proper subset of G if $H < G$ and $H \neq G$

Trivial subgroup: {e}, G

Index [i]

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

Maximal subgroup

H is a maximal subgroup of G if **NO** intermediate subgroup Z exist such that:

$$H < Z < G$$

Coset decomposition G : H

Group-subgroup pair H < G

left coset decomposition: $G = H + g_2H + \ldots + g_iH, \quad g_i \notin H$

i = index of H in G

first coset $\mathcal{H} =$	second coset $g_2\mathcal{H} =$	third coset $g_3\mathcal{H} =$	... ...	ith coset $g_i\mathcal{H} =$
$e = h_1$	$g_2\, e$	$g_3\, e$	...	$g_i\, e$
h_2	$g_2\, h_2$	$g_3\, h_2$	...	$g_i\, h_2$
h_3	$g_2\, h_3$	$g_3\, h_3$	...	$g_i\, h_3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
h_n	$g_2\, h_n$	$g_3\, h_n$	...	$g_i\, h_n$

Total of i cosets. Each of them contains the same number of elements.
No one contains elements of another coset

right coset decomposition $G = H + Hg_2 + \ldots + Hg_i, \quad g_i \notin H$

i = index of H in G

Conjugate subgroups

Conjugate subgroups

Subgroups H_1, $H_2 < G$ are called *conjugated subgroups* in G, if there exists an element $g_m \in G$ such that

$$g_m^{-1} H_1 g_m = H_2$$

The length of the conjugacy class $|L(H)|$ is a divisor of $|G|/|H|$

Normal subgroups

Let $H < G$, if $g_m^{-1} H g_m = H$ holds for all $g_m \in G$, H is called a *normal subgroup* of G, designated $H \lhd G$

Subgroups types

H < G is called a *translationengleiche subgroup* if G and H have the same group of translations, $T_H = T_G$ and H belongs to a crystal class of lower symmetry than G, $P_H < P_G$

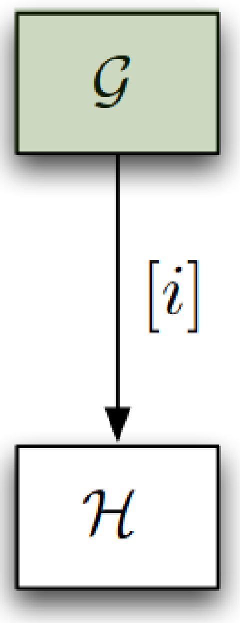
H < G is called a *klassengleiche subgroup*, if G and H belong to the same crystal class, $P_H = P_G$; therefore, H has fewer translations than G, $T_H < T_G$

H is called *general subgroup* of G, if $T_H < T_G$ and $P_H < P_G$

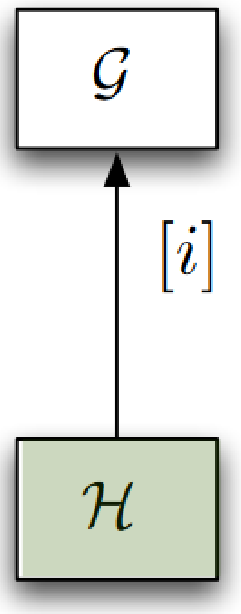
Group-subgroup relations

Applications

Group-subgroup relations



Group-supergroup relations



- Possible low symmetry structures
- Domain structure analysis
- Prediction of new structures

- Possible high-symmetry structures
- Prediction of phase transitions
- Determination of prototype structures

MAXIMA 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)
(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 $P_G = \{I, W_2, W_3,\ldots,W_i\}$

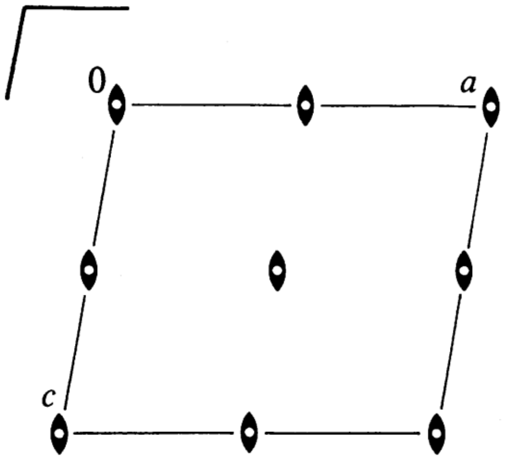
Example: P 1 2/m 1 (No. 10)

Coset decomposition G : T_G

Factor group $G/T_G \simeq P_G$

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

G = P2/m



T_G	T_G2	$T_G\bar{1}$	T_Gm
(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)
...	...	...	...

Translationengleiche subgroups H<G

H is called a ***translationengleiche subgroup*** if $T_G=T_H$ and $P_H < P_G$

Example: P 1 2/m 1

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

Translationengleiche subgroups H<G

H is called a ***translationengleiche subgroup*** if $T_G = T_H$ and $P_H < P_G$

Example: P 1 2/m 1

Coset decomposition

T_G	T_G2	$T_G\bar{1}$	T_Gm
$(1,0)$	$(2,0)$	$(\bar{1},0)$	$(m,0)$
$(1,t_1)$	$(2,t_1)$	$(\bar{1},t_1)$	(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**

$H_1 = T_G \cup T_G2$

P 1 2 1

Translationengleiche subgroups H<G

H is called a ***translationengleiche subgroup*** if $T_G = T_H$ and $P_H < P_G$

Example: P 1 2/m 1

Coset decomposition

T_G	T_G2	$T_G\bar{1}$	T_Gm
(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**

$H_1 = T_G \cup T_G2$
P 1 2 1

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

Translationengleiche subgroups $H<G$

H is called a ***translationengleiche subgroup*** if $T_G=T_H$ and $P_H < P_G$

Example: P 1 2/m 1

Coset decomposition

T_G	T_G2	$T_G\bar{1}$	T_Gm
(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**

$H_1 = T_G \cup T_G2$
P 1 2 1

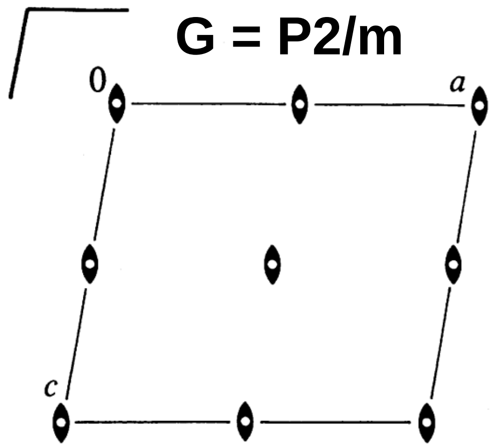
$H_2 = T_G \cup T_G\bar{1}$
P $\bar{1}$

$H_3 = T_G \cup T_Gm$
P 1 m 1

Example: P 1 2/m 1 (No. 10)

Translationengleiche subgroups H<G:

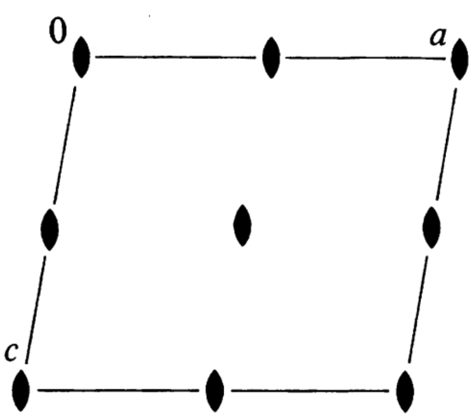
G = P2/m

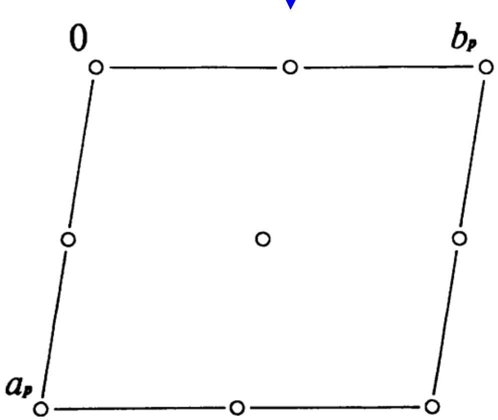


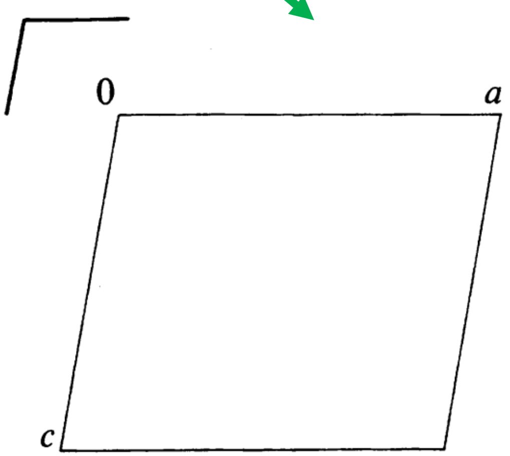
P121 = T_G U $T_G 2$

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

P1m1 = T_G U $T_G m$

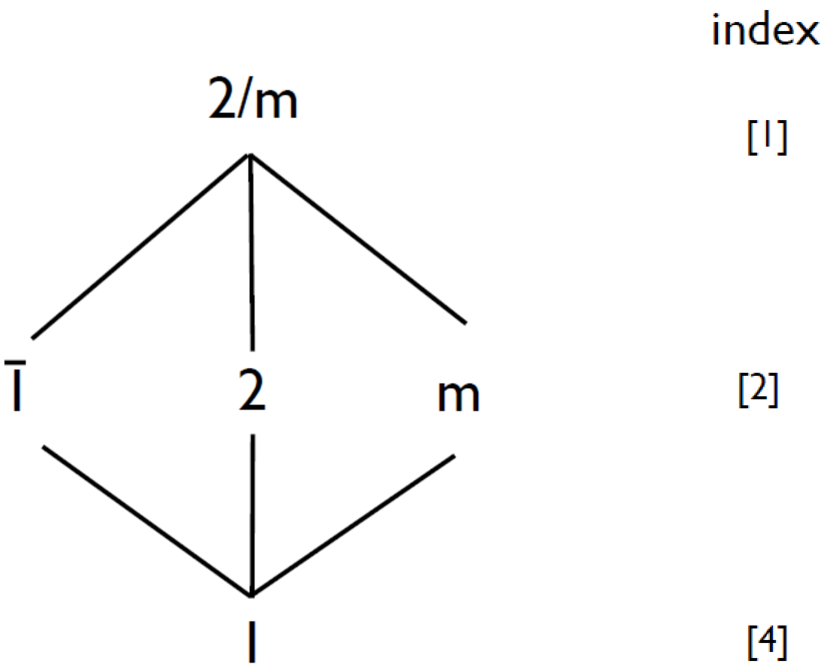




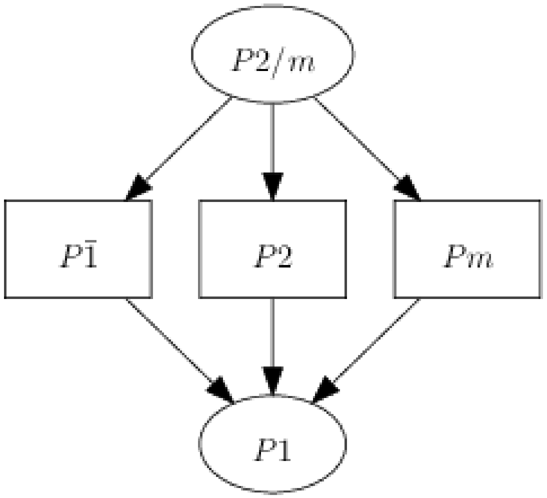


Example: P 1 2/m 1 (No. 10)

Translationengleiche subgroups H<G:



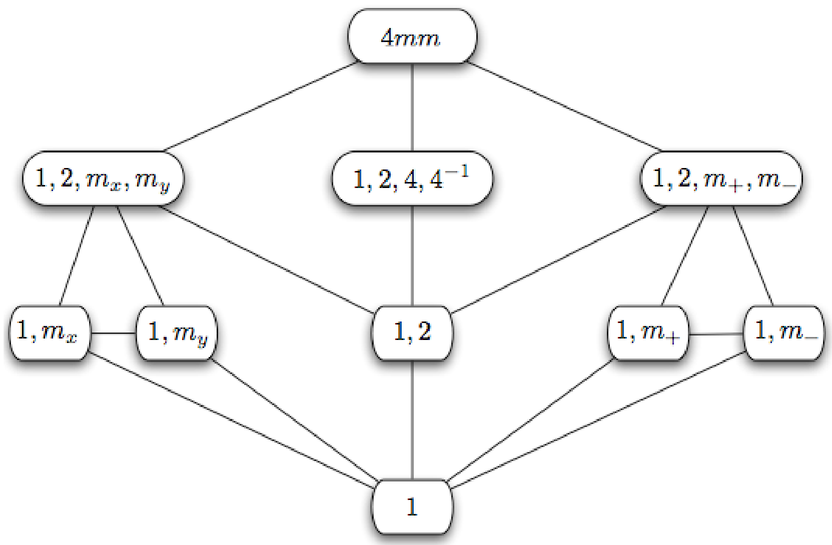
Subgroup diagram of pointgroup 2/m



Translationengleiche subgroups of space group *P*2/m

Exercise 2.25

Construct the diagram of the *t*-subgroups of P4mm using the `analogy' with the subgroup diagram of the group 4mm. Give the standard Hermann-Mauguin symbols of the *t*-subgroups of P4mm.



Maximal subgroups of space groups

International Tables for Crystallography, Vol. A1
ed. H. Wondratschek, U. Mueller

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	$\mathbf{a-b, a+b, c}$	
[2] $P2m1$ (25, $Pmm2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$	
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$	
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$	
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a, b, 2c}$	
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C4md$ (100, $P4bm$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a-b, a+b, c}$	
$C4md$ (100, $P4bm$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a-b, a+b, c}$	1/2, 1/2, 0
$C4mm$ (99, $P4mm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a-b, a+b, c}$	
$C4mm$ (99, $P4mm$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a-b, a+b, c}$	1/2, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F4mc$ (108, $I4cm$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a-b, a+b, 2c}$	
$F4mc$ (108, $I4cm$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,1)\rangle$	$\mathbf{a-b, a+b, 2c}$	1/2, 1/2, 0
$F4mm$ (107, $I4mm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a-b, a+b, 2c}$	
$F4mm$ (107, $I4mm$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a-b, a+b, 2c}$	1/2, 1/2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a, b, 3c}$	

Maximal subgroups of P4mm (No. 99)

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

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

General position

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

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	

Remarks

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

{ braces for conjugate subgroups

(P, p): $(\mathbf{a}_H, \mathbf{b}_H, \mathbf{c}_H) = (\mathbf{a}_G,\mathbf{b}_G,\mathbf{c}_G)\mathbf{P}$

$O_H = O_G + \mathbf{p}$

Subgroups of Space Groups

SUBGROUPGRAPH http://www.cryst.ehu.es/cryst/subgroupgraph.html

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:	10
Enter subgroup number (H) or choose it:	1
Enter the index [G:H] (optional):	4

Construct the lattice

Input:
- Group number (G)
- Subgroup number (H)
- The index [i] (optional)

Subgroups of Space Groups

Chains of maximal subgroups from *P2/m* (No. 10) [unique axis b] to *P1* (No. 1) with index 4

Chains of subgroups ...

For each chain of maximal subgroups relating G = *P2/m* and H = *P1* with index 4, there is a set of transformation matrices (P_j, p_j), where each matrix corresponds to a subgroup H_j isomorphic to H.

Click over "transformation" to see the list with the transformation matrices, obtained following the corresponding chain of maximal subgroups.

To see the contracted graph representing the chains, click on **[Show contracted graph]**.

To view the list with different subgroups of a given type and its distribution into the classes of conjugate subgroups click over **[Classify]** buttons.

The program distributes the subgroups into classes by comparing directly their elements in the group basis.

N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	010 003 001 [2 2]	*P2/m* > *P2* > *P1*	4	transformation...
2	010 006 001 [2 2]	*P2/m* > *Pm* > *P1*	2	transformation...
3	010 002 001 [2 2]	*P2/m* > *P*-1 > *P1*	2	transformation...

Print this table.

Show contracted graph

Classify (with a complete graph of all subgroups)

Classify (with complete graphs for individual subgroups)

Subgroups of Space Groups

Chains of maximal subgroups from *P2/m* (No. 10) [unique axis b] to *P1* (No. 1) with index 4

Chains of subgroups ...

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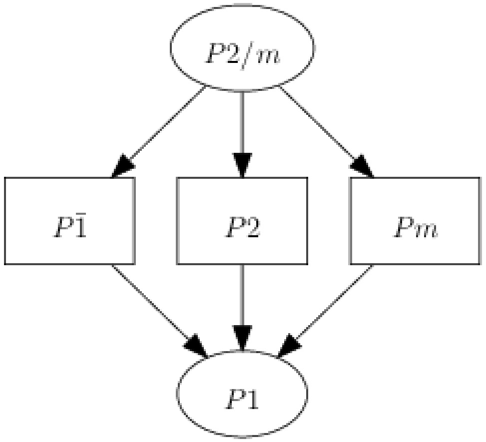
N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	010 003 001 [2 2]	*P2/m* > *P2* > *P1*	4	transformation...
2	010 006 001 [2 2]	*P2/m* > *Pm* > *P1*	2	transformation...
3	010 002 001 [2 2]	*P2/m* > *P-1* > *P1*	2	transformation...

Print this table.

Show contracted graph

Classify (with a complete graph c

Classify (with complete graphs for in



Exercise 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).

MAXIMA SUBGROUPS OF SPACE GROUPS

II. MAXIMAL KLASSENGLEICHE SUBGROUPS

Klassengleiche subgroups H < G

H is called a ***klassenglieche subgroup*** of G if $T_G > T_H$ and $P_H = P_G$

Example: P 1 (No. 1) – isomorphic k-subgroups

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

Coset decomposition

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

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

T_e	$T_e t_a$
$(1,0)$	$(1,t_a)$
$(1,t_1)$	$(1,t_1+t_a)$
$(1,t_2)$	$(1,t_2+t_a)$
...	...
$(1,t_j)$	$(1,t_j+t_a)$
...	...

Klassengleiche subgroups H < G

H is called a ***klassengleiche subgroup*** if $T_G > T_H$ and $P_H = P_G$

Example: P 1 (No. 1) – isomorphic k-subgroups

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

Coset decomposition

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

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

isomorphic *k*-subgroups:

P1(2***a***,***b***,***c***)

T_e	$T_e t_a$
$(1,0)$	$(1,t_a)$
$(1,t_1)$	$(1,t_1+t_a)$
$(1,t_2)$	$(1,t_2+t_a)$
...	...
$(1,t_j)$	$(1,t_j+t_a)$
...	...

$H = T_e$

Klassengleiche subgroups H < G

Example: P 1 (No. 1) – isomorphic k-subgroups

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

- Coset decomposition

P1=T_e + $T_e t_a$

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

- Isomorphic *k*-subgroups:

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.

H=T_e $\mathbf{t}_a$=(1,0,0)

$\mathbf{T_e}$	$\mathbf{T_e t_a}$
(1,0)	(1,t_a)
(1,t_1)	(1,t_1+t_a)
(1,t_2)	(1,t_2+t_a)
...	...
(1,t_j)	(1,t_j+t_a)
...	...

INFINITE number of maximal isomorphic subgroups

Series of maximal isomorphic subgroups

International Tables for Crystallography, Vol. A1

ed. H. Wondratschek, U. Mueller

Example: P-1 (No. 2)

$P\bar{1}$	No. 2	$P\bar{1}$	C_i^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	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

INFINITE number of maximal isomorphic subgroups

Klassengleiche subgroups H < G

Non-isomorphic subgroups

Example: C2 (No. 5)

- Coset decomposition

$C2 = T_c + T_c2$

$T_c = T_i + T_it_c$

T_i=integer

t_c=1/2,1/2,0

T_c		T_c2	
T_i	T_it_c	T_i2	T_it_c2
(1,0)	(1,0)	(2,0)	(2,0)
$(1,t_1)$	$(1, t_1+t_c)$	$(2,t_1)$	$(2,t_1+t_c)$
$(1,t_2)$	$(1,t_2+t_c)$	$(2,t_2)$	$(2,t_2)$
...	...	...	...
$(1,t_j)$	$(1,t_j+t_c)$	$(2,t_j)$	$(2,t_j)$
...	...	...	...

Klassengleiche subgroups H < G

Non-isomorphic subgroups

Example: C2 (No. 5)

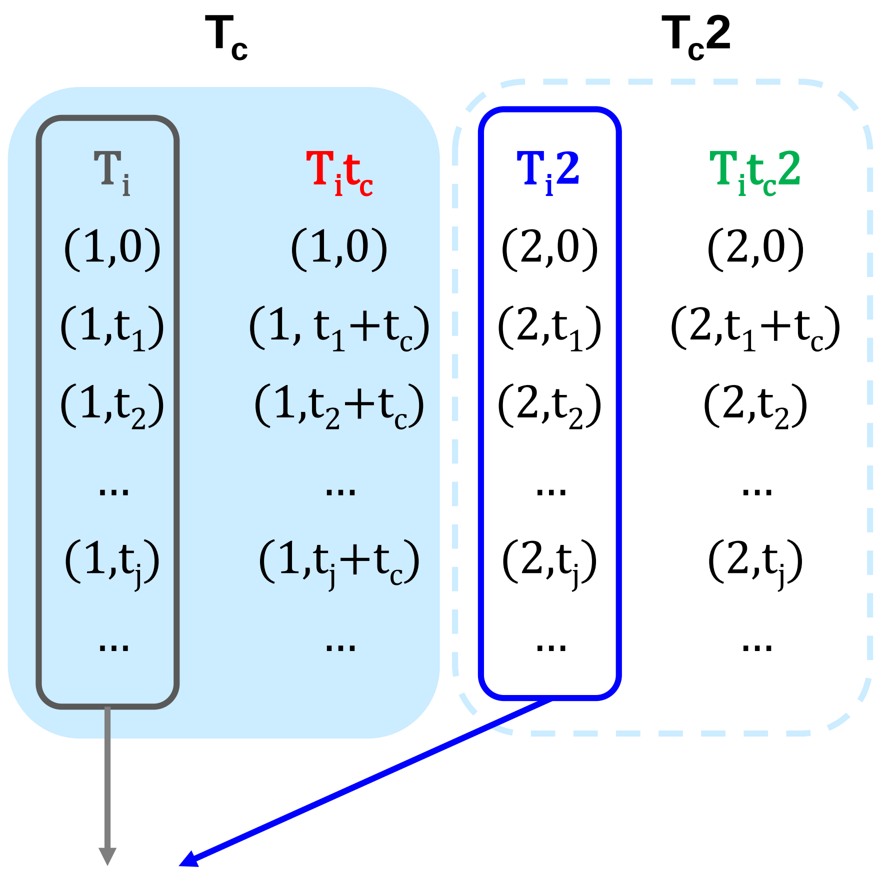
- Coset decomposition

$C2 = T_c + T_c2$

$T_c = T_i + T_i t_c$

T_i=integer

t_c=1/2,1/2,0



- Non-isomorphic *k*-subgroups: $H_1 = T_i \cup T_i2$

P2

Klassengleiche subgroups H < G

Non-isomorphic subgroups

Example: C2 (No. 5)

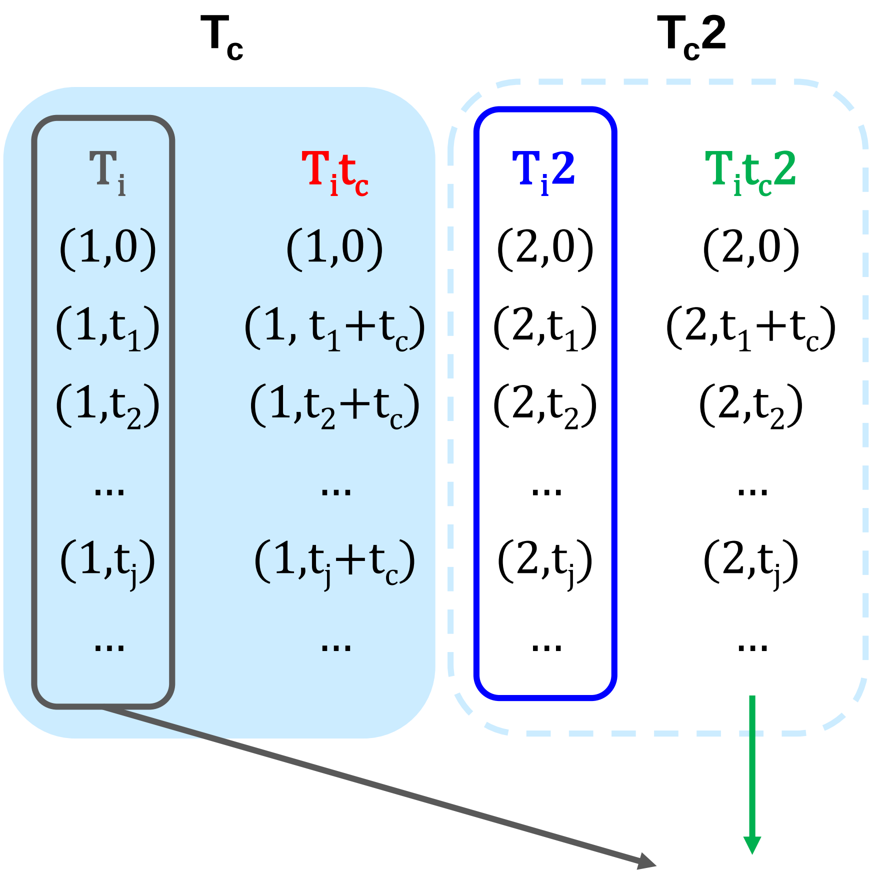
- Coset decomposition

  $C2 = T_c + T_c2$

  $T_c = T_i + T_it_c$

  T_i=integer

  t_c=1/2,1/2,0



- Non-isomorphic *k*-subgroups:

$H_1 = T_i \cup T_i2$ P2

$H_2 = T_i \cup T_it_c2$ $P2_1$

Maximal subgroups of space groups

International Tables for Crystallography, Vol. A1

ed. H. Wondratschek, U. Mueller

C^1_{4v} $P4mm$ No. 99 $P4mm$

I Maximal *translationengleiche* subgroups

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

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

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

$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a, b, 2c}$
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a, b, 2c}$

- **Series of maximal isomorphic subgroups**

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

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

[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 isomorphic subgroups

SERIES http://www.cryst.ehu.es/cryst/series.html

Series of Maximal Isomorphic Subgroups

Series of maximal isomorphic subgroups

For each space group you can obtain the list with its maximal isomorphic subgroups. The list contains the numbers and the symbols of the maximal subgroups as well as, the corresponding index and the transformation matrix that relates the basis of the group with that of the subgroup. It is worth to take account of:

- the program uses the default choice for the group setting.
- only maximal isomorphic subgroups with index less or equal to 27 are displayed (125, in the case of cubic groups)

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.

If you are interested in other publications related to Bilbao Crystallographic Server, click here

space group

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A [choose it] 87

NOTE: Other possibility is to define a maximum index for the parametric series of maximal isomorphic subgroups.

[Show series]

static databases

Maximal isomorphic subgroups

Series of maximal isomorphic subgroups of group *I4/m* (No. 87)

Note: Only series with an index less or equal to 27 are displayed

Series 1

Parametric form of the series 1 of maximal isomorphic subgroups of space group *I4/m* (No. 87)

Subgroup	Index	Transformation	Conditions
I4/m (87)	p	[1 0 0 0] [0 1 0 0] [0 0 p u]	prime p > 2 0 <= u < p

Static Databases

Number of conjugate subgroups: p conjugate subgroups

Click over **[show..]** to view a specific transformation for a given index

N	IT number	HM symbol	Index	Transformations
1	87	*I4/m*	3	show..
2	87	*I4/m*	5	show..
3	87	*I4/m*	7	show..
4	87	*I4/m*	11	show..
5	87	*I4/m*	13	show..
6	87	*I4/m*	17	show..
7	87	*I4/m*	19	show..
8	87	*I4/m*	23	show..

Maximal subgroups of space groups

MAXSUB http://www.cryst.ehu.es/cryst/maxsub.html

Maximal Subgroups of Space Groups

List with the maximal subgroups

For each one of the space group you can obtain the list with its maximal subgroups. This list contains the numbers and the symbols of these subgroups as well as the corresponding index and the transformation matrix that relates the basis of the group with that of the subgroup.

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.

If you are interested in other publications related to Bilbao Crystallographic Server, click here

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A — choose it — 139

Show WP Splittings? ☐

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

Show maximal subgroups

space group

Default settings of the space groups

static databases

Maximal subgroups of space groups

Maximal subgroups of group *I4/mmm* (No. 139)

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

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

N	IT number	HM symbol	Index	Transformations
1	69	*Fmmm*	2	show..
2	71	*Immm*	2	show..
3	87	*I4/m*	2	show..
4	97	*I422*	2	show..
5	107	*I4mm*	2	show..
6	119	*I-4m2*	2	show..
7	121	*I-42m*	2	show..
8	123	*P4/mmm*	2	show..
9	126	*P4/nnc*	2	show..
10	128	*P4/mnc*	2	show..
11	129	*P4/nmm*	2	show..
12	131	$P4_2/mmc$	2	show..
13	134	$P4_2/nnm$	2	show..
14	136	$P4_2/mnm$	2	show..
15	137	$P4_2/nmc$	2	show..
16	139	*I4/mmm*	3	show..
17	139	*I4/mmm*	5	show..
18	139	*I4/mmm*	7	show..
19	139	*I4/mmm*	9	show..

Maximal subgroups of space groups

Maximal subgroup(s) of type *Fmmm* (No. 69) of index 2

for Space Group *I4/mmm* (No. 139)

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

Conjugacy class a

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

(P, p)

[Click here for the Maximal Subgroups of group 69]

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

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

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

(P, p)

Exercise 2.26

The retrieval tool MAXSUB gives an access to the database on maximal subgroups of space groups as listed in *IT*A1. Determine the maximal subgroups of the group *P*4*mm* (No. 99) using the program MAXSUB.

Use the program SERIES to and determine the isomorphic subgroups of the group P4mm (No. 99).

GENERAL SUBGROUPS OF SPACE GROUPS

General subgroups H < G

- **Definition:**

  H is called a *general subgroup* of G, if $T_H < T_G$ and $P_H < P_G$ hold

  A general subgroup is neither translationengleiche or klassengleiche

- **Theorem of Hermann:**

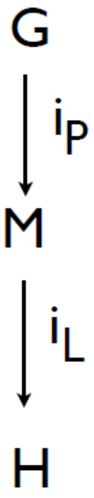
  A *maximal subgroup* of a space group is either *translationengleiche* or *klassengleiche*

  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

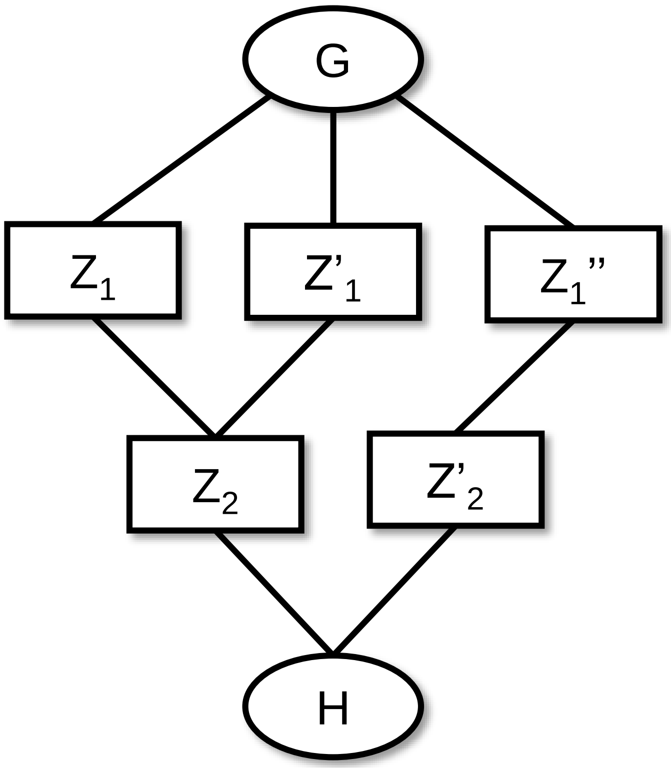
  H is a *k*-subgroup of M

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



General subgroups H < G

Chains of maximal subgroups



Group-subgroup pair

G > H : G, H, [i], (**P**, **p**)

Pairs: group - maximal subgroup

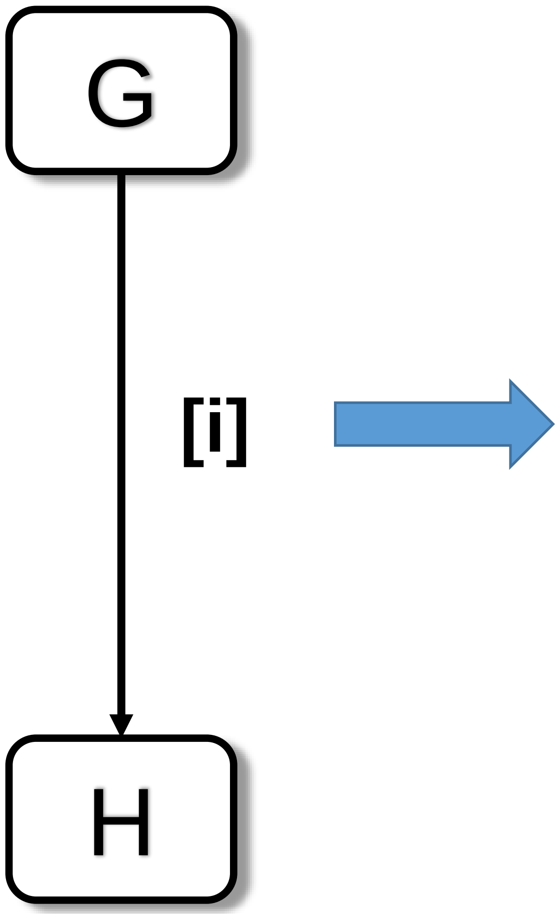
$Z_K > Z_{K+1}$, $(P, p)_K$

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

Exercise 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.

Domain-structure analysis



number of domain states

twins and antiphase domains

twinning operation

symmetry groups of the domain states

multiplicity and degeneracy

Domain-structure analysis

Homogeneous phase (parent)	G ⟶ H	Deformed phase Domain structure

Domains

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.

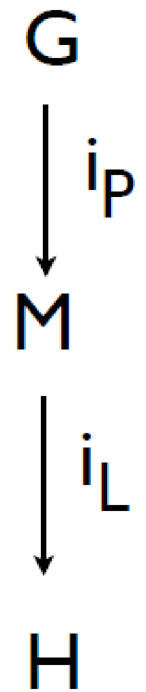
Domain-structure analysis

Hermann

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

M is a *t*-subgroup of G

H is a *k*-subgroup of M



The index is defined as $\mathbf{[i] = [i_P] \cdot [i_L]}$

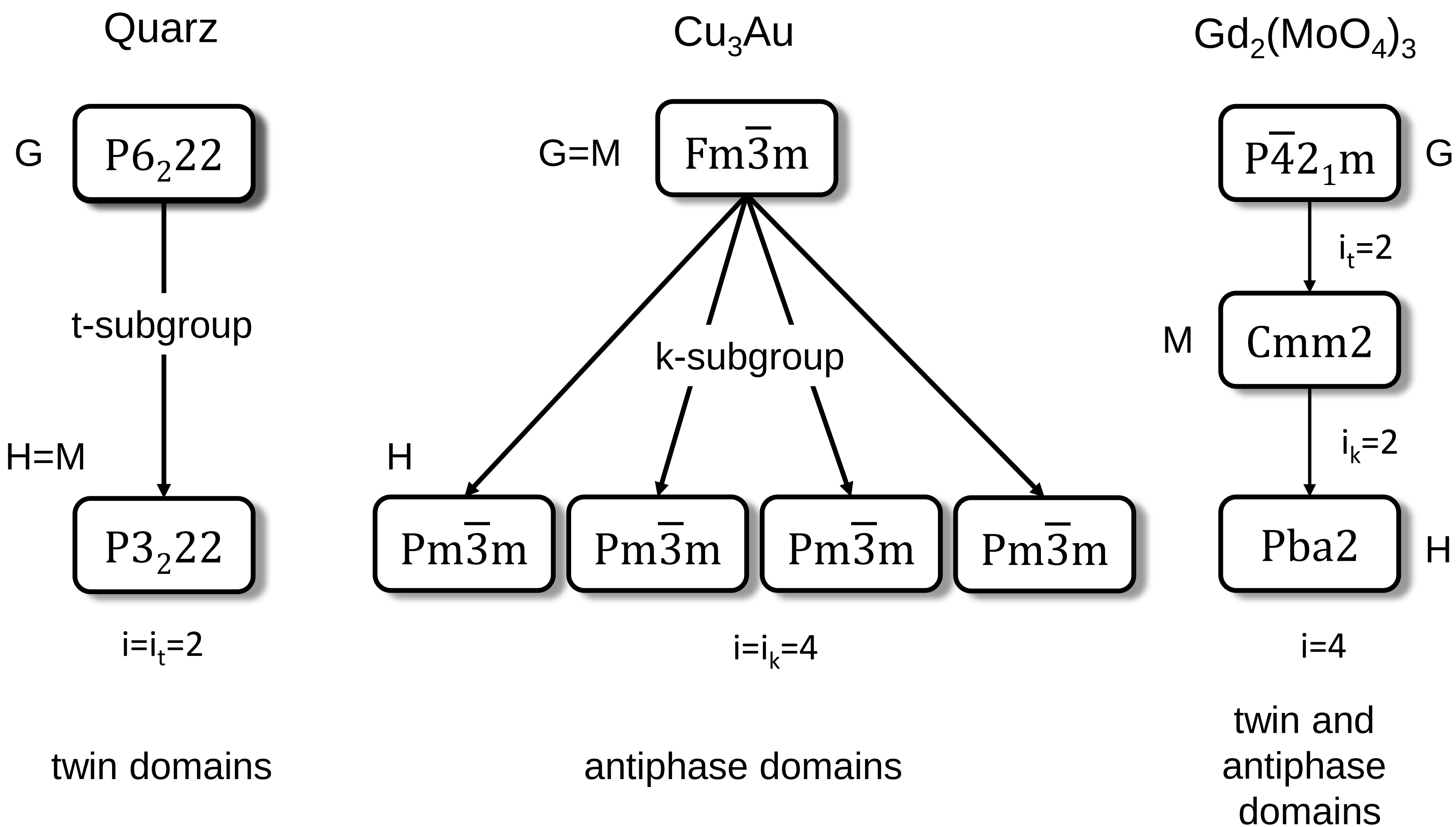
where

$i_P = P_G/P_H$ twins

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

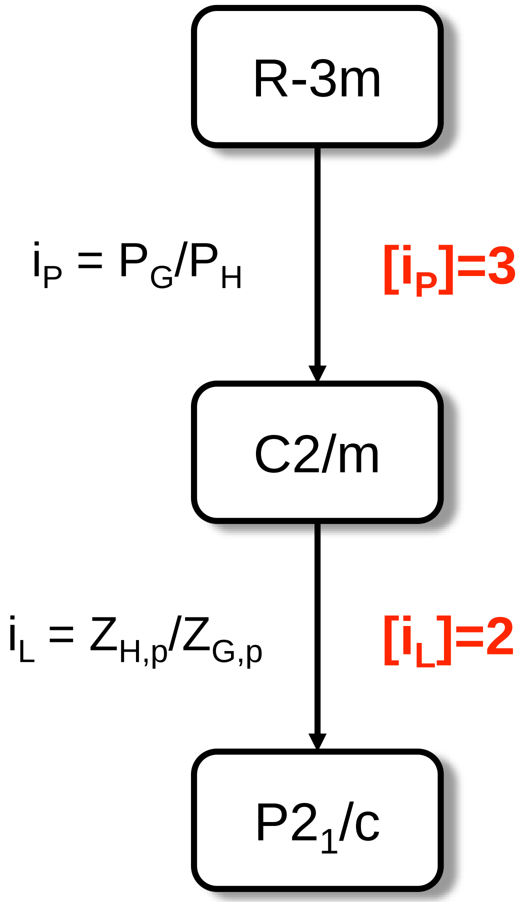
Classification of Domains

HERMANN http://www.cryst.ehu.es/cryst/hermann.html



Example: Lead vanadate Pb3(VO4)2

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



High-symmetry phase

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

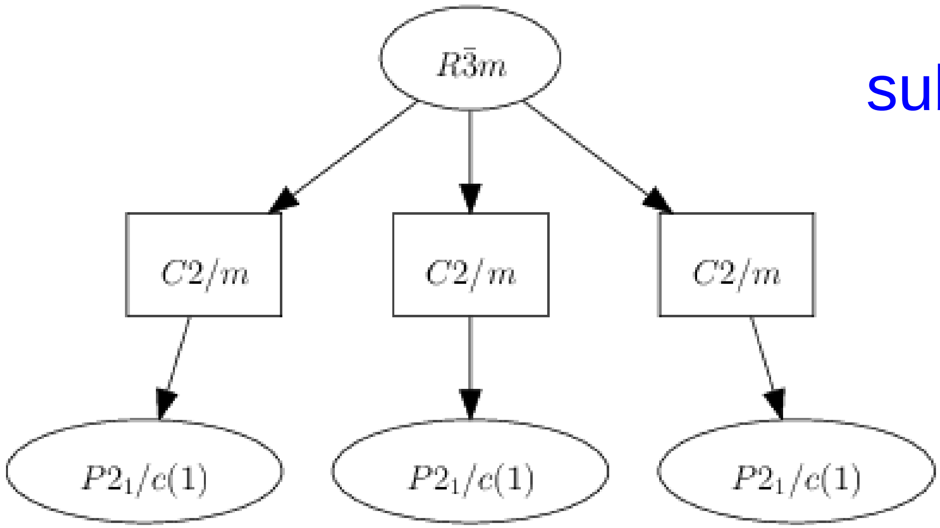
Low-symmetry phase

14
7.5075 6.0493 9.4814 90. 115.162 90.
7

Pb	1	2a	0.000000	0.000000	0.000000
Pb	2	4e	0.383500	0.581500	0.287900
PV	1	4e	0.207100	0.014300	0.399900
O	1	4e	0.287200	0.255900	0.015900
O	2	4e	0.259800	0.797900	0.021600
O	3	4e	0.319400	0.978400	0.282300
O	4	4e	0.033500	0.543100	0.209100

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

SUBGROUPGRAPH



Maximal subgroup graph

- number of domains= index [i] = $[i_P] \cdot [i_L]$=6
- number of ferroelastic domains: $i_P = 3$
- number of different subgroups $P2_1/c$: 3

Exercise 2.29

Domain-structure analysis

Determine the type and number of domain states in structural phase transitions specified by:

1. High-symmetry phase: P2/m
   Low-symmetry phase: P1 with small unit-cell deformation;
2. High-symmetry phase: P2/m
   Low-symmetry phase: P1 with duplication of the unit cell;
3. High-symmetry phase: P4mm
   Low-symmetry phase: P2 of index 8;
4. High-symmetry phase: $P4_2bc$
   Low-symmetry phase: $P2_1$ of index 8.

Exercise 2.30

Phase transitions in $BaTiO_3$

At high temperatures, $BaTiO_3$ has the cubic perovskite structure, space group *Pm*3*m*. Upon cooling it is distorted, adopting the space group *P*4*mm*. Will the crystals of the low-symmetry structure be twinned? If so, with how many kinds of domains?

What INPUT data should be introduced?

What program can be used?

Hint: The program INDEX could be useful

Exercise 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 *I*4/*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.

SUPERGROUPS OF SPACE GROUPS

Supergroups of space groups

Definitions

- 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

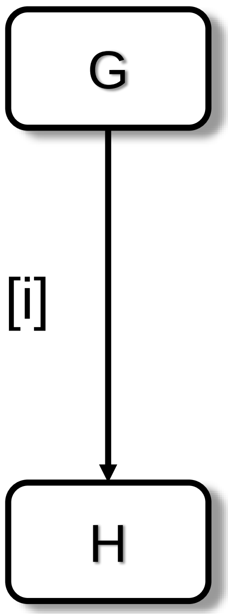
- translationengleiche (*t*-type)
- klassengleiche (*k*-type) → non-isomorphic / isomorphic

ITA1 data

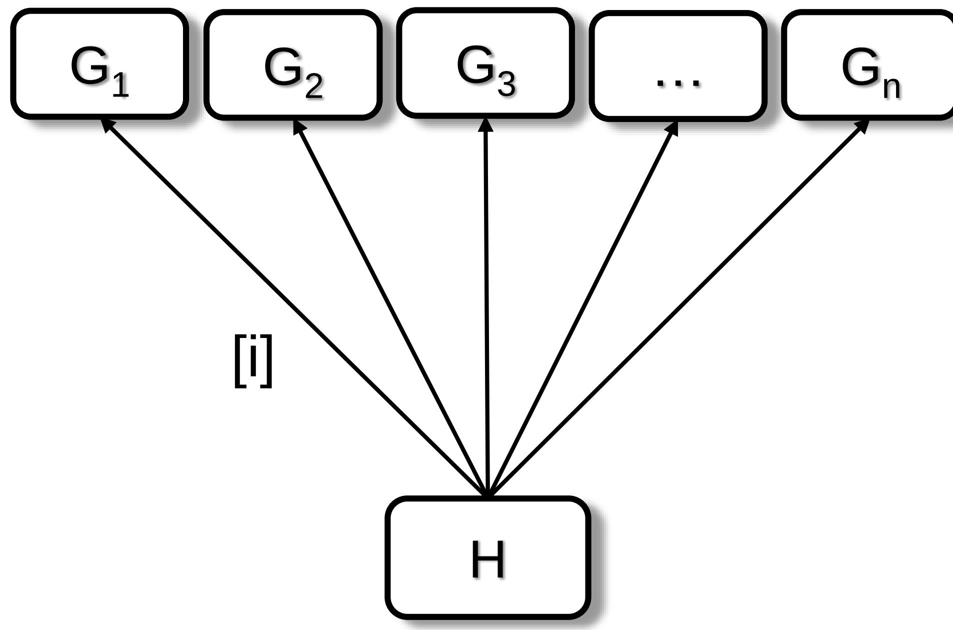
- minimal non-isomorphic *k*- and *t*-supergroups types

The Supergroup Problem

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



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

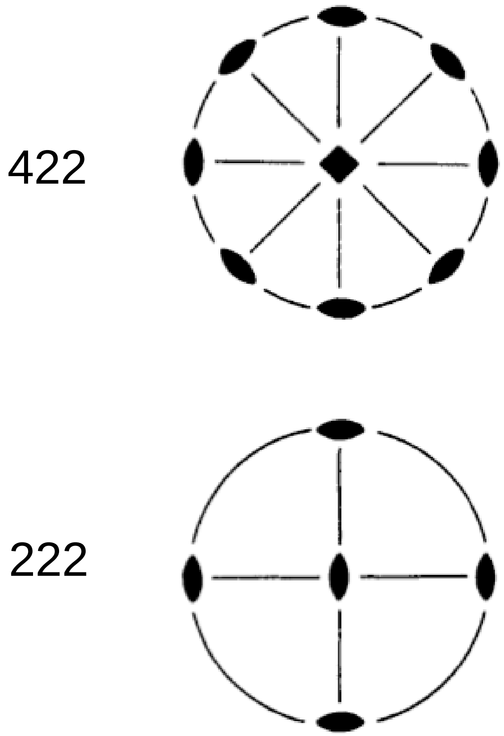


all G_k > H contain H as subgroup

$G_k = H + H g_2 + \ldots + Hg_{ik}$

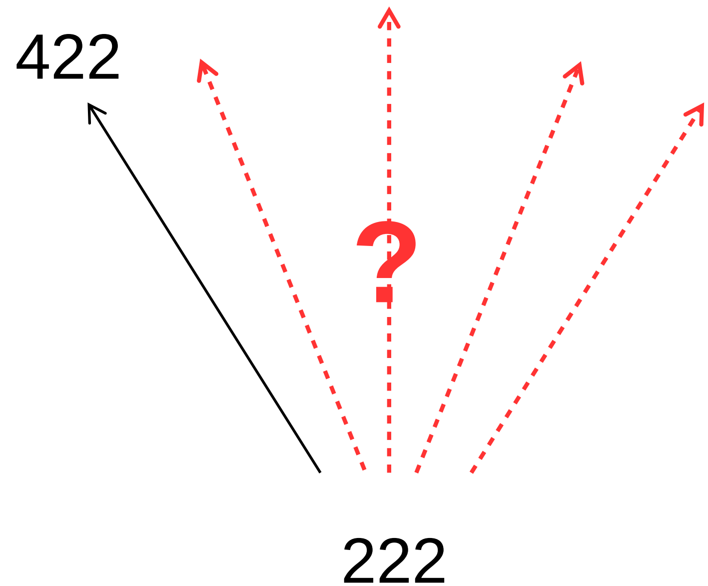
The Supergroup Problem

Group-subgroup
pair 422 > 222



How many are the
subgroups 222 of 422?

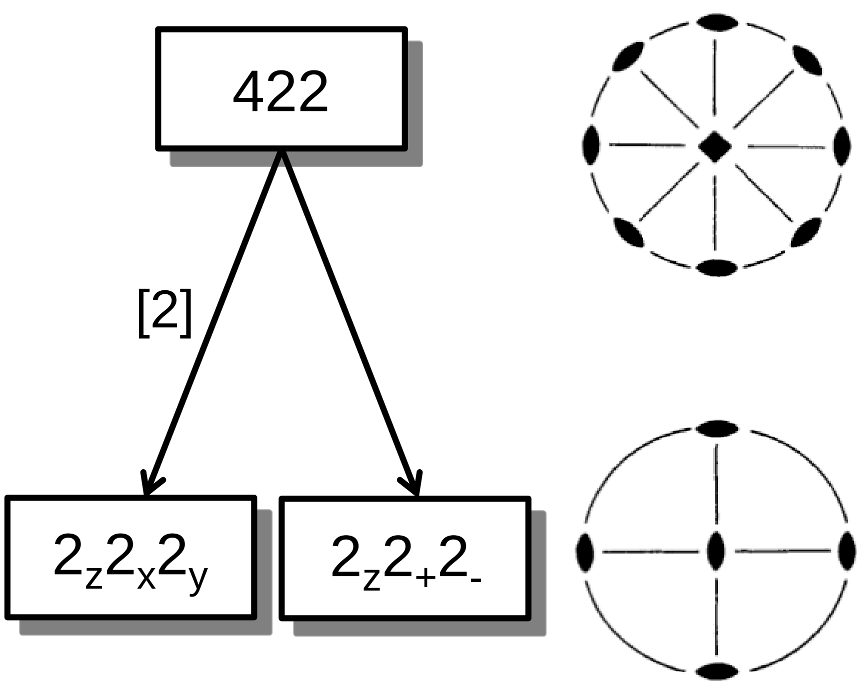
Supergroups 422
of the group 222



How many are the
supergroups 422 of 222?

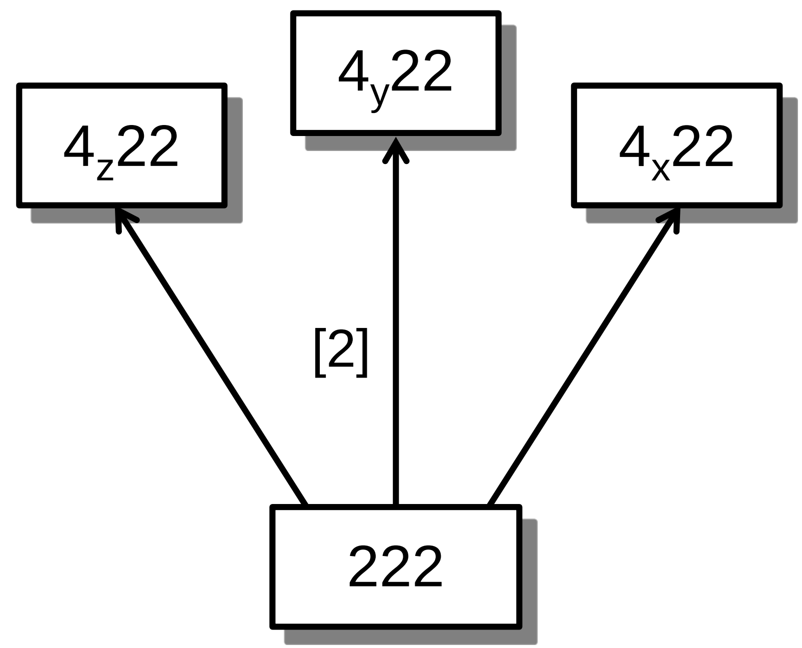
The Supergroup Problem

Group-subgroup pair 422 > 222



$$4_z22 = 2_z2_x2_y + 4_z(2_z2_x2_y)$$
$$4_z22 = 2_z2_+2_- + 4_z(2_z2_+2_-)$$

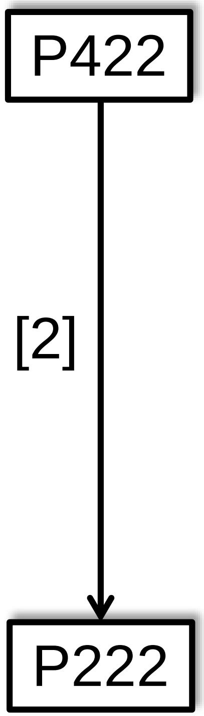
Supergroups 422 of the group 222

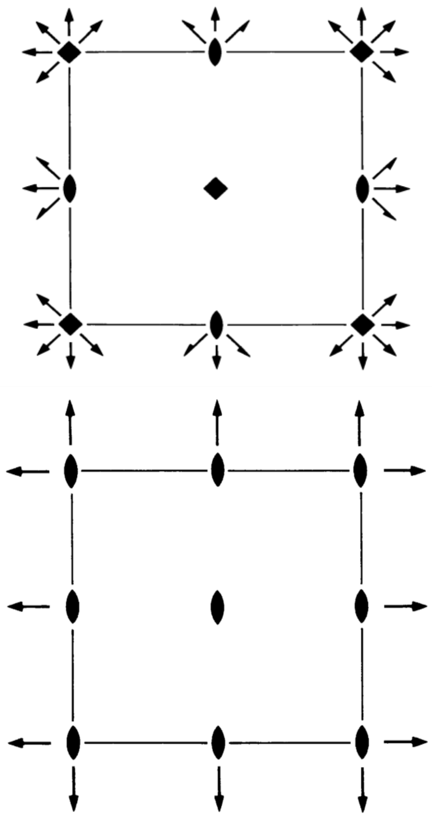


$$4_z22 = 222 + 4_z(222)$$
$$4_y22 = 222 + 4_y(222)$$
$$4_x22 = 222 + 4_x(222)$$

The Supergroup Problem

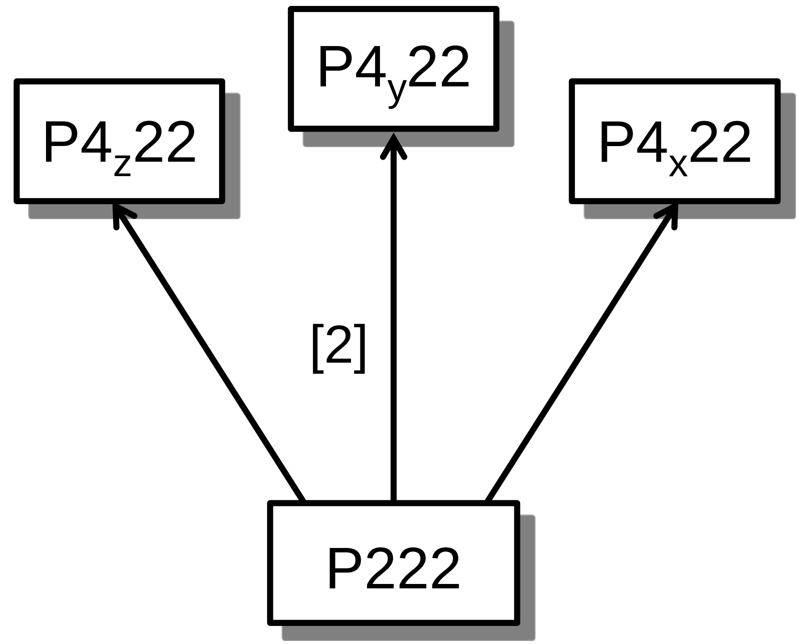
Group-subgroup pair P422 > P222





$$P422 = P222 + P222(4,0)$$

Supergroups 422 of the group 222

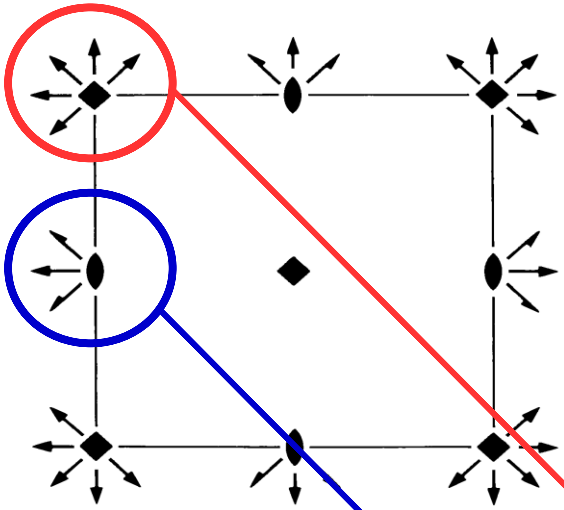


$$4_z22 = 222 + 4_z(222)$$
$$4_y22 = 222 + 4_y(222)$$
$$4_x22 = 222 + 4_x(222)$$

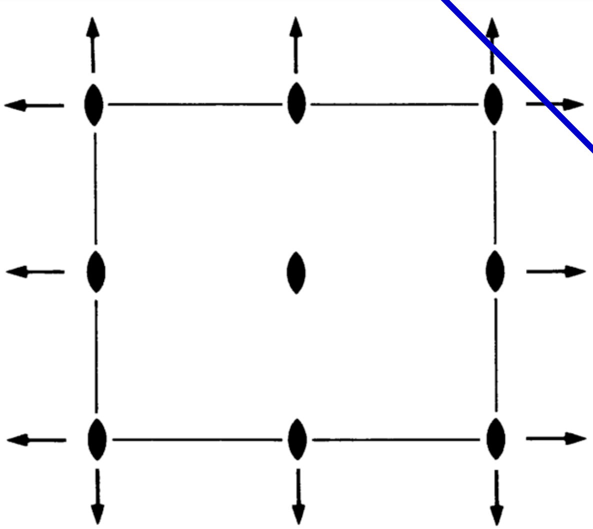
Are there more supergroups P422 of P222?

Example: Supergroups P422 of P222

P422



P222



H = P222
G = P422

P422 = P222 + (4|w)P222

	4	w	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	(1/2,0,0)	(-1/2,-1/2,0)	$(P422)'_1$
4_y	(1/2,0,0)	(-1/2,0,-1/2)	$(P422)'_2$
4_x	(0,1/2,0)	(0,-1/2,-1/2)	$(P422)'_3$

Minimal supergroups data

International Tables for Crystallography, Vol. A1
ed. H. Wondratschek, U. Mueller

*P*222 No. 16 *P*222 D_2^1

I Minimal *translationengleiche* supergroups

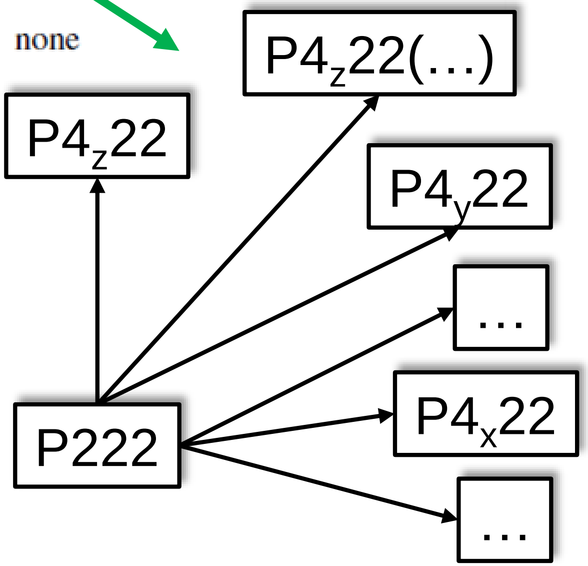
[2] *Pmmm* (47); [2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *P*422 (89); [2] $P4_222$ (93); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2m$ (111);
[3] *P*23 (195)

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

Minimal supergroups

MINSUP http://www.cryst.ehu.es/cryst/minsup.html

Minimal Supergroups of Space Groups

List with the minimal supergroups

For each one of the space group you can obtain the list with its minimal supergroups. This list contains the numbers and the symbols of these supergroups as well as the corresponding index and the transformation matrix that relates the basis of the group with that of the supergroup.

Also, there is a possibility to obtain all of the different supergroups of the same type.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it : 16

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

Show minimal supergroups

[Bilbao Crystallographic Server Main Menu]

Minimal supergroups

MINSUP http://www.cryst.ehu.es/cryst/minsup.html

Minimal Supergroups of Space Groups

List with the minimal supergroups

For each one of the space group you can obtain the list with its minimal supergroups. This list contains the numbers and the symbols of these supergroups as well as the corresponding index and the transformation

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it : 16

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

Show minimal supergroups

	N	HM symbol	ITA number	Index	Type	Subgroup data
○	1	*Pmmm*	47	2	t	transformation...
○	2	*Pnnn*	48	2	t	transformation...
○	3	*Pccm*	49	2	t	transformation...
○	4	*Pban*	50	2	t	transformation...
◉	5	*P*422	89	2	t	transformation...
○	6	$P4_222$	93	2	t	transformation...
○	7	*P*-42*c*	112	2	t	transformation...
○	8	*P*-42*m*	111	2	t	transformation...
○	9	*P*23	195	3	t	transformation...
○	10	*C*222	21	2	k	transformation...
○	11	*I*222	23	2	k	transformation...
○	12	*P*222	16	3	k	transformation...
○	13	*P*222	16	2	k	transformation...

show

rystallographic Server Main Menu]

Minimal supergroups

MINSUP http://www.cryst.ehu.es/cryst/minsup.html

Minimal Supergroups of Space Groups

List with the minimal supergroups

For each one of the space group you can obtain the list with its minimal supergroups. This list contains the numbers and the symbols of these supergroups as well as the corresponding index and the transformation

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it : 16

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

Show minimal supergroups

	N	HM symbol	ITA number	Index	Type	Subgroup data
○	1	*Pmmm*	47	2	t	transformation...
○	2	*Pnnn*	48	2	t	transformation...
○	3	*Pccm*	49	2	t	transformation...
○	4	*Pban*	50	2	t	transformation...
◉	5	*P*422	89	2	t	transformation...
○	6	$P4_222$	93	2	t	transformation...
○	7	*P*-42*c*	112	2	t	transformation...
○	8	*P*-42*m*	111	2	t	transformation...
○	9	*P*23	195	3	t	transformation...
○	10	*C*222	21	2	k	transformation...
○	11	*I*222	23	2	k	transformation...
○	12	*P*222	16	3	k	transformation...
○	13	*P*222	16	2	k	transformation...

show

rystallographic Server Main Menu]

N	Transformation matrix	Coset representatives	Wyckoff Splitting	More...
1	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	(x, y, z) (-y-1/2, x+1/2, z)	WP splitting	Full cosets
2	$\begin{pmatrix} 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	(x, y, z) (x, -z-1/2, y+1/2)	WP splitting	Full cosets
3	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	(x, y, z) (z-1/2, y, -x-1/2)	WP splitting	Full cosets
4	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	(x, y, z) (x, -z, y)	WP splitting	Full cosets
5	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	(x, y, z) (-y, x, z)	WP splitting	Full cosets
6	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	(x, y, z) (z, y, -x)	WP splitting	Full cosets

Supergroups of spce groups

SUPERGROUPS http://www.cryst.ehu.es/cryst/supergroups.html

Supergroups of a Given Type

Different supergroups ...

The program SUPERGROUPS will give you all of the different supergroups of the same type with specified index for a given group-supergroup pair.

As an input data you should give (or select) the numbers of the group and the supergroup, and the index.

The procedure for the calculation of all of the supergroups is based on the normalizers of the space groups. By default the Euclidean normalizers are used. If you want to use other normalizer, please select it from the list.

How to obtain a valid index ?

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	Subgroup normalizer
Euclidean normalizer	Euclidean normalizer

Find the Supergroups

Input:

- supergroup
- subgroup
- index
- option normalizers

Supergroups of spce groups

Output of the program **SUPERGROUPS**

Supergroups (of index 2) isomorphic to the group *P*422 (No. 89) of the group *P*222 (No. 16)

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

Normalizer of H in G

Normal subgroup

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

Normalizer of H in G, H < H

$N_{G(H)} = \{ g \in G$, if $g^{-1}Hg = H\}$

$G \geq N_{G(H)} \geq H$

What is the normalizer $N_{G(H)}$ if H G?

⇨ Number of subgroups $H_i < G$ in a conjugate class $n = [G:N_{G(H)}]$

Normalizer of H in G

Normal subgroup

Applications:

Equivalent point configurations

Wyckoff sets

Equivalent structure descriptions

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

Normalizer of H in G, H < H

$$N_{G(H)} = \{\, g \in G, \text{ if } g^{-1}Hg = H \}$$

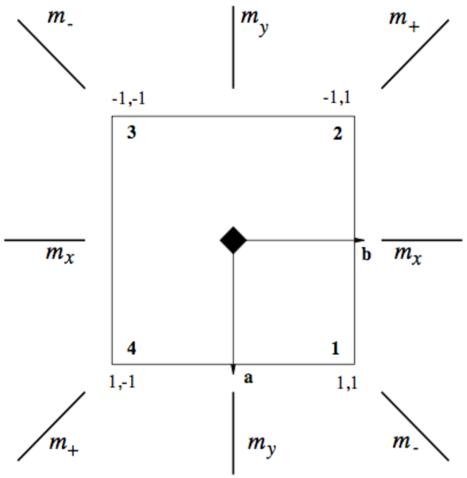
$$G \geq N_{G(H)} \geq H$$

What is the normalizer $N_{G(H)}$ if H G?

Number of subgroups H_i<G in a conjugate class $n=[G:N_{G(H)}]$

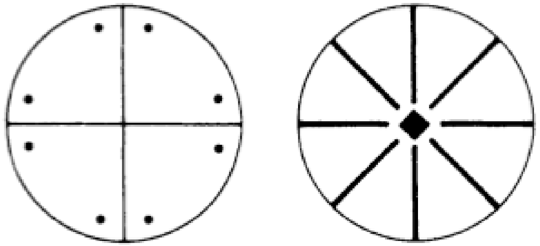
Exercise 2.10

Consider the group *4mm* and its subgroups of index 4. Determine their **normalizers** in *4mm*. Comment on the relation between the distribution of subgroups into conjugacy classes and their normalizers.



4mm	*1*	*2*	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
1	*1*	*2*	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
2	*2*	*1*	4^-	4^+	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
4^+	4^+	4^-	*2*	*1*	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
4^-	4^-	4^+	*1*	*2*	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	*1*	*2*	4^-	4^+
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	*2*	*1*	4^+	4^-
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^+	4^-	*1*	*2*
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^-	4^+	*2*	*1*

Hint: The stereographic projections could be rather helpful



Normalizers of space groups

Euclidean normalizer

The Euclidean normalizer $N_E(G)$ is the set of all isometries $h_i \in E$ mapping the space group G as a whole onto itself by conjugation:

$$N_E(G) = \{h_j \in E \mid h_j G h_j^{-1} = G\}$$

The Euclidean normalizer $N_E(G)$ is a supergroup of G, *i.e.* $G \leq N_E(G)$

Affine normalizer

The affine normalizer $N_A(G)$ is defined for each space group G as:

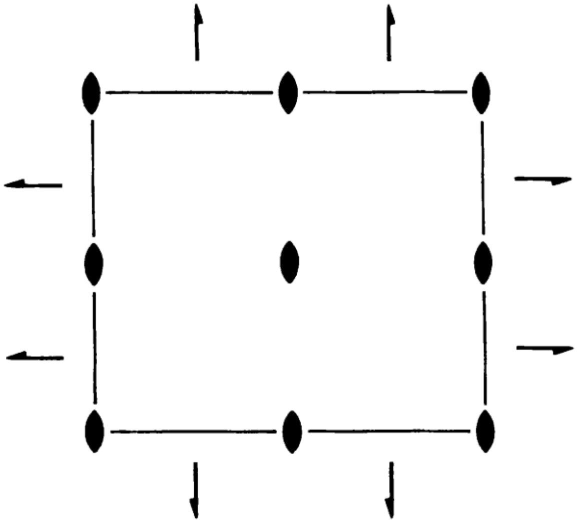
$$N_A(G) = \{h_j \in A \mid h_j G h_j^{-1} = G\}$$

It corresponds to the symmetry of the set of symmetry elements of G if their distances are neglected.

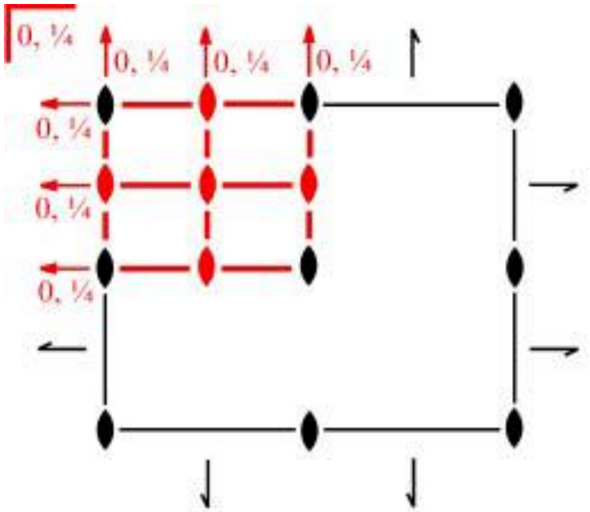
Normalizers of space groups

Normalizers of crystallographic groups may be considered as something like **the symmetry of symmetry**

Example: $P2_12_12$ (No. 18)



The symmetry elements of $P2_12_12$ (No.18)

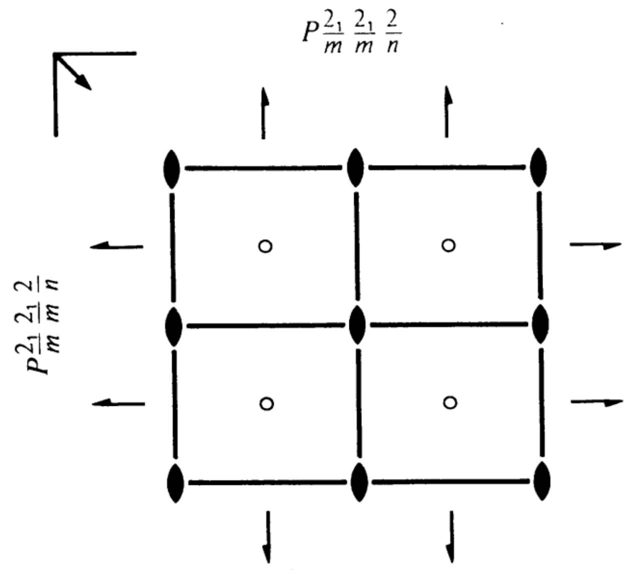


All symmetry elements are mapped onto another by isometries of the Euclidean normalizer which is also a space group: Pmmm (1/2**a**,1/2**b**,1/2**c**)

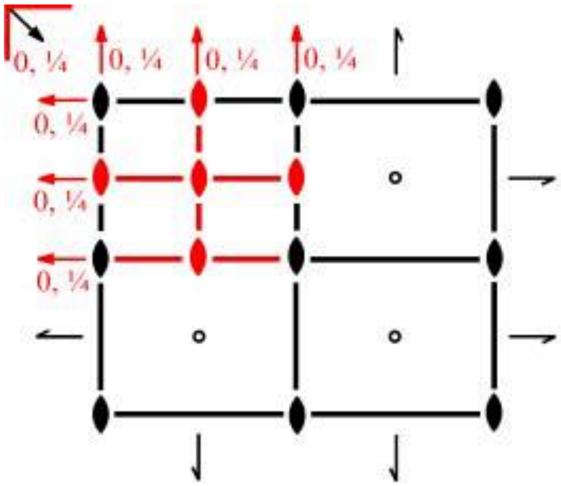
Normalizers of space groups

Normalizers of crystallographic groups may be considered as something like **the symmetry of symmetry**

Example: Pmmn (No. 59)



The symmetry elements of Pmmn (No. 59)

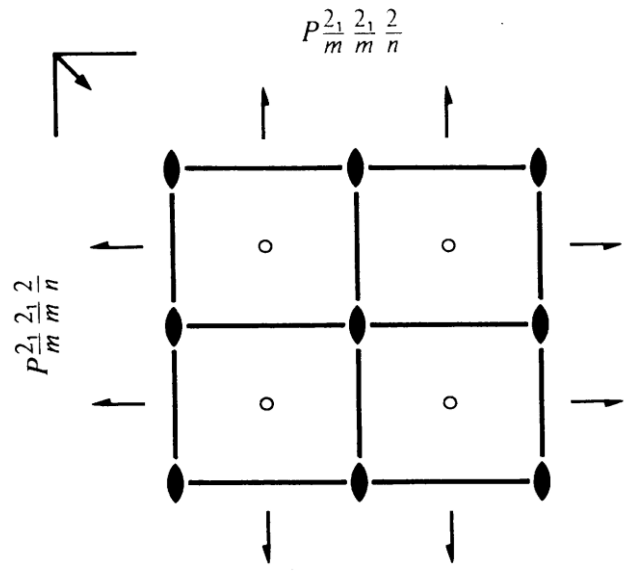


In the general case the Euclidean normalizer is orthorrombic: Pmmm (1/2**a**,1/2**b**,1/2**c**)

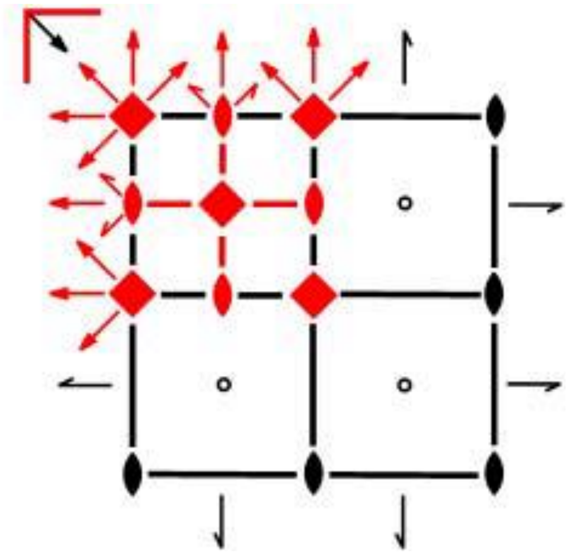
Normalizers of space groups

Normalizers of crystallographic groups may be considered as something like **the symmetry of symmetry**

Example: Pmmn (No. 59)



The symmetry elements of Pmmn (No. 59)



If the metric is specialized a=b, the Euclidean normalizer is tetragonal: P4/mmm (1/2**a**,1/2**b**,1/2**c**)

Normalizers of space groups

International Tables for Crystallography, Vol. A, Chapter 15

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*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$

Normalizers of space groups

NORMALIZER http://www.cryst.ehu.es/cryst/get_nor.html

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]**.

Part of the symmetry data shown by the program **NORMALIZER** is based on the data of normalizers of space groups given in:

Koch, E., Fischer, W. & Muller, U. (2016). *Normalizers of space groups and their use in crystallography. International Tables for Crystallography*, Vol.A, *Space-Group Symmetry*, edited by M. I. Aroyo, Chapter 3.5, 6th ed. Chichester: Willey.

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

Choose:

- Euclidean (general metric): ○
- Enhanced Euclidean (specialized metric): ◉
- Affine: ○

Hint: Further information on normalizers can be found under WYCKSETS

[Show]

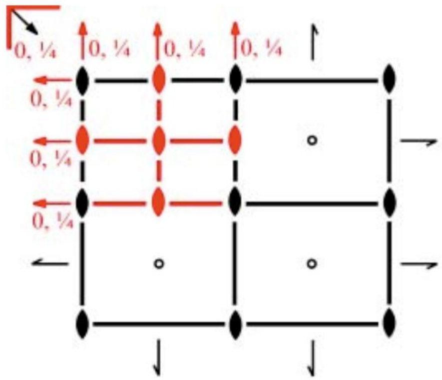
Enhanced Euclidean normalizer (specialized metrics)

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

[Show]

Example: Space group Pnnm (No. 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*.

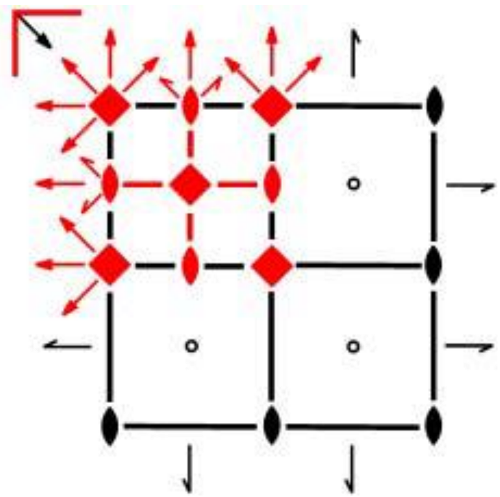
x+1/2,y,z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	*t* (1/2,0,0)
x,y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	*t* (0,1/2,0)
x,y,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	*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: Space group Pnnm (No. 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**) with respect to the Euclidean normalizer *Pmmm*.

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

WYCKSETS http://www.cryst.ehu.es/cryst/get_set.html

Wyckoff Sets

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

If you are interested in other publications related to Bilbao Crystallographic Server, click here

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

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

Hint: Other possibility is to check the full table of Wyckoff Sets for space groups.

[Show]

Symmetry-equivalent Wyckoff positions

Transformation of the Wyckoff Positions of *Pmmn* (059) [origin choice 2] under the coset representatives of its affine normalizer

Index: 16

No. #	Coset Representative		Transformed WP
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	a b c d e f g
2	x+1/2,y,z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	b a c d e f g
3	x,y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	b a c d e f g
4	x,y,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	a b d c e f g
5	x+1/2,y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	a b c d e f g

a ↔ b

Symmetry-equivalent Wyckoff positions

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 *Pmmn* (No. 59) [origin choice 2]

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

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

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Crystallographic Server

Exercise 2.36

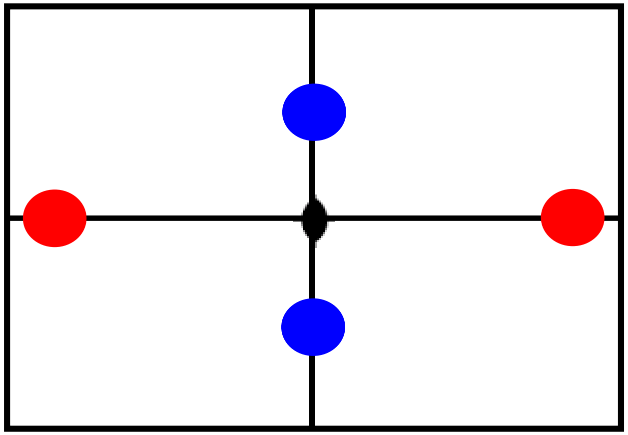
Using the computer tool NORMALIZER determine the Euclidean normalizer of the group *P*222 (No. 16) (general metric) and the Euclidean normalizers of enhanced symmetry for the cases of specialized metric of *P*222.

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.

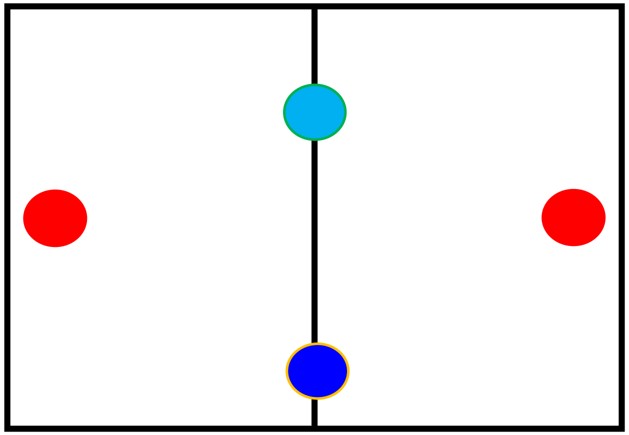
RELATIONS BETWEEN WYCKOFF POSITONS

Relation between Wyckoff positions

G = Pmm2 > H = Pm, [i] = 2



G = Pmm2



H = Pm

G = Pmm2				H = Pm		
2h	m..	(0,y,z)	→	2c	1	(x,y,z)
2f	.m.	(x,0,z)	→	1b	m	$(x_1,0,z_1)$
			→	1b	m	$(x_2,0,z_2)$

Splitting of Wyckoff positions

Example

Consider the group-subgroup pair *P4mm > Pmm2*

Determine the splitting schemes for WPs 1a,1b, 2c, 4d, 4e
[i]=2, ***a’=a, b’=b, c’=c***

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	$4mm$	$0,0,z$			

Group *Pmm2*

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

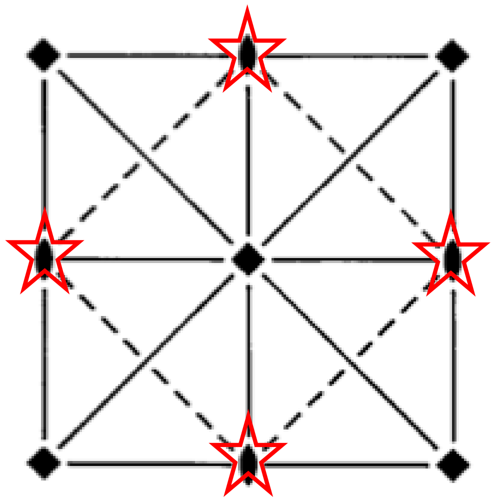
Positions

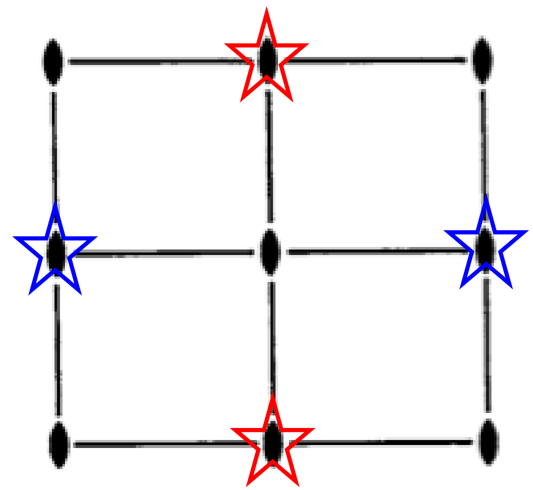
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
2	h	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
2	g	$m..$	$0,y,z$	$0,\bar{y},z$		
2	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$		
2	e	$.m.$	$x,0,z$	$\bar{x},0,z$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

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

Determine the splitting schemes for WPs 1a,1b, 2c, 4d, 4e
[i]=2, ***a'=a, b'=b, c'=c***





2c 2mm. 1/2 0 z
0 1/2 z

→ 1c mm2 1/2 0 z
→ 1b mm2 0 1/2 z'

Data on Relations between Wyckoff Positions

International Tables for Crystallography, Vol. A1

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

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$2c$	$4d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups									
[2] $P4$ (75)			$1a$	$1b$	$2c$	$4d$	$4d$	$4d$	$2\times4d$
[2] $Pmm2$ (25)			$1a$	$1d$	$1b;1c$	$4i$	$2e;2g$	$2f;2h$	$2\times4i$
[2] $Cmm2$ (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a$	$2b$	$4c$	$4d;4e$	$8f$	$8f$	$2\times8f$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $I4cm$ (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4a$	$4b$	$8c$	$16d$	$16d$	$2\times8c$	$2\times16d$
[2] $I4cm$ (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$4a$	$8c$	$16d$	$2\times8c$	$16d$	$2\times16d$
[2] $I4mm$ (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times2a$	$4b$	$8c$	$2\times8d$	$2\times8c$	$16e$	$2\times16e$
[2] $I4mm$ (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$2\times2a$	$8c$	$2\times8d$	$16e$	$2\times8c$	$2\times16e$
[2] $P4_2mc$ (105)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$2\times2c$	$8f$	$2\times4d$	$2\times4e$	$2\times8f$
[2] $P4cc$ (103)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$8d$	$8d$	$8d$	$2\times8d$
[2] $P4_2cm$ (101)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$2\times4d$	$8e$	$8e$	$2\times8e$

Wyckoff Positions Splitting

WYCKSPLIT http://www.cryst.ehu.es/cryst/wpsplit.html

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)			
Linear part:	1	1	0
	-1	1	0
	0	0	1
Origin shift:	0	0	0

Show group-subgroup data.

Input:

- space-group number
- subgroup number
- transformation matrix (**P**,**p**)

Wyckoff Positions Splitting

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)
☐ 4c (0, 1/2, 0)	4f (1/4, 1/4, 1/2)
☐ 2b (0, 0, 1/2)	4e (1/4, 1/4, 0)
☐ 2a (0, 0, 0)	2d (0, 0, 1/2)
	2c (1/2, 0, 1/2)
	2b (1/2, 0, 0)
	2a (0, 0, 0)

Choose of the Wyckoff positions

Wyckoff Positions Splitting

P4$_2$/mnm **(No. 136) > *Cmmm* (No. 65)**

	Wyckoff position(s)		
	Group	Subgroup	More...
	16k	16r 16r	Relations
	8j	8n 8o	Relations
	8i	8p 8q	Relations
	8h	8m 8m	Relations
	4g	4g 4j	Relations
	4f	4i 4h	Relations
	4e	4k 4l	Relations
8	4d	8m	Relations
9	4c	4e 4f	Relations
10	2b	2d 2b	Relations
11	2a	2a 2c	Relations

Wyckoff Positions Splitting

Wyckoff Positions Splitting

P4_2*/mnm* (No. 136) > *Cmmm* (No. 65)

Splitting of Wyckoff position 4f

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, x, 0)	(0, x, 0)	$4i_1$	(0, y_1, 0)
2	(-x, -x, 0)	(0, -x, 0)		(0, -y_1, 0)
3	(1+x, x, 0)	(1/2, 1/2+x, 0)		(1/2, 1/2+y_1, 0)
4	(1-x, -x, 0)	(1/2, 1/2-x, 0)		(1/2, 1/2-y_1, 0)
5	(1/2-x, 1/2+x, 1/2)	(-x, 1/2, 1/2)	$4h_1$	(1/2+x_2, 1/2, 1/2)
6	(1/2+x, 1/2-x, 1/2)	(x, 1/2, 1/2)		(1/2-x_2, 1/2, 1/2)
7	(1/2-x, -1/2+x, 1/2)	(1/2-x, 0, 1/2)		(x_2, 0, 1/2)
8	(1/2+x, -1/2-x, 1/2)	(1/2+x, 0, 1/2)		(-x_2, 0, 1/2)

Relation between coordinate triplets

Exercise 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.