IUCr Commission on Crystallographic Computing

Mieres 2011:

Crystallographic Computing School

Computing Commission

IUCr

Crystallographic Computing School

Oviedo, Spain

16 August - 22 August 2011

Bilbao Crystallographic Server

Symmetry algorithms and their implementation

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Euskal Herriko Unibertsitatea

Bilbao Crystallographic Server

http://www.cryst.ehu.es

FCT/ZTF

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

IT On! 2011
rkshop on the Online Edition of International Tables for Crystallography
31 August - 3 September 2011
Bilbao / SPAIN

Aperiodic Crystals for Beginners
Aperiodic Crystals for Beginners
IUCr Satellite Meeting
31 August - 1 September 2011
Alcalá de Henares / SPAIN

ons

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symme

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

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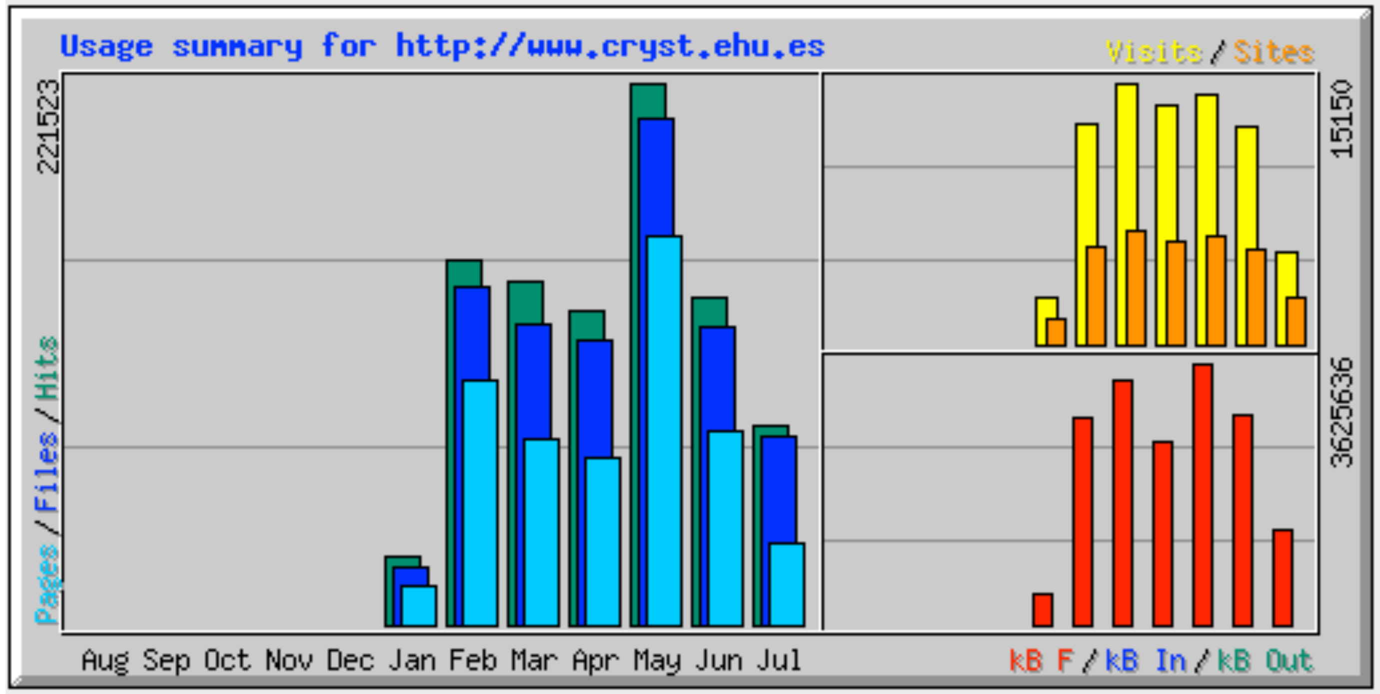
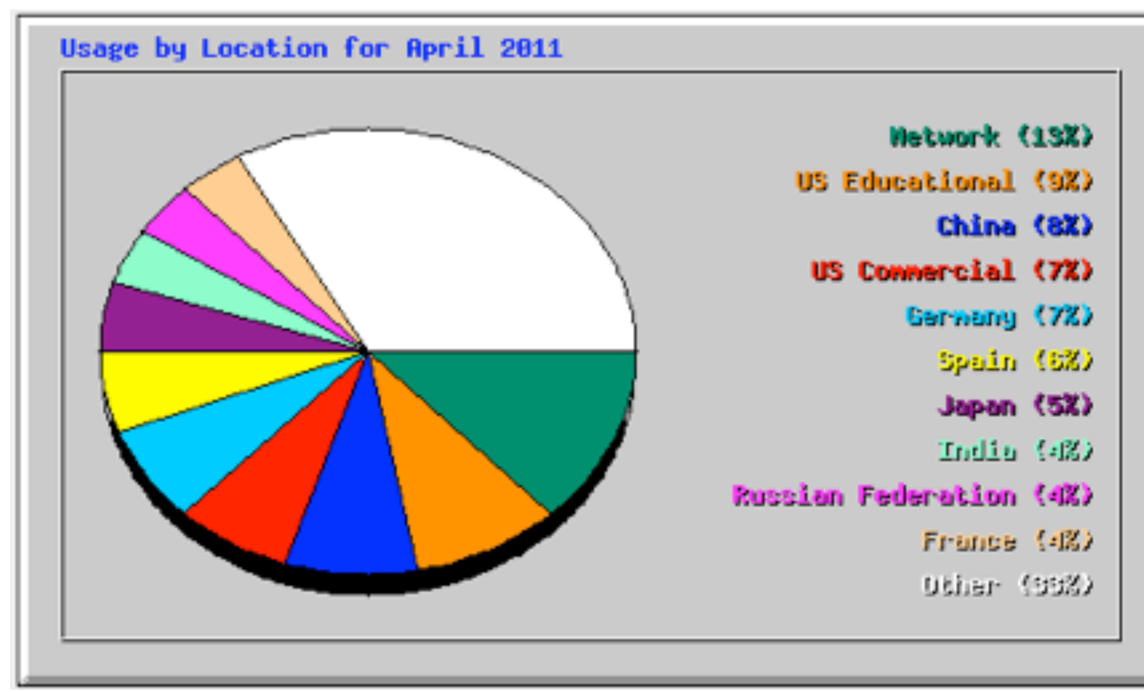
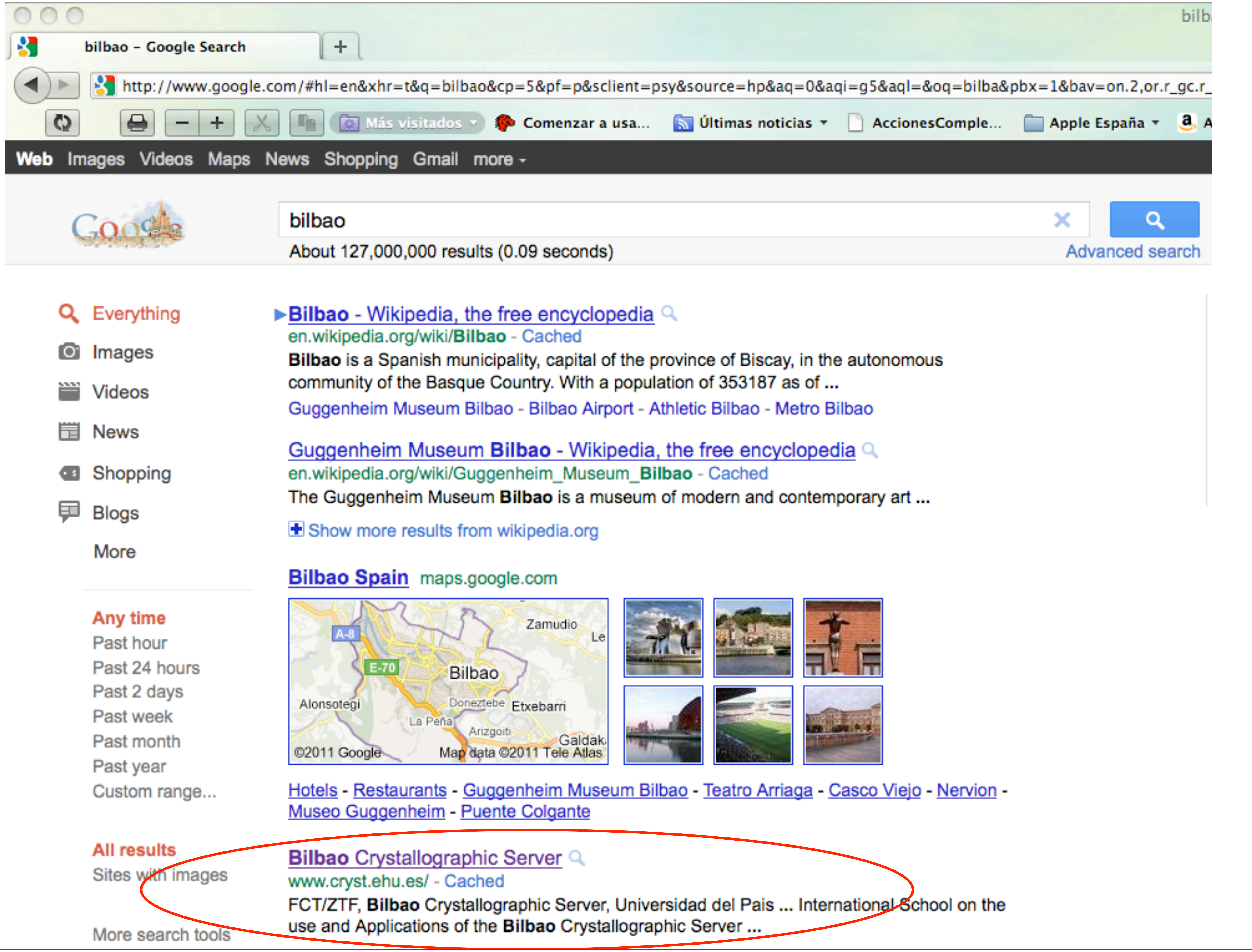
Bilbao Crystallographic Server usage statistics



Summary by Month

Month	Daily Avg				Monthly Totals							
	Hits	Files	Pages	Visits	Sites	kB F	kB In	kB Out	Visits	Pages	Files	Hits
Jul 2011	5836	5462	2357	383	2721	1294908	0	0	5372	33003	76469	81715
Jun 2011	4450	4045	2629	422	5445	2899230	0	0	12660	78872	121358	133527
May 2011	7145	6674	5111	464	6232	3625636	0	0	14413	158466	206921	221523
Apr 2011	4289	3864	2290	458	5996	2551734	0	0	13762	68724	115930	128685
Mar 2011	4517	3946	2461	488	6541	3376796	0	0	15150	76320	122339	140041
Feb 2011	5304	4914	3573	456	5699	2863785	0	0	12776	100064	137617	148524
Jan 2011	902	758	495	85	1515	409096	0	0	2656	15362	23517	27988
Totals						**17021181**	0	**0**	**76789**	**530811**	**804151**	**882003**




bilbao - Google Search
http://www.google.com/#hl=en&xhr=t&q=bilbao&cp=5&pf=p&sclient=psy&source=hp&aq=0&aqi=g5&aql=&oq=bilba&pbx=1&bav=on.2,or.r_gc.r_
Más visitados
Comenzar a usa...
Últimas noticias
AccionesComple...
Apple España
Web Images Videos Maps News Shopping Gmail more
bilbao
About 127,000,000 results (0.09 seconds)
Advanced search
Everything
Images
Videos
News
Shopping
Blogs
More
Any time
Past hour
Past 24 hours
Past 2 days
Past week
Past month
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Custom range...
All results
Sites with images
More search tools
Bilbao - Wikipedia, the free encyclopedia
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Bilbao is a Spanish municipality, capital of the province of Biscay, in the autonomous community of the Basque Country. With a population of 353187 as of ...
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Guggenheim Museum Bilbao - Wikipedia, the free encyclopedia
en.wikipedia.org/wiki/Guggenheim_Museum_Bilbao - Cached
The Guggenheim Museum Bilbao is a museum of modern and contemporary art ...
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E-70
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Alonsotegi
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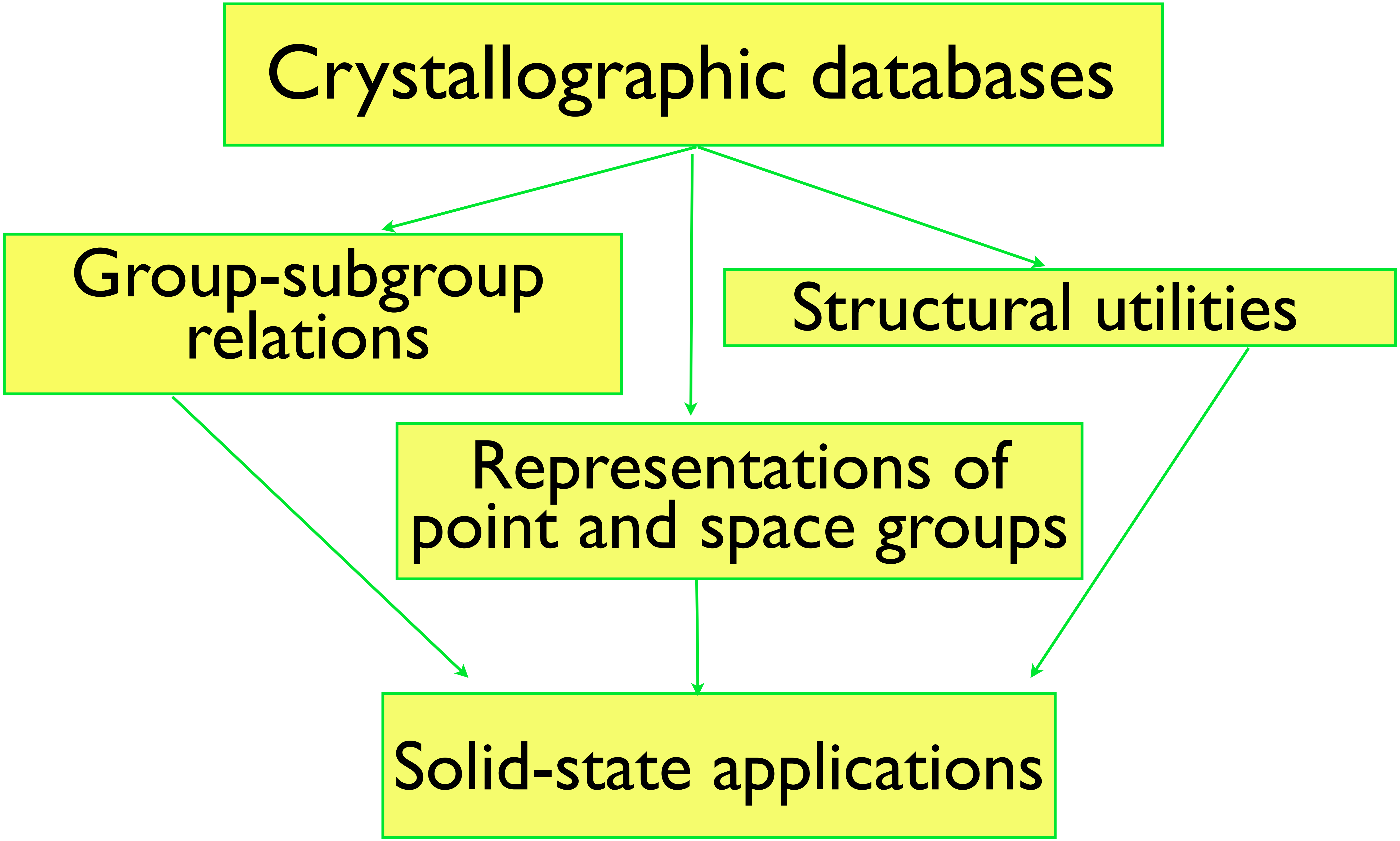
www.cryst.ehu.es/ - Cached
FCT/ZTF, Bilbao Crystallographic Server, Universidad del Pais ... International School on the use and Applications of the Bilbao Crystallographic Server ...

Bilbao Crystallographic Server



Symmetry Operations and Space Groups

Notation and Formalism

Crystal pattern: infinite, idealized crystal structure (without disorder, dislocations, impurities, etc.)

Symmetry operations: The isometries that map a crystal pattern onto itself are called crystallographic *symmetry operations*

Space group G: The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $H \lhd G$: The infinite set of all translations that are symmetry operations of the crystal pattern

Description of isometries

Matrix formalism

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$$

linear/matrix part

translation column part

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w}$$

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\,\boldsymbol{x} \quad \text{or} \quad \tilde{\boldsymbol{x}} = \{\boldsymbol{W} \mid \boldsymbol{w}\}\,\boldsymbol{x}$$

matrix-column pair

Seitz symbol

Matrix formalism: 4x4 matrices

$$\boldsymbol{x} \rightarrow \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right) ; \; \tilde{\boldsymbol{x}} \rightarrow \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right)$$

augmented matrices:

$$(\boldsymbol{W}, \boldsymbol{w}) \rightarrow \mathbb{W} = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

$\text{point } X \longrightarrow \text{point } \tilde{X} :$

$$\tilde{\mathbb{x}} = \mathbb{W}\,\mathbb{x} \qquad \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right) = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right)$$

Presentation of Space groups

General position of G

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

Factor group G/T_G

isomorphic to the point group P_G of G

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

Decomposition $G:(T_{int})_G$

CRYSTALLOGRAPHIC DATABASES

Crystallographic Databases

International Tables for Crystallography

Space-group Data

International Tables for Crystallography

Volume A: Space-group symmetry

generators
Wyckoff positions
Wyckoff sets
normalizers

Volume A1: Symmetry Relations between space groups

maximal subgroups of index 2,3 and 4
series of isomorphic subgroups

Retrieval tools

ITA space group *P4mm*

GENPOS

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				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

WYCKPOS

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2]$P411$ ($P4$, 75) 1; 2; 3; 4
[2]$P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2]$P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2]$P4_2mc$($\mathbf{c}'=2\mathbf{c}$)(105); [2]$P4cc$($\mathbf{c}'=2\mathbf{c}$)(103); [2]$P4_2cm$($\mathbf{c}'=2\mathbf{c}$)(101); [2]$C4md$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$)($P4bm$, 100); [2]$F4mc$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$)($I4cm$, 108); [2]$F4mm$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$)($I4mm$, 107)

MAXSUB

Maximal isomorphic subgroups of lowest index

IIc [2]$P4mm$($\mathbf{c}'=2\mathbf{c}$)(99); [2]$C4mm$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$)($P4mm$, 99)

SERIES

Minimal non-isomorphic supergroups

I [2]$P4/mmm$(123); [2]$P4/nmm$(129)

II [2]$I4mm$(107)

MINSUP

CIF DATABASE

CIF Dictionary for the
Bilbao Crystallographic Server
1994 -1996

CIF_SYM Dictionary
IUCr
1998 - 2001

XVII IUCr congress, Seattle 1996
Acta Cryst A52 (1996) Suppl., C-577

International Tables, Volume G
Definition and exchange of
crystallographic data, 2005

CIF workshop

MSWK.CF.13 CIF DATA FOR INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY; VOL: A1 [SUBGROUP DATA] (TO APPEAR) AND VOL: A. Wondratschek, H.; Institut fuer Kristallographie, Universitaet, D-76128 Karlsruhe, Germany; Madariaga, G. and Aroyo, M. I., Dpto. de Fisica de la Materia Condensada, Facultad de Ciencias, Universidad del Pais Vasco, Apdo. 644, 48080 Bilbao, Spain

space-group information
Wyckoff positions
symmetry operations

CIF DATABASE on the Bilbao Crystallographic Server

DATA for SPACE GROUPS

Headline
Generators
General Position
Maximal Subgroups
- HM symbols
- Index
- Transformation matrix

Minimal supergroups
- HM symbols
- Index

Series of maximal subgroups (parametric form)

Subperiodic groups: rod and layer groups

International Tables for Crystallography, Volume E: Subperiodic groups

generators
general postitions
Wyckoff positions

Data on maximal subgroups (Aroyo & Wondratschek)

maximal subgroups of index 2,3 and 4
series of isomorphic subgroups

Retrieval tools

CIF DATABASE on the Bilbao Crystallographic Server

DATA for SUBPERIODIC GROUPS

Headline
Generators
General Position
Special Wyckoff positions
Maximal Subgroups
- HM symbols
- Index
- Transformation matrix

Minimal supergroups
- HM symbols
- Index

Series of maximal subgroups (parametric form)

XML DATABASE on the Bilbao Crystallographic Server

XML dictionary ⟷ CIF dictionary

DATA for SPACE and SUBPERIODIC GROUPS

Headline
Generators
General Position
Special Wyckoff positions (multiplicity, Wyckoff letter, site symmetry, representatives)
Maximal Subgroups
- HM symbols
- Index
- Transformation matrix
- Wyckoff posicion splittings

Minimal supergroups
- HM symbols
- Index

Series of maximal subgroups (parametric form)

Representation Database

Representations of space and point groups

wave-vector data

Brillouin zones
representation domains
parameter ranges

POINT

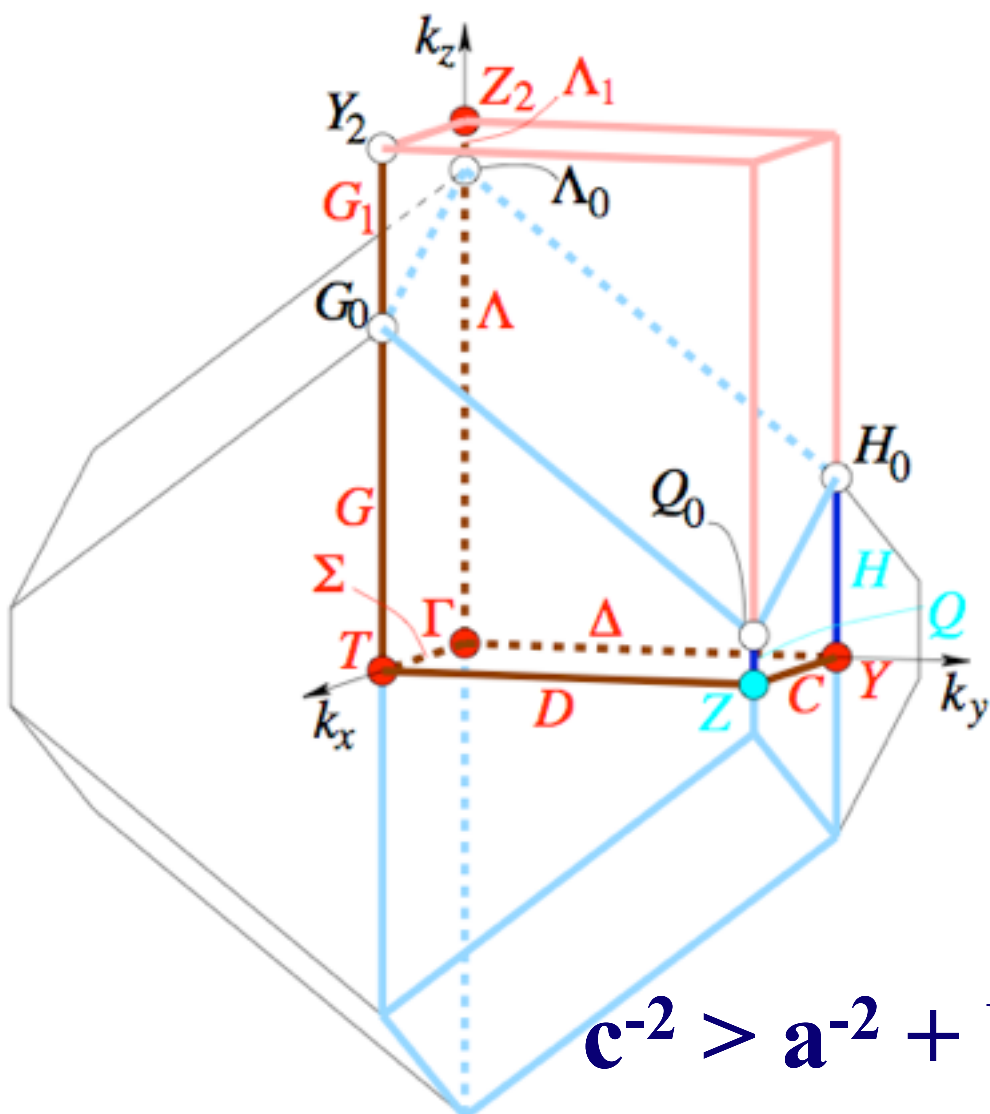
character tables
multiplication tables
symmetrized products

Databases

Retrieval tools

Brillouin Zone Database
Crystallographic Approach

Reciprocal space groups		Symmorphic space groups
Brillouin zones	↔	IT unit cells
Representation domain		Asymmetric unit
Wave-vector symmetry		Wyckoff positions



$c^{-2} > a^{-2} + b^{-2}$

The k-vector Types of Group 22 [*F*222]

k-vector description			Wyckoff Position			ITA description
CDML*		Conventional-ITA	ITA			Coordinates
Label	Primitive					
GM	0,0,0	0,0,0	a	2	222	0,0,0
T	1,1/2,1/2	0,1,1	b	2	222	0,1/2,1/2
T~T$_2$			b	2	222	1/2,0,0
Z	1/2,1/2,0	0,0,1	c	2	222	0,0,1/2
Y	1/2,0,1/2	0,1,0	d	2	222	0,1/2,0
Y~Y$_2$			d	2	222	1/2,0,1/2
SM	0,u,u ex	2u,0,0	e	4	2..	x,0,0 : 0 < x <= sm$_0$
U	1,1/2+u,1/2+u ex	2u,1,1	e	4	2..	x,1/2,1/2 : 0 < x < u$_0$
U~SM$_1$=[SM$_0$ T$_2$]			e	4	2..	x,0,0 : 1/2-u$_0$=sm$_0$ < x < 1/2
SM+SM$_1$=[GM T$_2$]			e	4	2..	x,0,0 : 0 < x < 1/2
A	1/2,1/2+u,u ex	2u,0,1	f	4	2..	x,0,1/2 : 0 < x <= a$_0$
C	1/2,u,1/2+u ex	2u,1,0	f	4	2..	x,1/2,0 : 0 < x < c$_0$

GROUP-SUBGROUP RELATIONS OF SPACE GROUPS

Bilbao Crystallographic Server — Group-subgroup relations of space groups

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: Some basic definitions (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

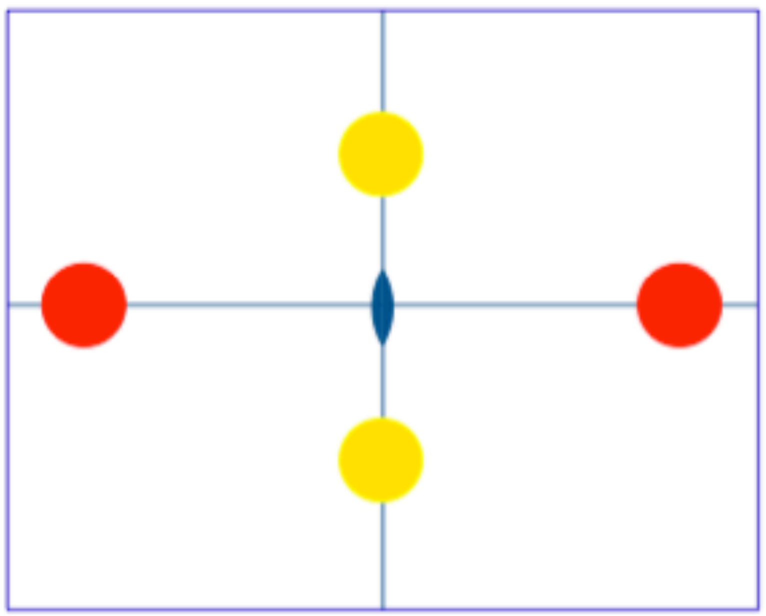
Index of the subgroup H in G: $[i]=|G|/|H|$
(order of G)/(order of H)

Maximal subgroup H of G
NO subgroup Z exists such that:
$H < Z < G$

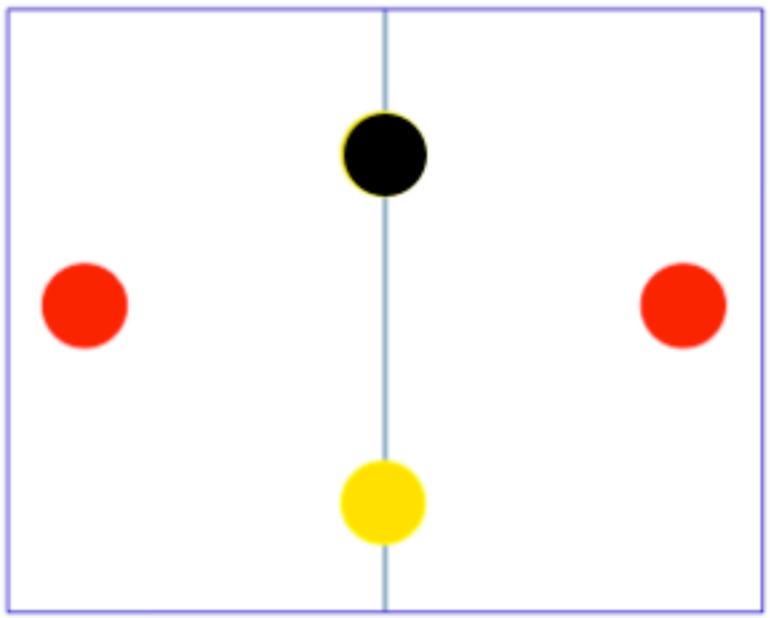
Problem: Subgroups of Space Groups

1. Subgroups of the same type

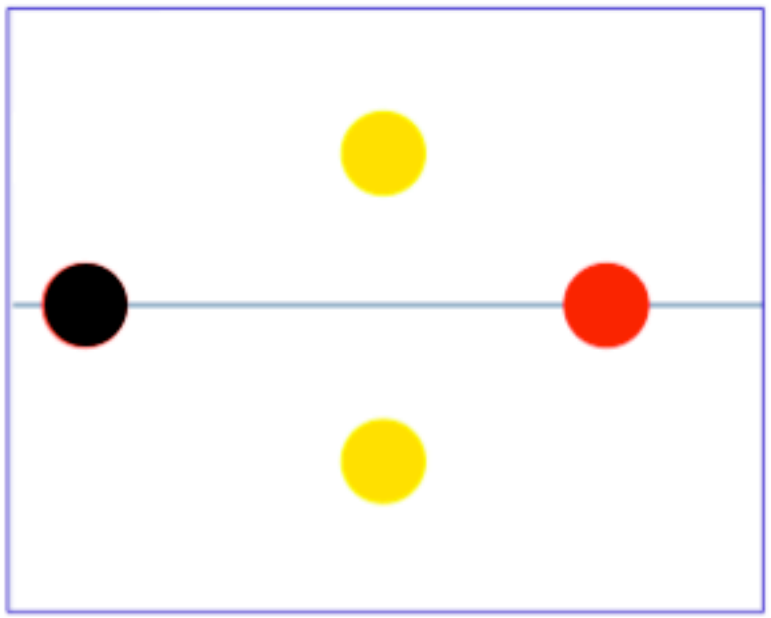
$$\mathcal{G} = \mathrm{P}mm2 > \mathcal{H} = \mathrm{P}m, \;\; [i] = 2$$



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



$S_1,\ \mathcal{H} = \mathrm{P}1m1$



$S_2,\ \mathcal{H} = \mathrm{P}m11$

$\mathcal{H} = \mathrm{P}m$, No. 6 en IT$A$

$\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H} \Leftrightarrow$ different low-symmetry structures

Conjugate subgroups

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

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

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

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

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

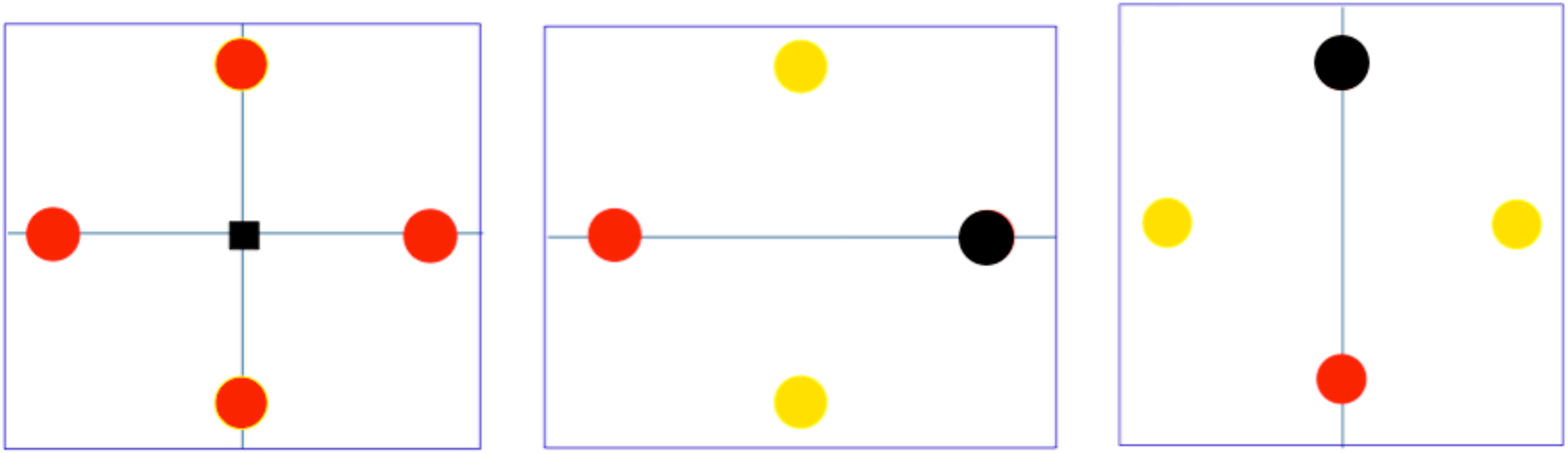
Normal subgroup

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

Problem: Subgroups of Space Groups

2. Conjugated subgroups

$$\mathcal{G} = \mathrm{P}4mm > \mathcal{H} = \mathrm{P}m, \ [i] = 4$$



$S_0, \ \mathcal{G} = \mathrm{P}4mm$ $S', \ \mathcal{H} = \mathrm{P}m11$ $S'', \ \mathcal{H} = \mathrm{P}1m1$

$\mathcal{H} = \mathrm{P}m$, No. 6 en ITA

$\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H}$ of the same class $\Leftrightarrow$ domain structure

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

Example ITA1: Space group *P4mm*

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

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

General position

GENPOS

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

MAXSUB

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

SERIES

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$ p prime no conjugate subgroups	$\mathbf{a,b,}p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4mm$ (99)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ prime $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

MINSUP

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

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

I Maximal *translationengleiche* subgroups

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

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

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

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

Remarks

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

{ braces for conjugate subgroups

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

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

DATA ITA1: Maximal Subgroups

Transformation matrix: (P,p)

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

↓

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

↓ (P,p)

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

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

Data on **maximal** subgroups of space groups in *The Bilbao Crystallographic Server*

Example: Space group *P4mm*

Maximal subgroup(s) of type 35 (*Cmm*2) of index 2

for Space Group 99 (*P4mm*)

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

Maximal subgroup(s) of type 107 (*I4mm*) of index 2

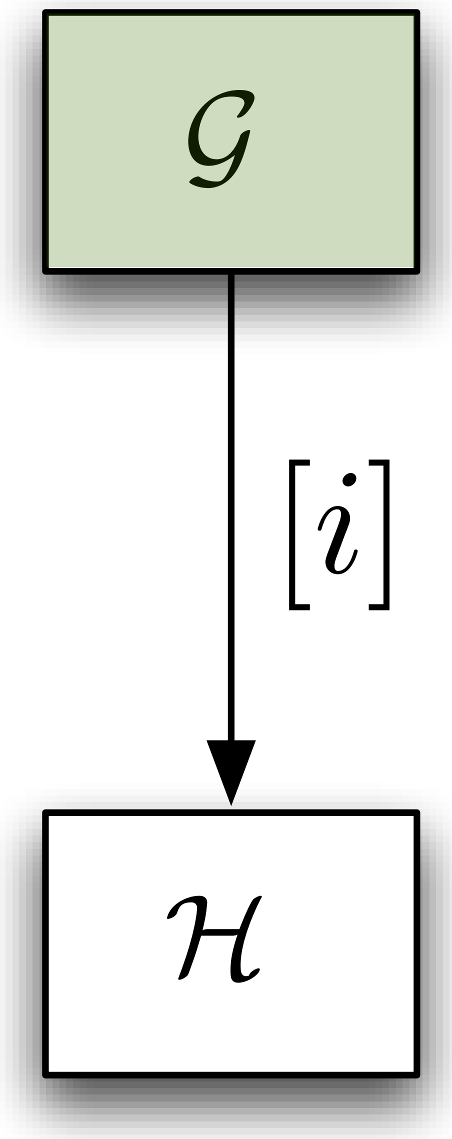
Conjugacy class a

Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1 & 1 & 0 & 1/2 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	ChBasis

Conjugacy class b

Subgroup(s)	Transformation Matrix	More...
group No 2	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	ChBasis

Group-Subgroup Relations



Applications

- ◇ Possible low-symmetry structures
- ◇ Domain structure
- ◇ Prediction of new structures
- ◇ Symmetry modes

Aim

$$\mathcal{G} > \mathcal{H},\ [i]$$

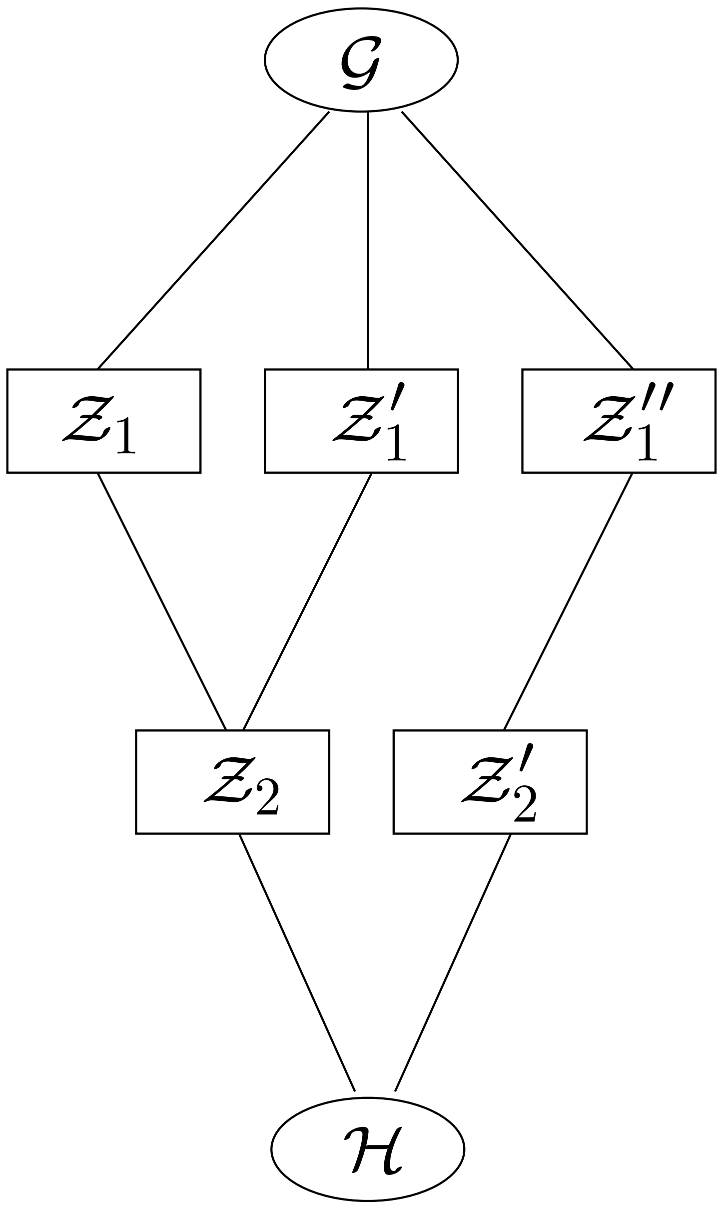
chains of maximal subgroups

$$\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H}$$

classification of $\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H}$

General idea

Any pair of space groups G>H of any index can be related via chains of maximal subgroups



Group-subgroup pair

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

Pairs: group - maximal subgroup

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

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

Graph of maximal subgroups

Subgroups calculation: SUBGROUPGRAPH

Chains of maximal subgroups

$$(\mathrm{P},\mathbf{p})_m \Rightarrow \mathcal{H}_m$$

↓

Direct comparison of the $\mathcal{H}_m$

$$\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H}$$

↓

$$\boldsymbol{\mathcal{G}} = \boldsymbol{\mathcal{H}} + \sum_{l=2}^{[i]} g_l \boldsymbol{\mathcal{H}}$$

Conjugation $\boldsymbol{\mathcal{H}_k}$ with g_l

Comparison of the subgroup elements

$\mathcal{G} > \mathcal{H},\ [i]$

Classes of $\mathcal{H}_k \overset{[i]}{\sim} \mathcal{H}$

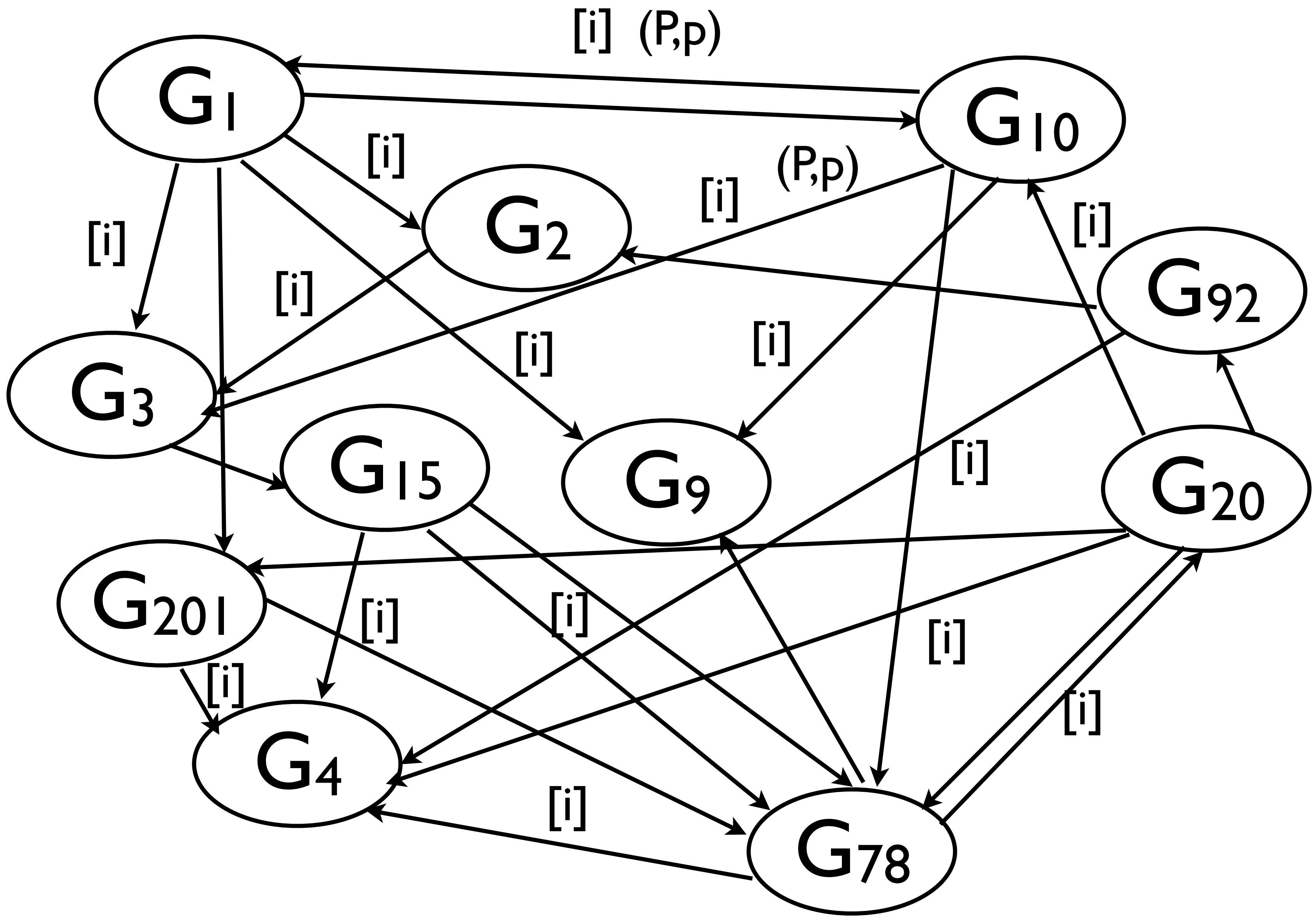
http://www.cryst.ehu.es/subgroupgraph.html

SUBGROUPGRAPH

Step 1:

ITA1 data of maximal subgroups

Graph of maximal subgroups



-230 nodes - space groups

-G>H: directed edges with attributes: [i], (P,p)

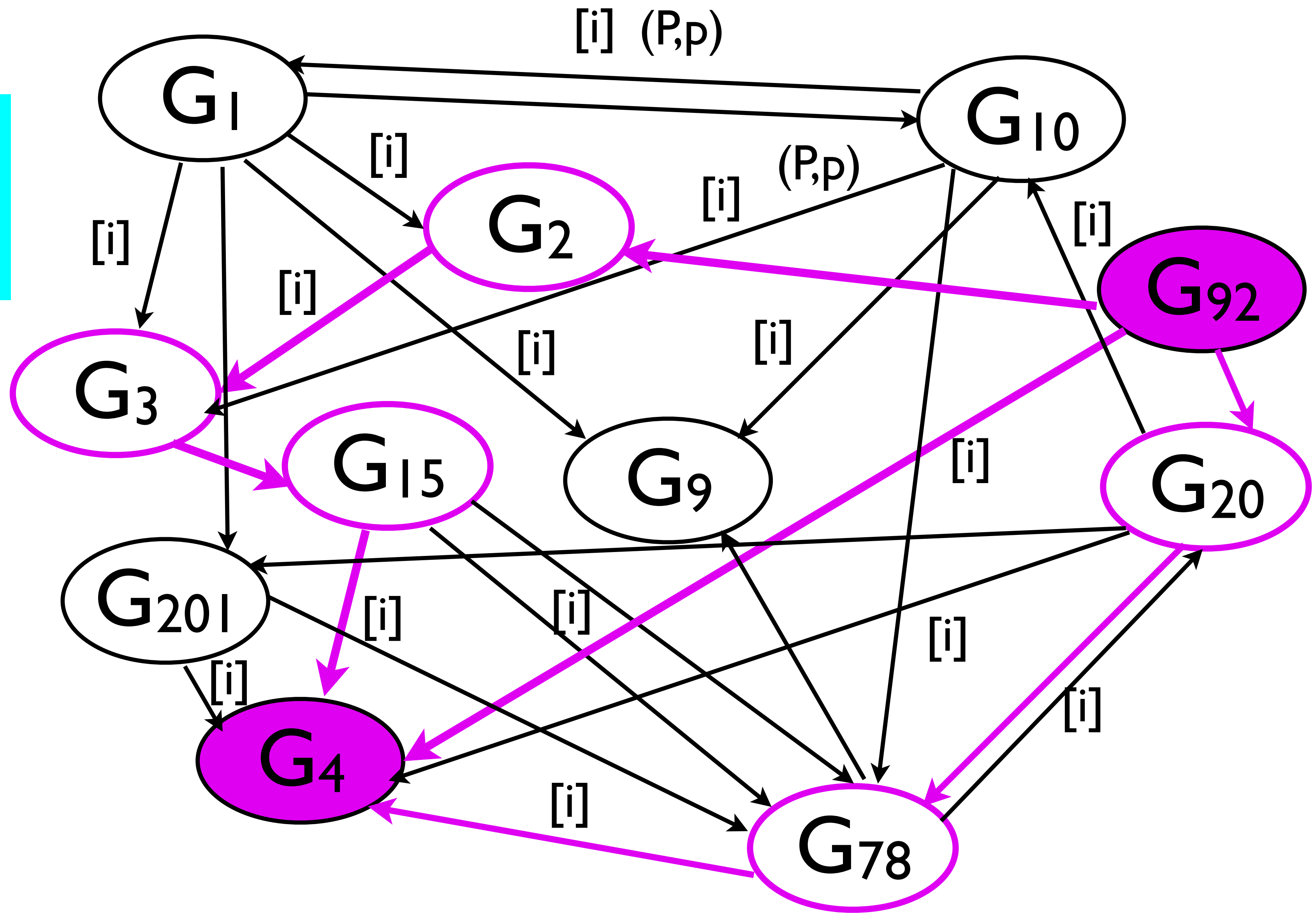
SUBGROUPGRAPH

Step 2:

Specification of G > H

⬇

Sub-graph of maximal subgroups



Sub-graph for G>H (contracted)

top vertex: $G=G_{92}$-node

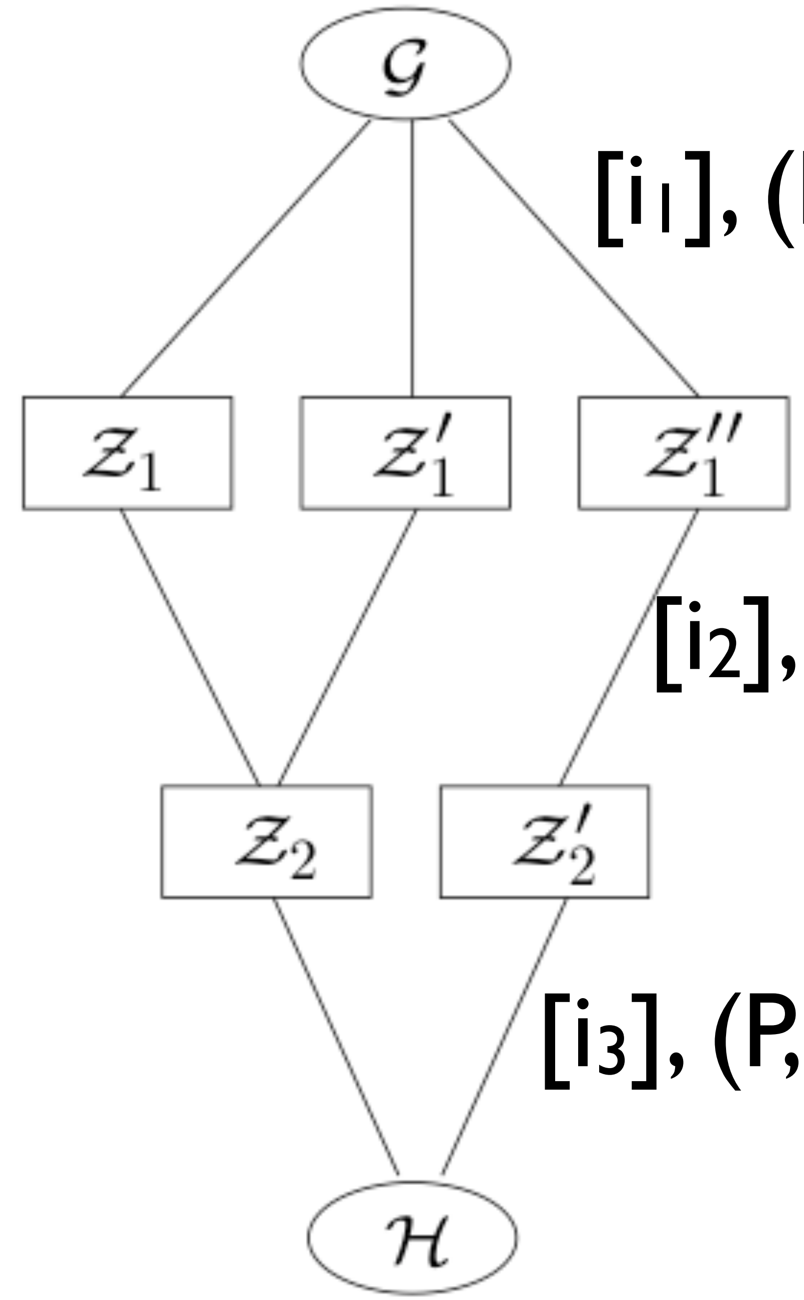
bottom vertex $H=G_4$-node

SUBGROUPGRAPH

Step 3:

Specification of the index [i] of G > H

Sub-graph of chains of maximal subgroups



$[i_1]$, $(P,p)_1$

$[i_2]$, $(P,p)_2$

$[i_3]$, $(P,p)_3$

Complete graph for G>H, [i], (P,p)

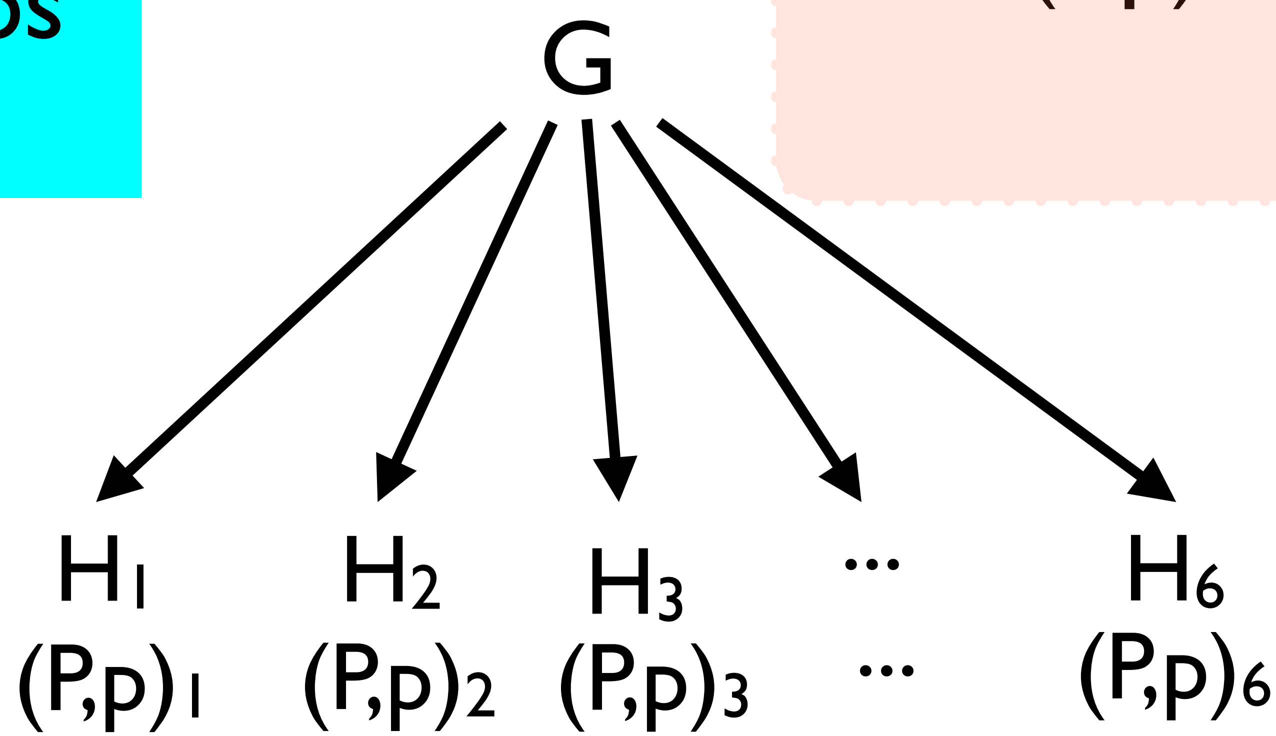
$[i] = [i_1].[i_2].[i_3]$

$(P,p) = (P,p)_1 . (P,p)_2 . (P,p)_3$

SUBGROUPGRAPH

Step 4a:

Identical Subgroups
$H_i \equiv H_j$



Identification of identical subgroups

$$(P,p)_i H (P,p)_i^{-1} = (P,p)_j H (P,p)_j^{-1}$$

$$H_i \overset{?}{\equiv} H_j$$

Step 4b:

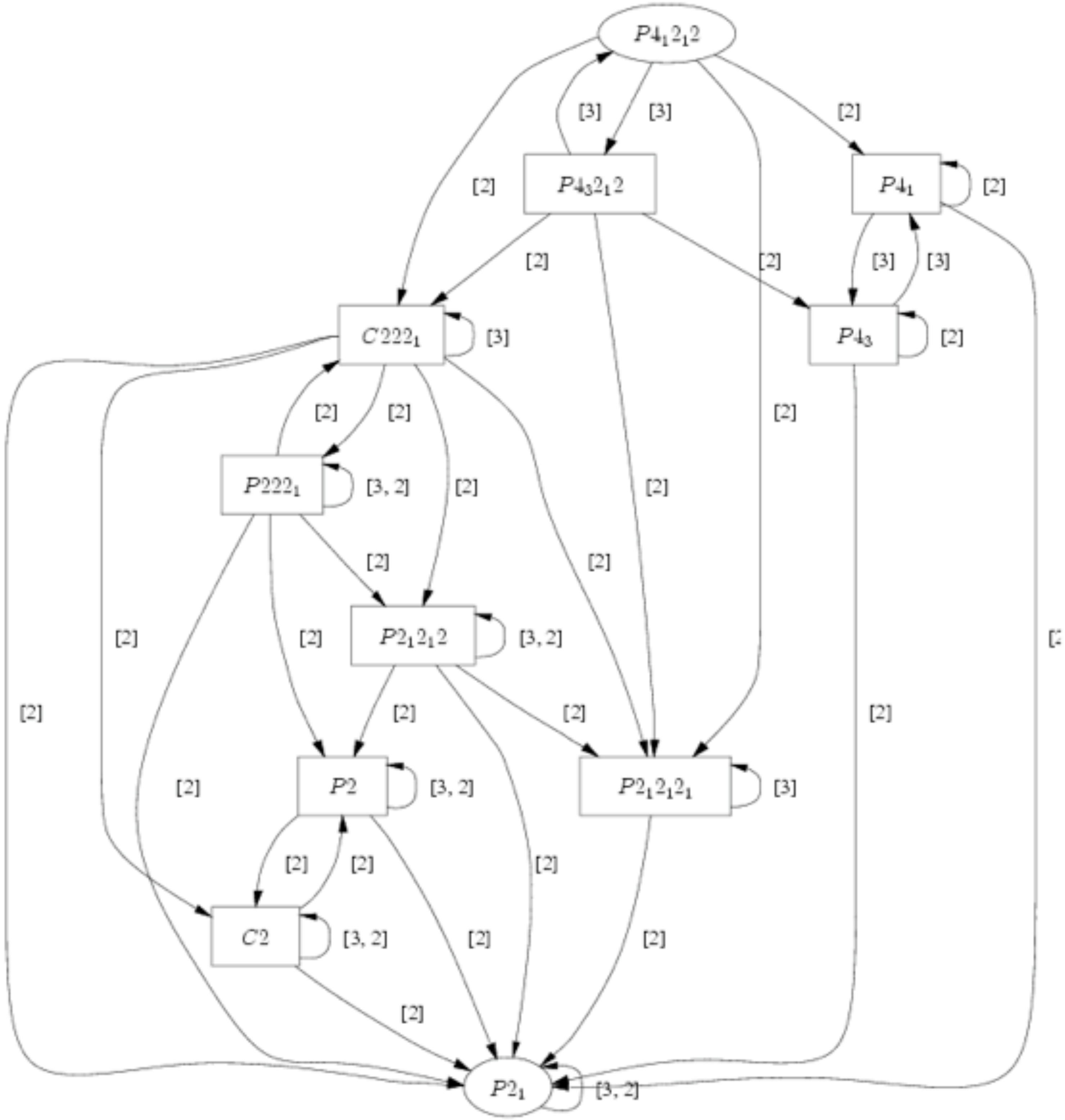
Conjugate subgroups
$H_i \sim H_j$

$$H_i \overset{?}{\sim} H_j$$

$$H_i = (W,w)_G^{-1} H_j (W,w)_G$$

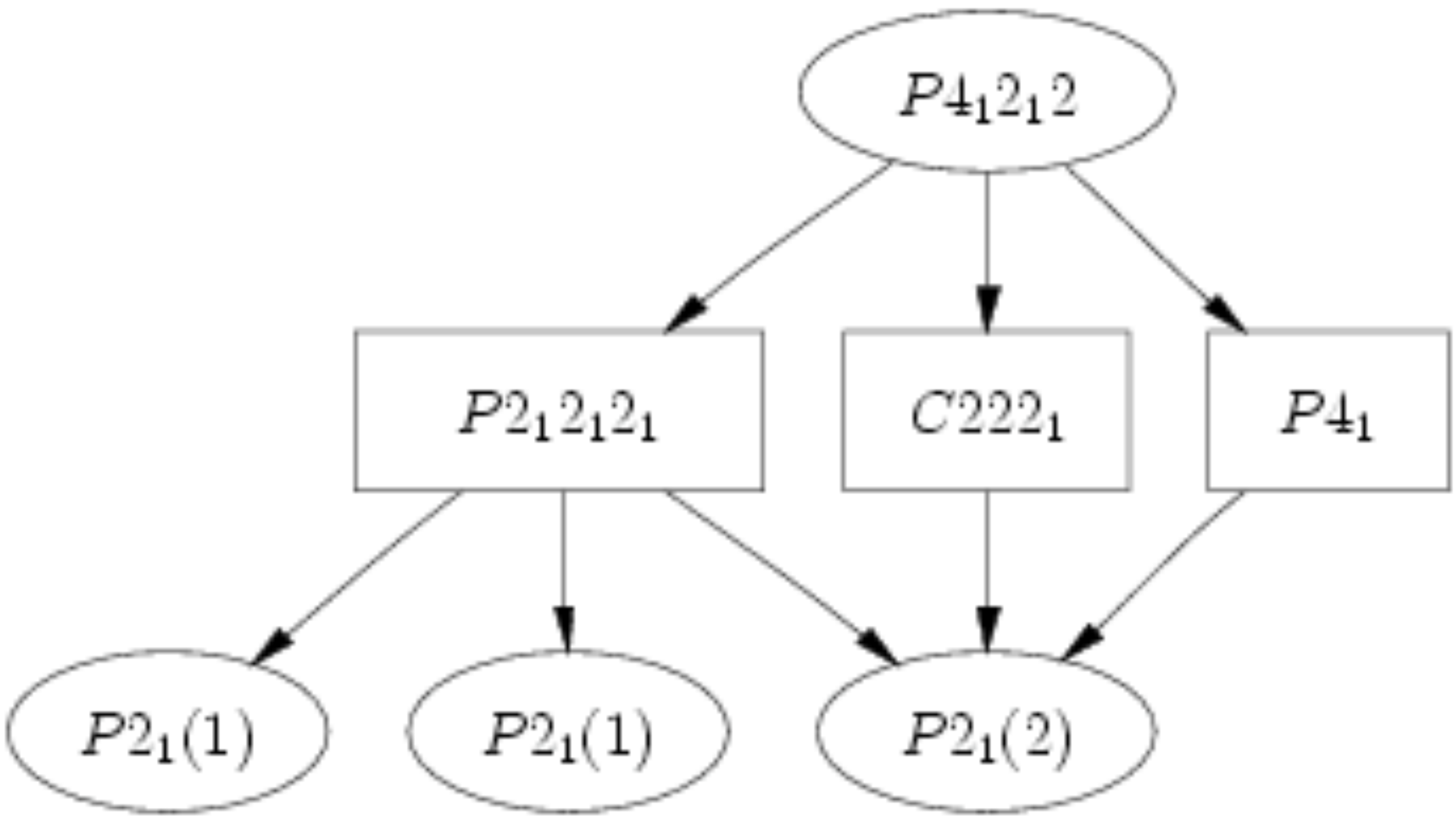
Classes of conjugate subgroups

Example SUBGROUPGRAPH: $P4_12_12 > P2_1$



General contracted graph for $P4_12_12 > P2_1$

Example SUBGROUPGRAPH: $P4_12_12 > P2_1$, index 4



Complete graph for $P4_12_12 > P2_1$, index 4.

Three $P2_1$ subgroups in ***two*** conjugacy classes

EXAMPLE:

SUBGROUPGRAPH: $P4_12_12 > P2_1$

Classification of the subgroups of type $P2_1(4)$ of group $P4_12_12(92)$ with index 4

Class 1

N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
1	092 019 004 [2 2]	$P4_12_12 > P2_12_12_1 > P2_1$	$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 5/8 \end{pmatrix}$	matrix 1	--
2	092 019 004 [2 2]	$P4_12_12 > P2_12_12_1 > P2_1$	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/4 \\ 1 & 0 & 0 & 3/8 \end{pmatrix}$	matrix 2	--

Class 2

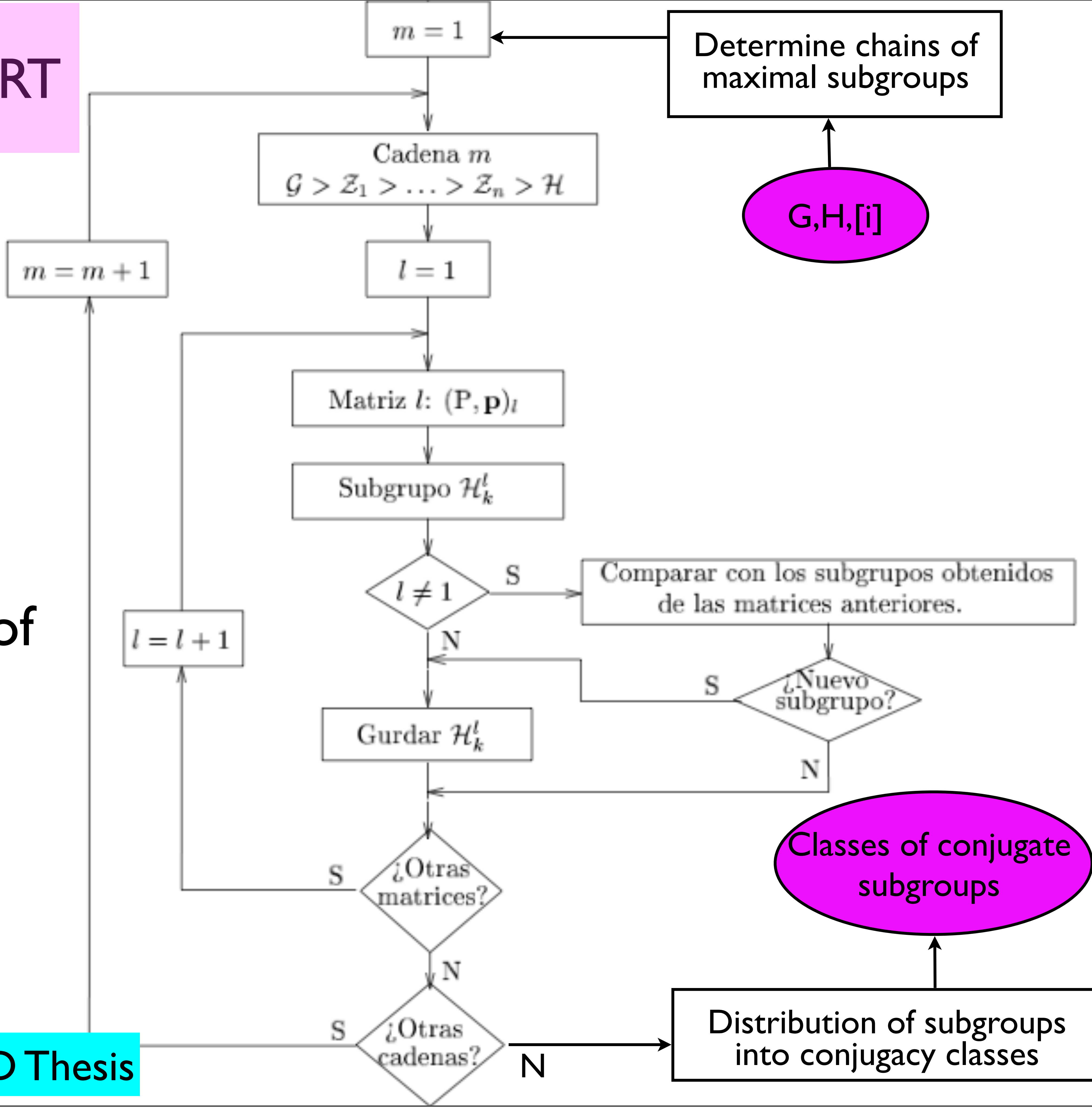
N	Chain [indices]	Chain with HM symbols	Transformation	Transform with	Identical
3	092 020 004 [2 2]	$P4_12_12 > C222_1 > P2_1$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1/4 \end{pmatrix}$	matrix 3	to group 3

normal subgroup

FLOW-CHART

SUBGROUP GRAPH

Calculation of Subgroups

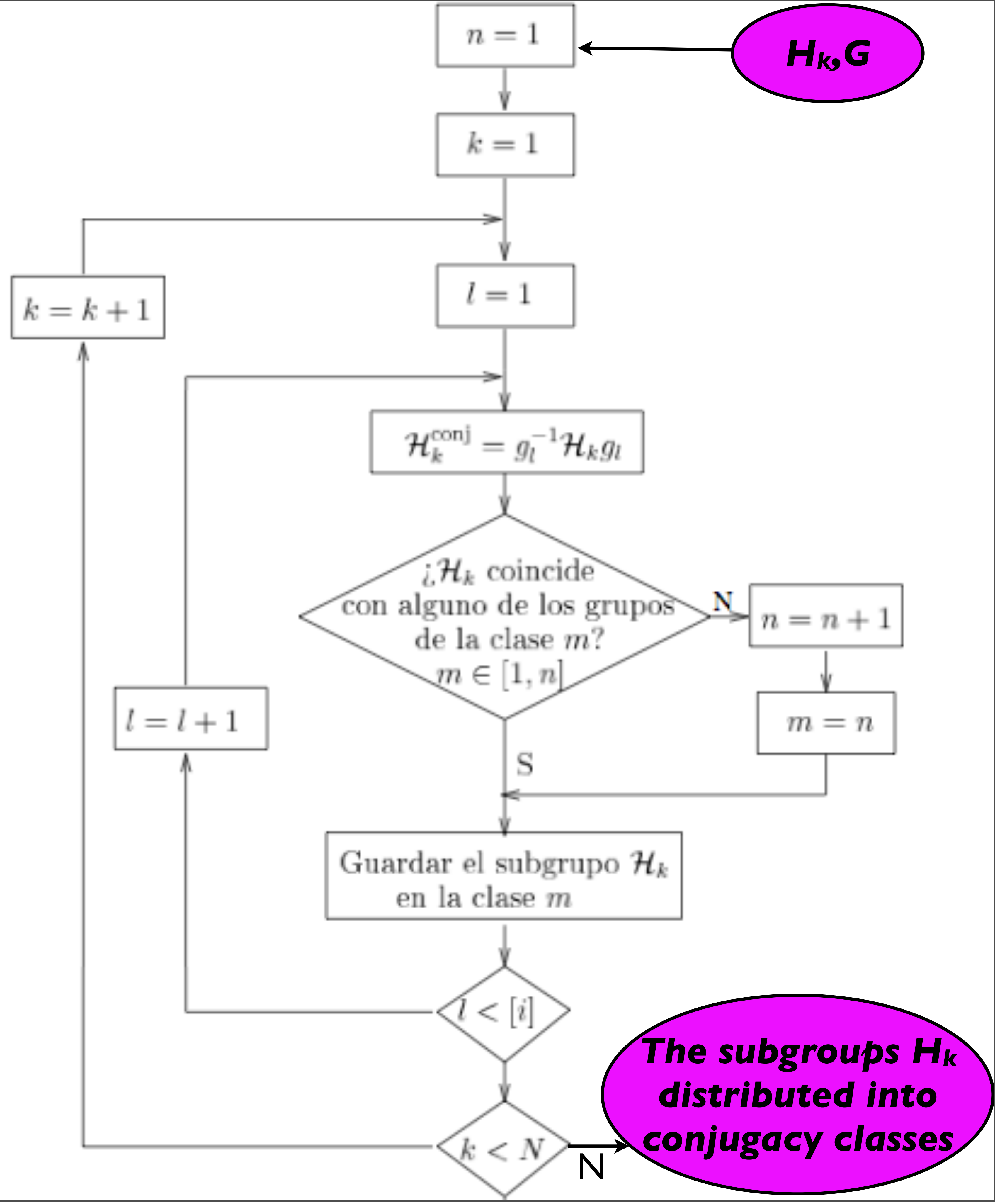


Eli Kroumova, PhD Thesis

FLOW-CHART

SUBGROUPGRAPH

Distribution of subgroups into conjugacy classes



Eli Kroumova, PhD Thesis

Calculation of Subgroups

General subgroups H<G: $\begin{cases} T_H < T_G \\ P_H < P_G \end{cases}$

Theorem HERMANN, 1929:

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

M is a *t-subgroup* of G: $T_G = T_M$

H is a *k-subgroup* of M: $P_M = P_H$

G

↓ $i_P = P_G/P_H$

M

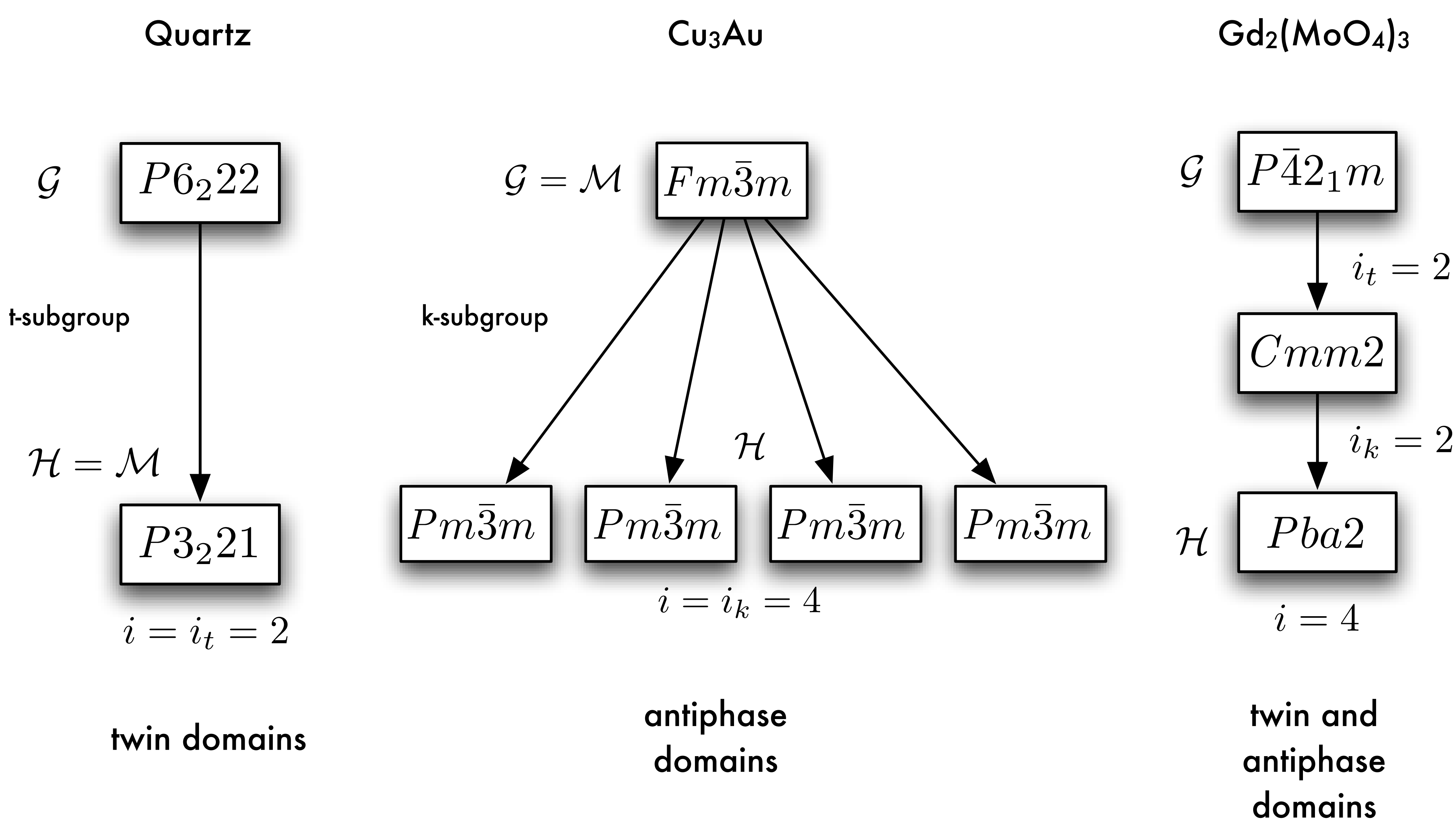
↓ $i_L = T_G/T_H$

H

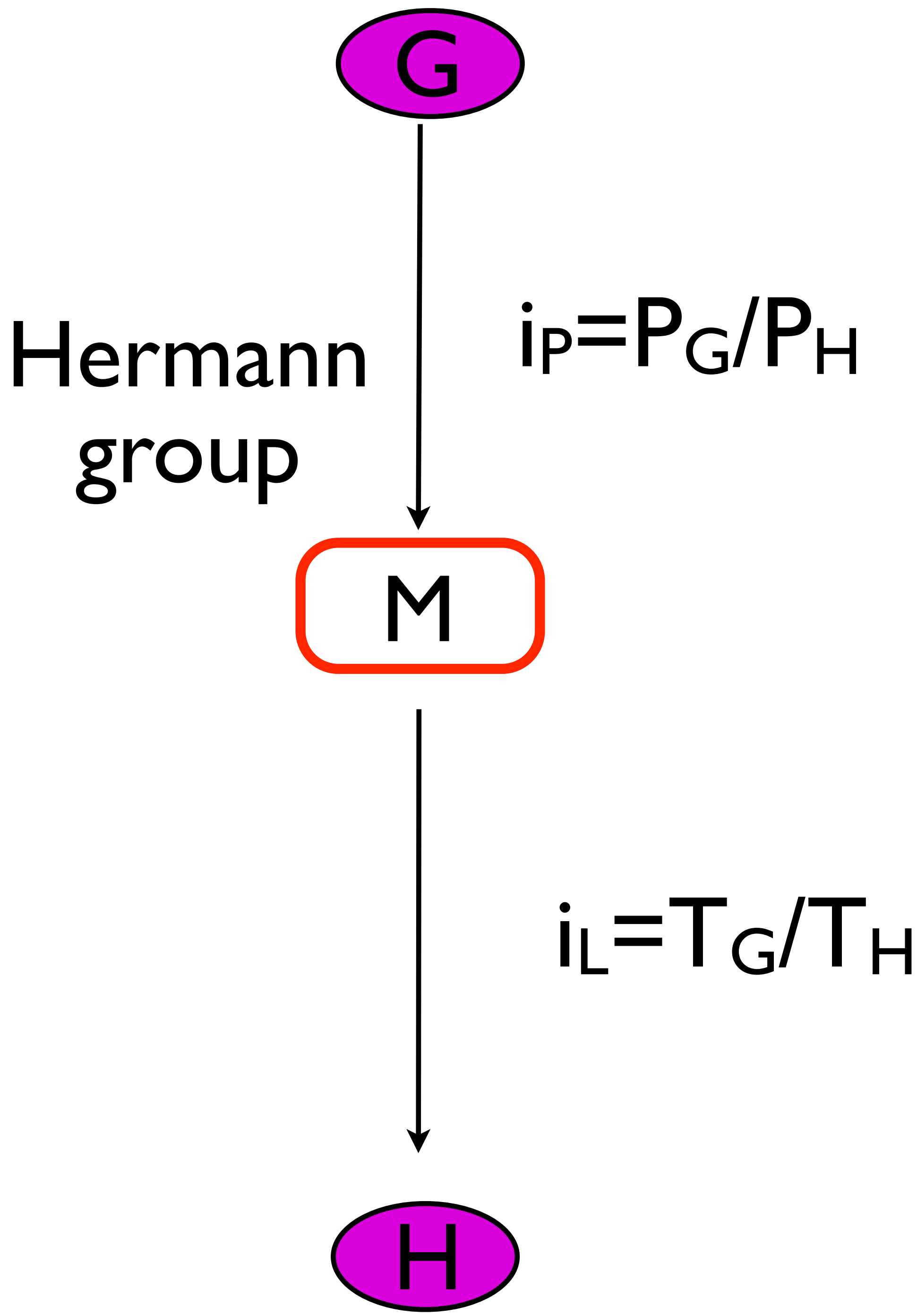
Corollary A maximal subgroup is either a *t*- or *k*-subgroup

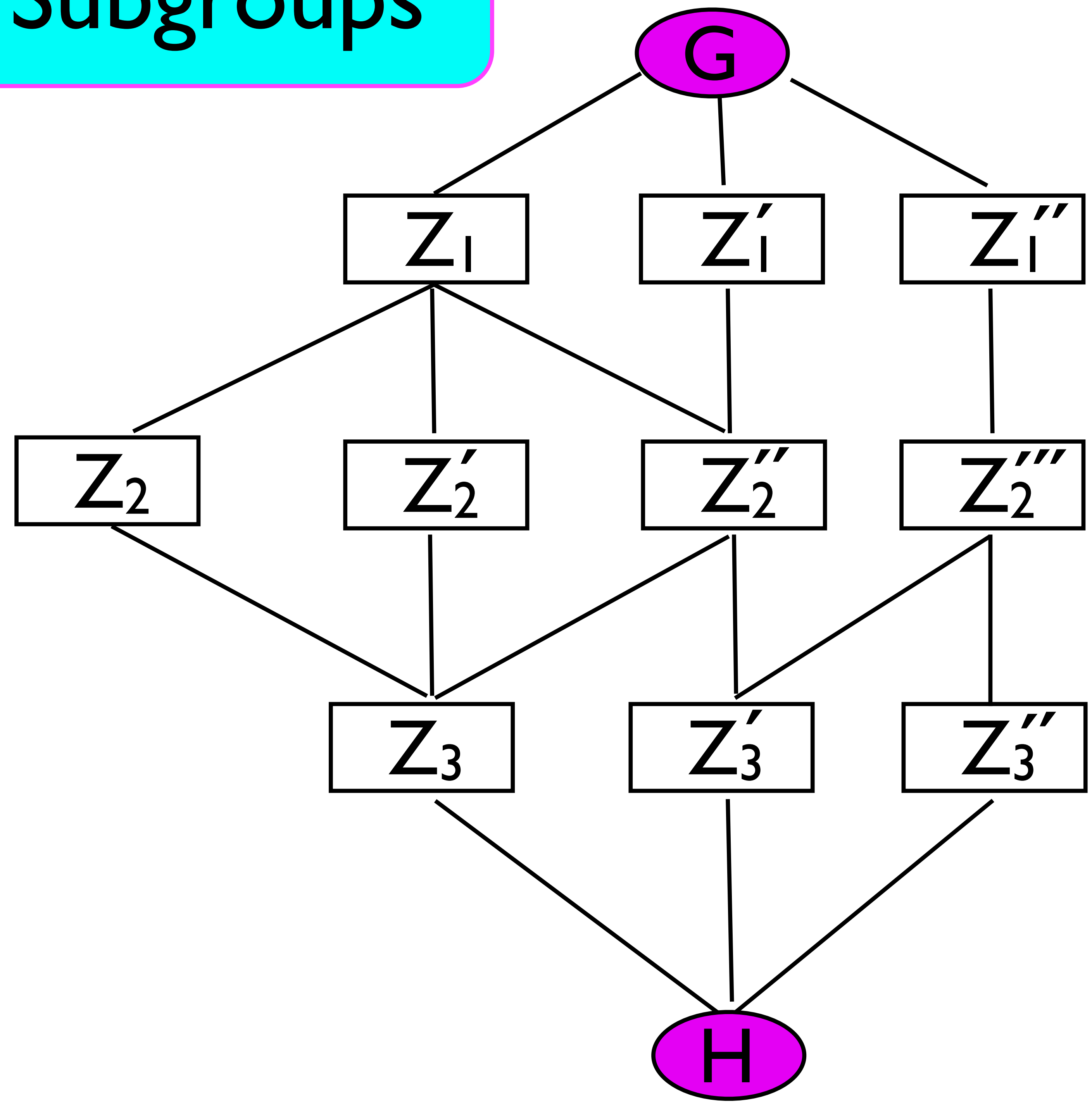
Problem: CLASSIFICATION OF DOMAINS

HERMANN



Calculation of Subgroups

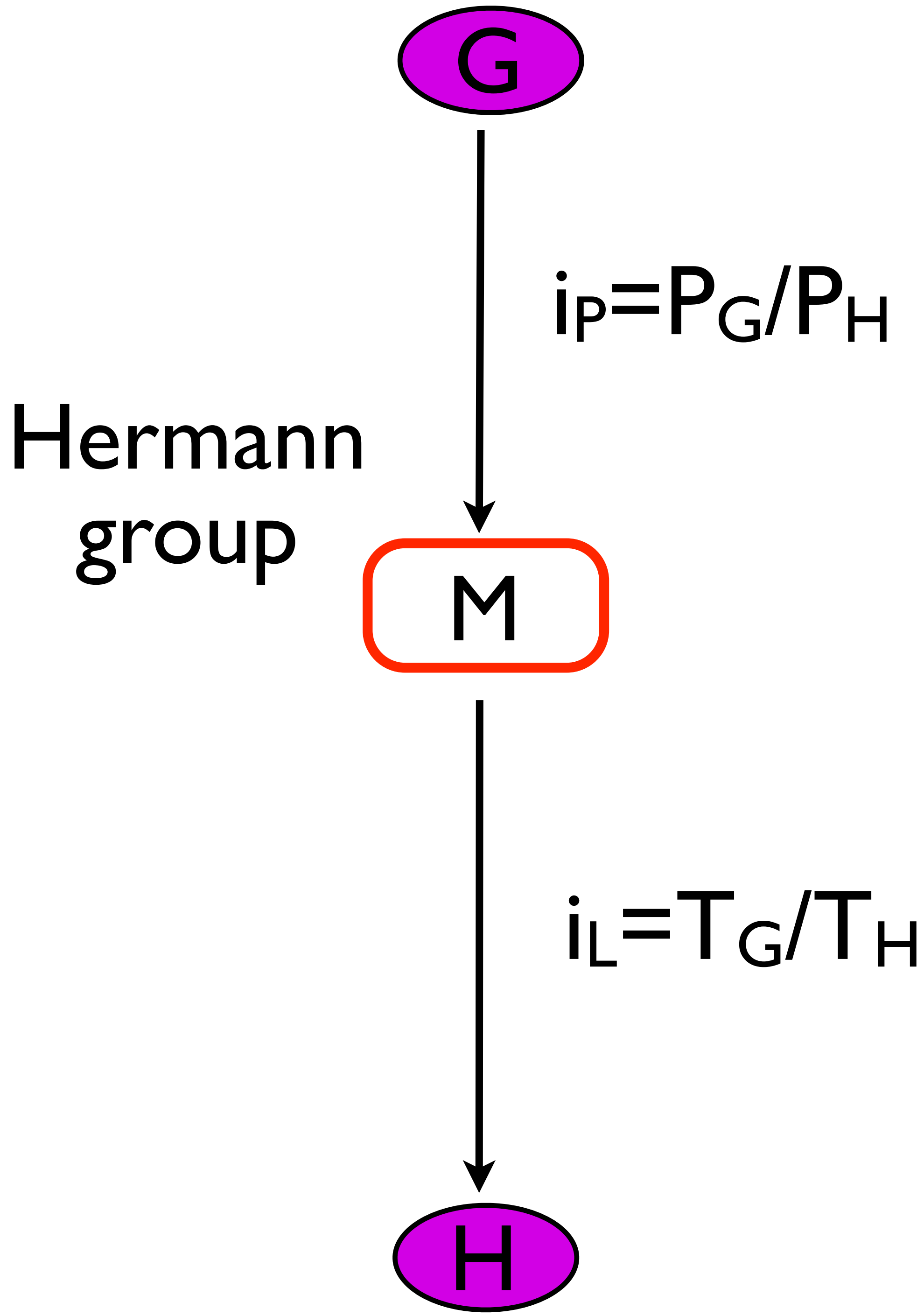


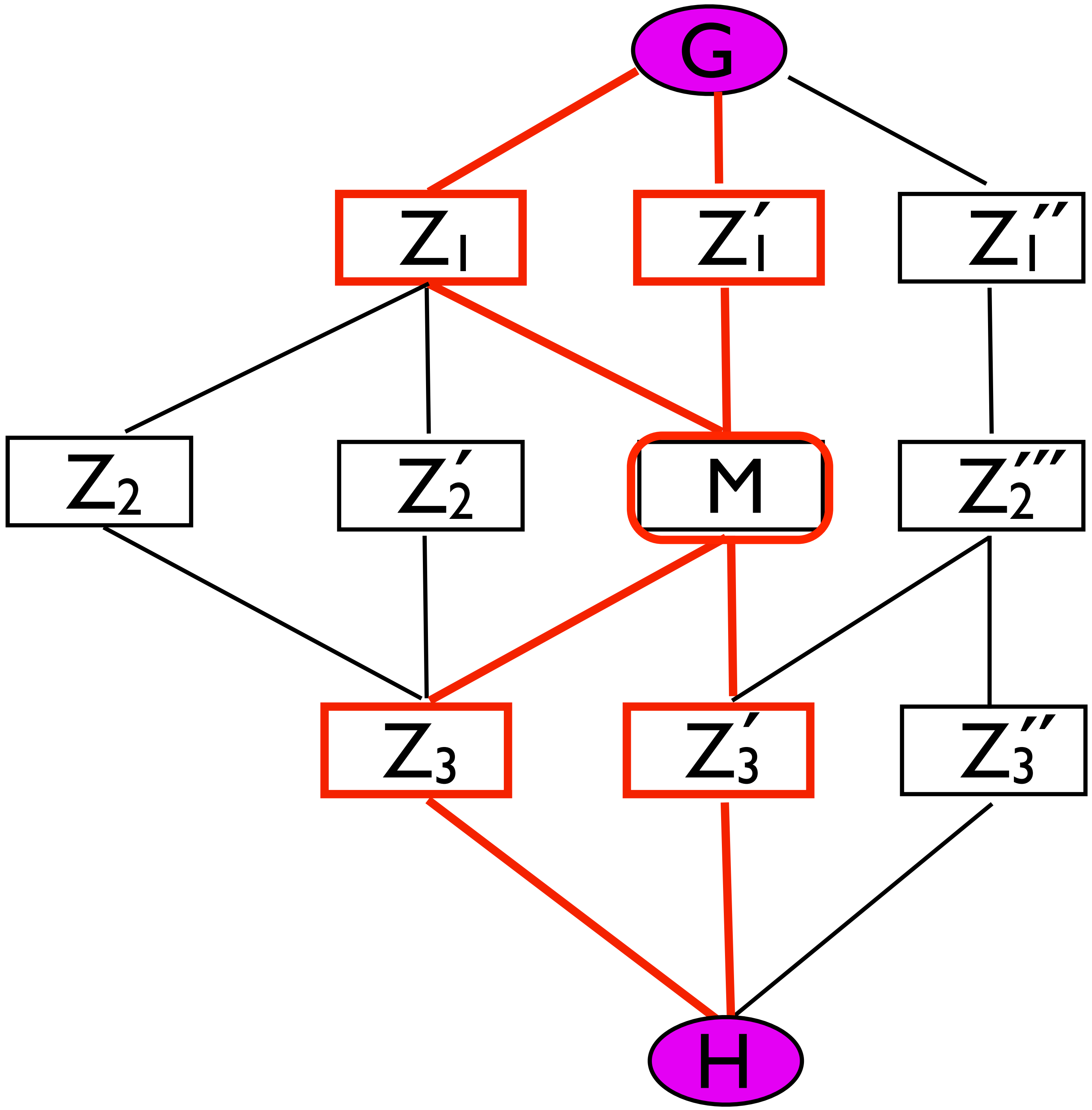


SUBGROUPGRAPH

Complete graph of maximal subgroups

Calculation of Subgroups: HERMANN



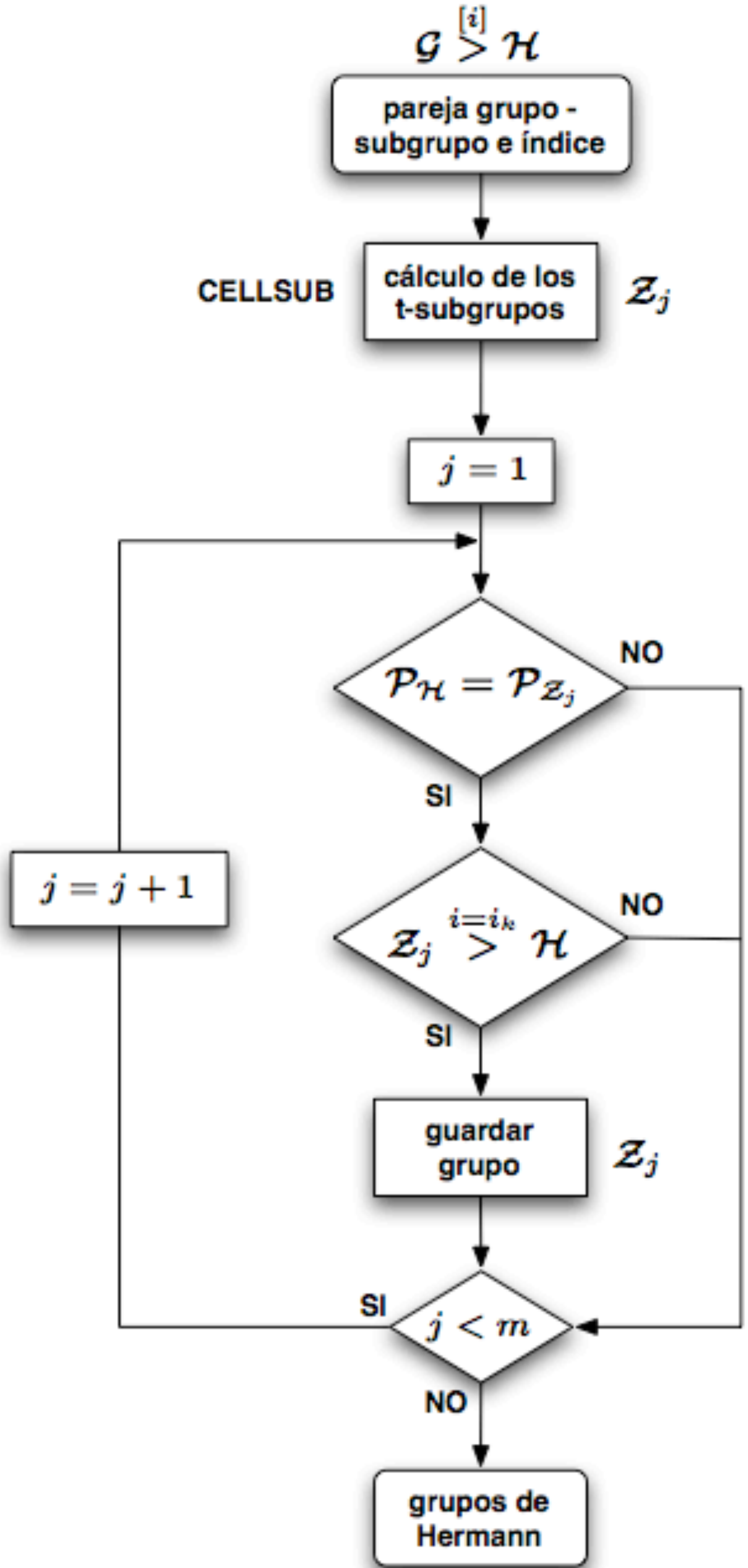


HERMANN
Graph of maximal subgroups

FLOW-CHART

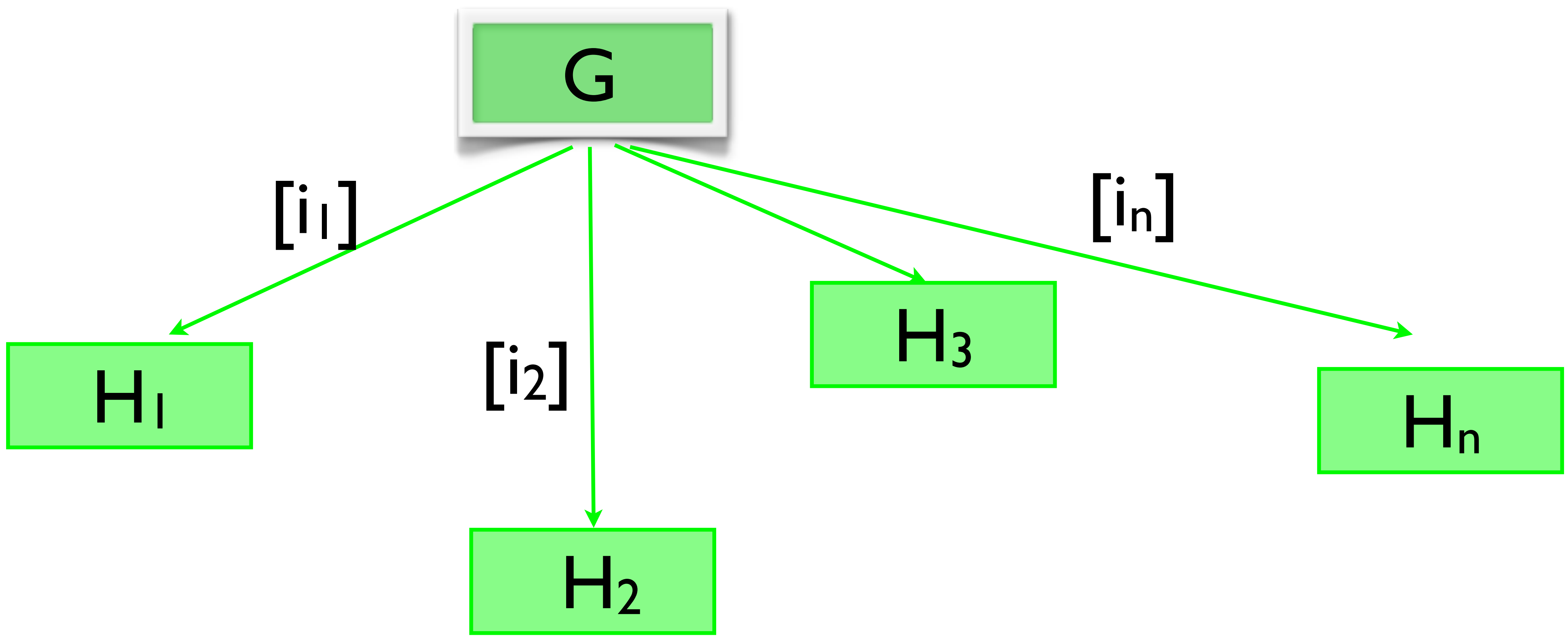
Calculation of Subgroups

HERMANN



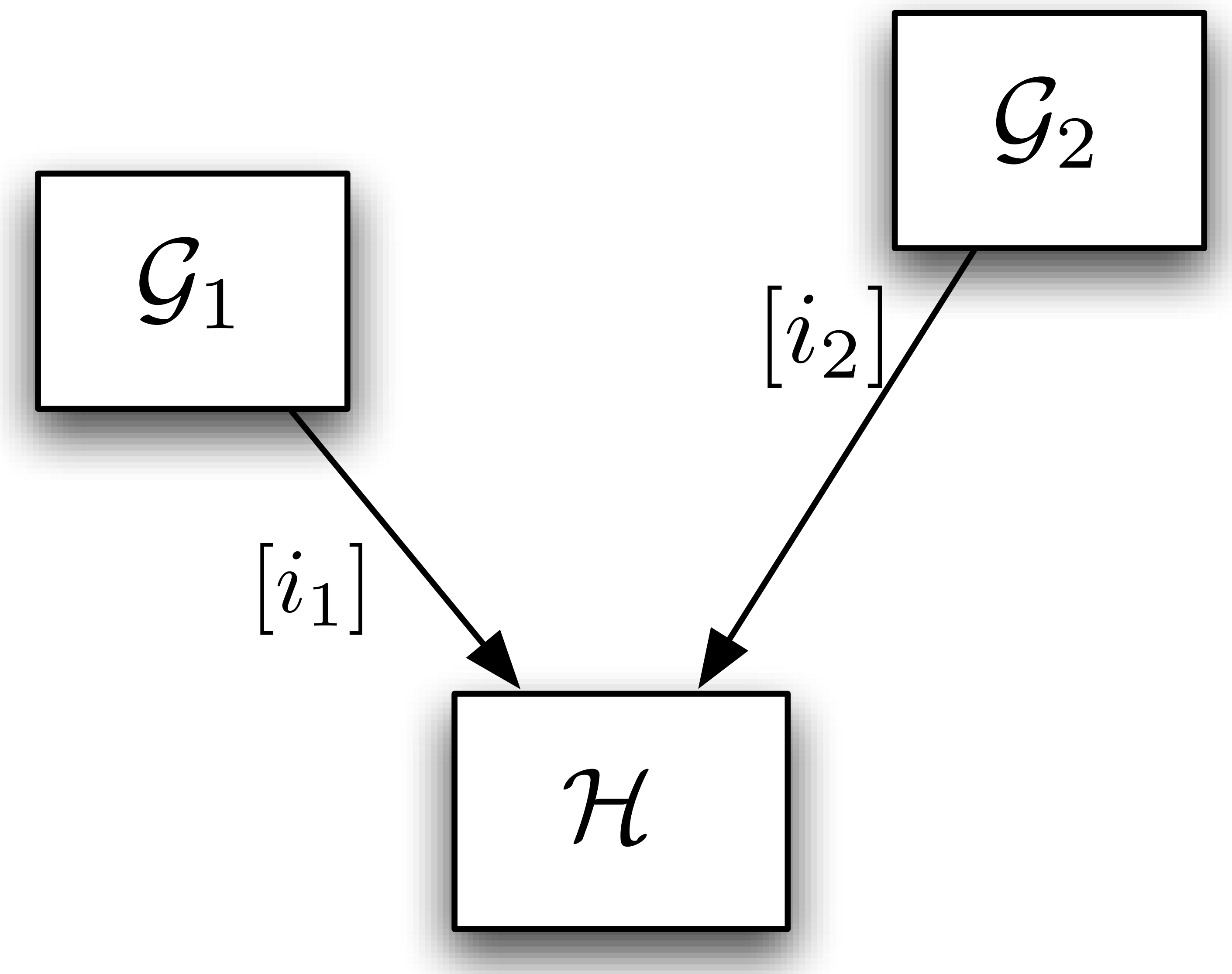
Cesar Capillas, PhD Thesis

Problem: Subgroups for a given cell multiplication — **CELLSUB**



$[i_L]$=const

Problem: Common subgroups — COMMONSUBS



$$Z_{\mathcal{H}_1} = Z_{\mathcal{H}_2}$$

$$i_1 = \frac{|\mathcal{P}_{\mathcal{G}_1}|}{|\mathcal{P}_{\mathcal{H}_1}|} \cdot \frac{Z^p_{\mathcal{H}_1}}{Z^p_{\mathcal{G}_1}}$$

$$i_2 = \frac{|\mathcal{P}_{\mathcal{G}_2}|}{|\mathcal{P}_{\mathcal{H}_2}|} \cdot \frac{Z^p_{\mathcal{H}_2}}{Z^p_{\mathcal{G}_2}}$$

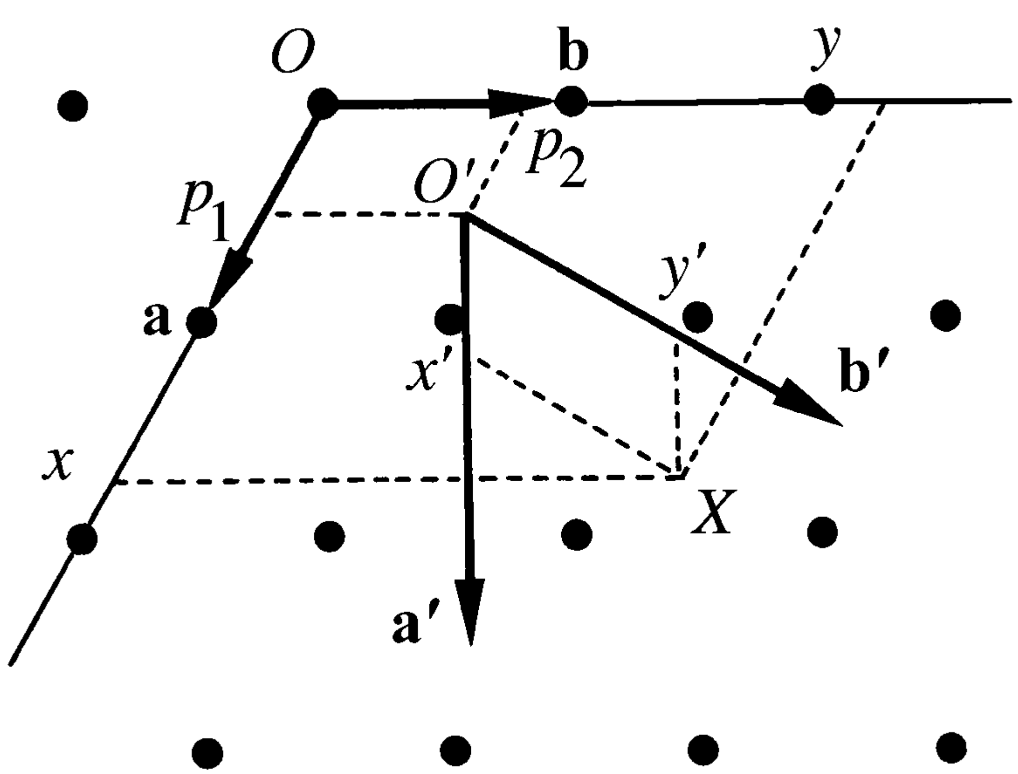
index condition

$$i_2 = i_1 \cdot \frac{Z_1}{Z_2} \cdot \frac{|\mathcal{P}_{\mathcal{G}_2}|}{|\mathcal{P}_{\mathcal{G}_1}|} \cdot \frac{f_{\mathcal{G}_2}}{f_{\mathcal{G}_1}}$$

the set of common subgroup types is finite if a maximum k-index is defined

Basic functions: TRANSFORM

General affine transformation



3-dimensional space

$(\mathbf{a}, \mathbf{b}, \mathbf{c})$, origin O: point $X(x, y, z)$

$$\downarrow (P,p)$$

$(\mathbf{a}', \mathbf{b}', \mathbf{c}')$, origin O': point $X(x', y', z')$

Transformation of symmetry operations (*W*,*w*):

$$(W',w')=(P,p)^{-1}(W,w)(P,p)$$

TRANSFORM

INPUT:

Space group $G=\{(W,w)_k, k=1,\dots,p\}$

Transformation matrix (P,p)

OUTPUT:

Case 1: det P=1

$\{(W,w)_k, k=1,\dots,p\}$

$\downarrow (P,p)$

$\{(W',w')_k, k=1,\dots,p\}$

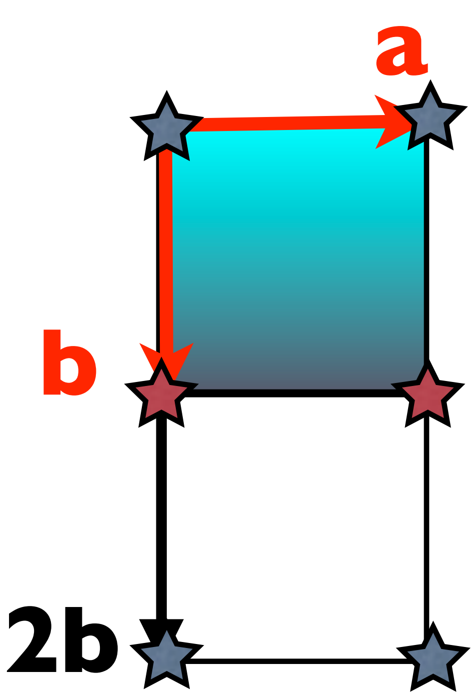
Case 2: det P>1 (subgroup basis)

$\{(W,w)_k, k=1,\dots,p\}$

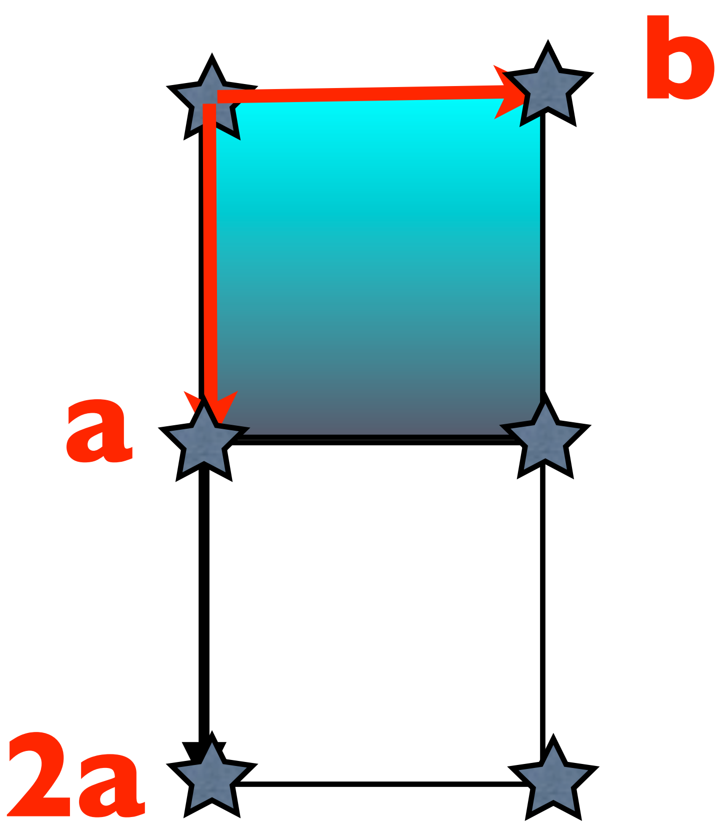
$\{(W',w')_k, k=1,\dots,p\}$

$t(0,1,0)$

$\{(W',w')_l, l=p+1,\dots,2p\}$



Example: **a'**=2**a**, **b'**=**b**, **c'**=**c**



$(P,p)=$

2	0	0
0	1	0
0	0	1

$(P,p)^{-1}=$

1/2	0	0
0	1	0
0	0	1

integer translations $t(1,0,0) \longrightarrow t(1/2,0,0)$ non-integer translations

$$(T_{int})_H \neq (P,p)^{-1}T_{int}(P,p)$$

$$(P,p)^{-1}T_{int}(P,p)$$

$(T_{int})_H$ $\qquad$ $t(1/2,0,0)(T_{int})_H$

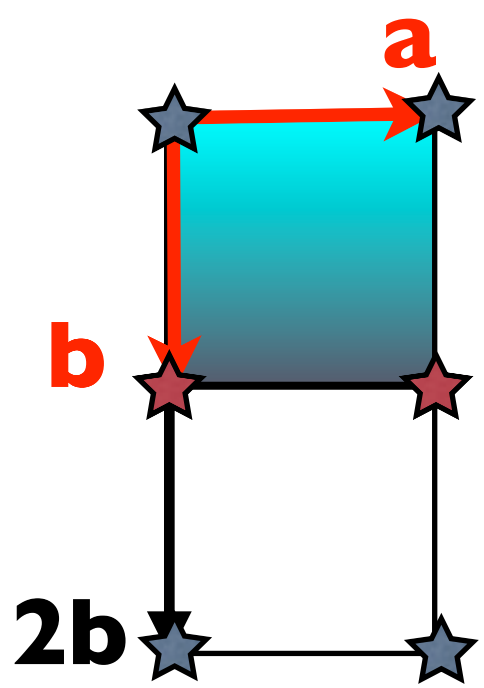
TRANSFORM

$P222_1(\mathbf{a},\mathbf{b},\mathbf{c})$

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&-1&0&0\\0&0&1&1/2\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&1&0&0\\0&0&-1&1/2\end{pmatrix}\quad\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\end{pmatrix}$$

$t(0,1,0)$

$$\begin{pmatrix}1&0&0&0\\0&1&0&1\\0&0&1&0\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&-1&0&1\\0&0&1&1/2\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&1&0&1\\0&0&-1&1/2\end{pmatrix}\quad\begin{pmatrix}1&0&0&0\\0&-1&0&1\\0&0&-1&0\end{pmatrix}$$



$$(P,p)\begin{pmatrix}1&0&0&0\\0&2&0&0\\0&0&1&0\end{pmatrix}$$

$P222_1(\mathbf{a},2\mathbf{b},\mathbf{c})$

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&-1&0&0\\0&0&1&1/2\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&1&0&0\\0&0&-1&1/2\end{pmatrix}\quad\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\end{pmatrix}$$

$$\begin{pmatrix}1&0&0&0\\0&1&0&1/2\\0&0&1&0\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&-1&0&1/2\\0&0&1&1/2\end{pmatrix}\quad\begin{pmatrix}-1&0&0&0\\0&1&0&1/2\\0&0&-1&1/2\end{pmatrix}\quad\begin{pmatrix}1&0&0&0\\0&-1&0&1/2\\0&0&-1&0\end{pmatrix}$$

Basic functions: COSETS

Coset decomposition G:H

Group-subgroup pair $H < G$

left coset decomposition $G=H+g_2H+...+g_mH, g_i \notin H,$
m=index of H in G

right coset decomposition $G=H+Hg_2+...+Hg_m, g_i \notin H$
m=index of H in G

Normal subgroups $Hg_j= g_jH$, for all $g_j=1, ..., [i]$

COSETS

GIVEN: Group-subgroup pair G>H
Transformation matrix (P,p)

PROCEDURE:

Step 1. Transformation of G to the H basis: TRANSFORM

$$\{(W,w)_G,\ k=1,\ldots,p\} \xrightarrow{(P,p)} \{(W',w')_{G(H)},\ k=1,\ldots,p\}$$

Step 2a. Right coset decomposition

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

Step 2b. Left coset decomposition

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

EXAMPLE:

COSETS: $P4_12_12 > P2_1$

Subgroup $P2_1$(normal): $(P,p)=\left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{array}\right]\left[\begin{array}{c} 0 \\ 0 \\ 1/4 \end{array}\right]$

Right coset decomposition

```
Coset 1:

(x,y,z)
(-x,y+1/2,-z)

Coset 2:

(z+1/2,y+1/4,-x+1/2)
(-z+1/2,y+3/4,x+1/2)

Coset 3:

(-x+1/2,-y+3/4,z+1/2)
(x+1/2,-y+1/4,-z+1/2)

Coset 4:

(-z,-y+1/2,-x)
(z,-y,x)
```

Hg=gH

Left coset decomposition

```
Coset 1:

(x,y,z)
(-x,y+1/2,-z)

Coset 2:

(z+1/2,y+1/4,-x-1/2)
(-z+1/2,y+3/4,x-1/2)

Coset 3:

(-x+1/2,-y-1/4,z-1/2)
(x+1/2,-y+1/4,-z-1/2)

Coset 4:

(-z,-y-1/2,-x)
(z,-y,x)
```

EXAMPLE:

COSETS: $P4_12_12 > P2_1$

Subgroup $P2_1$(not normal): $(P,p)=$
```
[      1      0      0 ] [      1/4]
[      0      1      0 ] [        0]
[      0      0      1 ] [      5/8]
```

Right coset decomposition

```
Coset 1:

(x,y,z)
(-x,y+1/2,-z)

Coset 2:

(-x+1/2,-y,z+1/2)
(x+1/2,-y+1/2,-z+1/2)

Coset 3:

(-y+1/4,x+3/4,z+1/4)
(y+3/4,x+1/4,-z+3/4)

Coset 4:

(y+1/4,-x+1/4,z+3/4)
(-y+3/4,-x+3/4,-z+1/4)
```

Left coset decomposition

```
Coset 1:

(x,y,z)
(-x,y+1/2,-z-1)

Coset 2:

(-x-1/2,-y,z+1/2)
(x+1/2,-y+1/2,-z-1/2)

Coset 3:

(-y+1/4,x+3/4,z+1/4)
(-y-1/4,-x-1/4,-z-3/4)

Coset 4:

(y+1/4,-x+1/4,z+3/4)
(y-1/4,x+1/4,-z-5/4)
```

$Hg \neq gH$

COSETS WARNING: tricky points

STEP 1. Transformation of G to a subgroup basis:

$$G = T + Tg_2 + Tg_3 + \ldots + Tg_k$$

$$T_{int} \quad T_{int}t_2 \quad \ldots \quad T_{int}t_j$$

(P,p)

$$(T)_H = (P,p)^{-1} T_{int} (P,p) + (P,p)^{-1} (T_{int} t_2)(P,p) + \ldots$$

$$(T_{int})_H \neq (P,p)^{-1} T_{int} (P,p)$$

$$(t_i)_H \neq (P,p)^{-1} t_i (P,p)$$

$$(T)_H = (T_{int})_H + (T_{int})_H (t_2)_H + \ldots + (T_{int})_H (t_k)_H$$

Example: Cccm(66) > P2/m(10), index 4

(P,p)=

1	0	1/2
1	0	-1/2
0	1	0

$(P,p)^{-1}$=

1/2	1/2	0
0	0	1
1	-1	0

Transformation of N(Cccm)=Pmmm(1/2,1/2,1/2)

(i) $(T_{int})_H \neq (P,p)^{-1} T_{int} (P,p)$

integer translations

t(1,0,0) ⟶ t(1/2,0,1)

t(0,1,0) ⟶ t(1/2,0,-1)

non-integer translations

(ii) $(t_i)_H \neq (P,p)^{-1} t_i (P,p)$

different cosets

t(1/2,0,0) ⟶ t(1/4,0,1/2)

t(0,1/2,0) ⟶ t(1/4,0,-1/2) ⟶ t(1/4,0,1/2)

the same coset

COSETS WARNING: tricky points

STEP 2. Decomposition of G with respect to H<G

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

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

$(W_G,w_G)\in G$ $\quad$ $(W_G,w'_G)\in G$

belong to the same coset?

$\Delta=w_G-w'_G$

right: $\Delta = t_H$ $\quad\rightarrow\quad$ $(W_i,w_i+t_H) \in H(W_i,w_i)$

left: $\Delta=V_it_H$ $\quad\rightarrow\quad$ $(V_i,v_i+V_it_H) \in (V_i,v_i)H$

EXAMPLE:

R-3m > P2$_1$/c, index 6

$$(3^+)_G = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \xrightarrow{(P,p)=\begin{pmatrix} \frac{2}{3} & 0 & -2 \\ \frac{1}{3} & 1 & -1 \\ \frac{1}{3} & 0 & 0 \end{pmatrix}} \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & -\frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} = (3^+)_H$$

coset representatives:

(...,...) $(3^+,000)$ $(3^+,\frac{1}{3}\frac{2}{3}\frac{2}{3})$ $(3^+,\frac{2}{3}\frac{1}{3}\frac{1}{3})$ (...,...)

$(3^+,000)$ $(3^+,100)$ $(3^+,2\frac{1}{2}\frac{1}{2})$

right: belong to the same coset

$\Delta = t_H$

left: belong to the same coset

$\Delta = V_i t_H$

$V_i = 3^+$, $t_H = (100)$

Bilbao Crystallographic Server

Ouput COSETS

Right cosets

Coset 1:

(x,y,z)
(-x,y+1/2,-z+1/2)
(-x,-y,-z)
(x,-y+1/2,z+1/2)

$(3^+,000)$

Coset 2:

(x,1/2x-1/2y-3/2z,1/2x+1/2y-1/2z)
(-x,1/2x-1/2y-3/2z+1/2,-1/2x-1/2y+1/2z+1/2)
(-x,-1/2x+1/2y+3/2z,-1/2x-1/2y+1/2z)
(x,-1/2x+1/2y+3/2z+1/2,1/2x+1/2y-1/2z+1/2)

Coset 3:

(x,-1/2x-1/2y+3/2z,1/2x-1/2y-1/2z)
(-x,-1/2x-1/2y+3/2z+1/2,-1/2x+1/2y+1/2z+1/2)
(-x,1/2x+1/2y-3/2z,-1/2x+1/2y+1/2z)
(x,1/2x+1/2y-3/2z+1/2,1/2x-1/2y-1/2z+1/2)

$(3^+,0 1/2 1/2)$

Coset 4:

(-x,1/2x-1/2y-3/2z,-1/2x-1/2y+1/2z)
(x,1/2x-1/2y-3/2z+1/2,1/2x+1/2y-1/2z+1/2)
(x,-1/2x+1/2y+3/2z,1/2x+1/2y-1/2z)
(-x,-1/2x+1/2y+3/2z+1/2,-1/2x-1/2y+1/2z+1/2)

Coset 5:

(-x,-1/2x-1/2y+3/2z,-1/2x+1/2y+1/2z)
(x,-1/2x-1/2y+3/2z+1/2,1/2x-1/2y-1/2z+1/2)
(x,1/2x+1/2y-3/2z,1/2x-1/2y-1/2z)
(-x,1/2x+1/2y-3/2z+1/2,-1/2x+1/2y+1/2z+1/2)

Coset 6:

(-x,y,-z)
(x,y+1/2,z+1/2)
(x,-y,z)
(-x,-y+1/2,-z+1/2)

Left cosets

Coset 1:

(x,y,z)
(-x+2,y+1/2,-z+1/2)
(-x,-y,-z)
(x+2,-y+1/2,z+1/2)

$(3^+,000)$

Coset 2:

(x,1/2x-1/2y-3/2z,1/2x+1/2y-1/2z)
(-x+1,-1/2x-1/2y+3/2z,-1/2x+1/2y+1/2z)
(-x,-1/2x+1/2y+3/2z,-1/2x-1/2y+1/2z)
(x+1,1/2x+1/2y-3/2z,1/2x-1/2y-1/2z)

Coset 3:

(x,-1/2x-1/2y+3/2z,1/2x-1/2y-1/2z)
(-x+1,1/2x-1/2y-3/2z,-1/2x-1/2y+1/2z)
(-x,1/2x+1/2y-3/2z,-1/2x+1/2y+1/2z)
(x+1,-1/2x+1/2y+3/2z,1/2x+1/2y-1/2z)

Coset 4:

(-x,1/2x-1/2y-3/2z,-1/2x-1/2y+1/2z)
(x+1,-1/2x-1/2y+3/2z,1/2x-1/2y-1/2z)
(x,-1/2x+1/2y+3/2z,1/2x+1/2y-1/2z)
(-x+1,1/2x+1/2y-3/2z,-1/2x+1/2y+1/2z)

$(3^+,100)$

Coset 5:

(-x,-1/2x-1/2y+3/2z,-1/2x+1/2y+1/2z)
(x+1,1/2x-1/2y-3/2z,1/2x+1/2y-1/2z)
(x,1/2x+1/2y-3/2z,1/2x-1/2y-1/2z)
(-x+1,-1/2x+1/2y+3/2z,-1/2x-1/2y+1/2z)

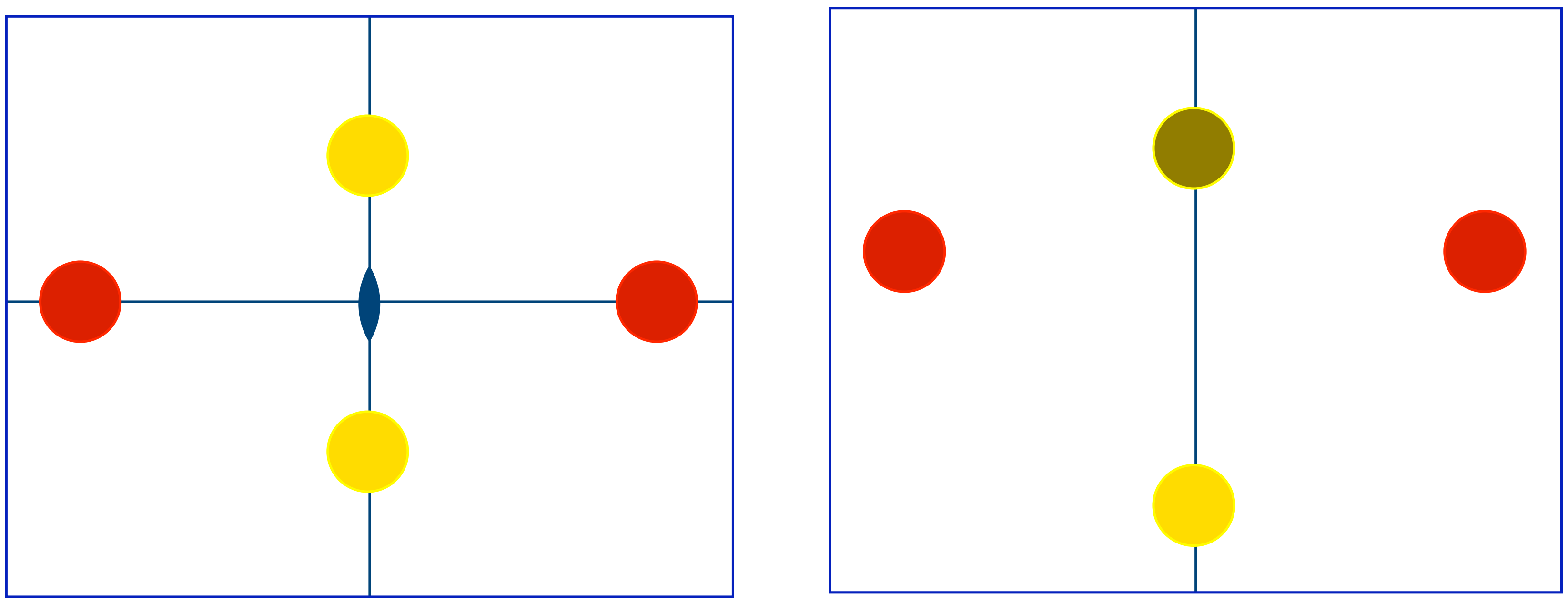
Coset 6:

(-x,y,-z)
(x+2,y+1/2,z+1/2)
(x,-y,z)
(-x+2,-y+1/2,-z+1/2)

SPLITTINGS OF WYCKOFF POSITIONS

Relations between Wyckoff positions

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



$S_0, \ \mathcal{G} = \mathrm{P}mm2$ $\qquad$ $S_1, \ \mathcal{H} = \mathrm{P}m$

2*h* m.. (1/2,y,z) → 2*c* 1 (x,y,z)

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

SYMMETRY REDUCTION

Splittings of Wyckoff positions

Applications

◇ Phase transitions

◇ Derivative structures

◇ Symmetry modes

AIM

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

◇ splitting of $\mathcal{W}^{\mathcal{G}}$ in suborbits

◇ relation between the suborbits and $\mathcal{W}_i^{\mathcal{H}}$

Splittings of Wyckoff positions

Example: Space group $P4_2/mnm$ (selection)

International Tables of Crystallography, Vol.A1

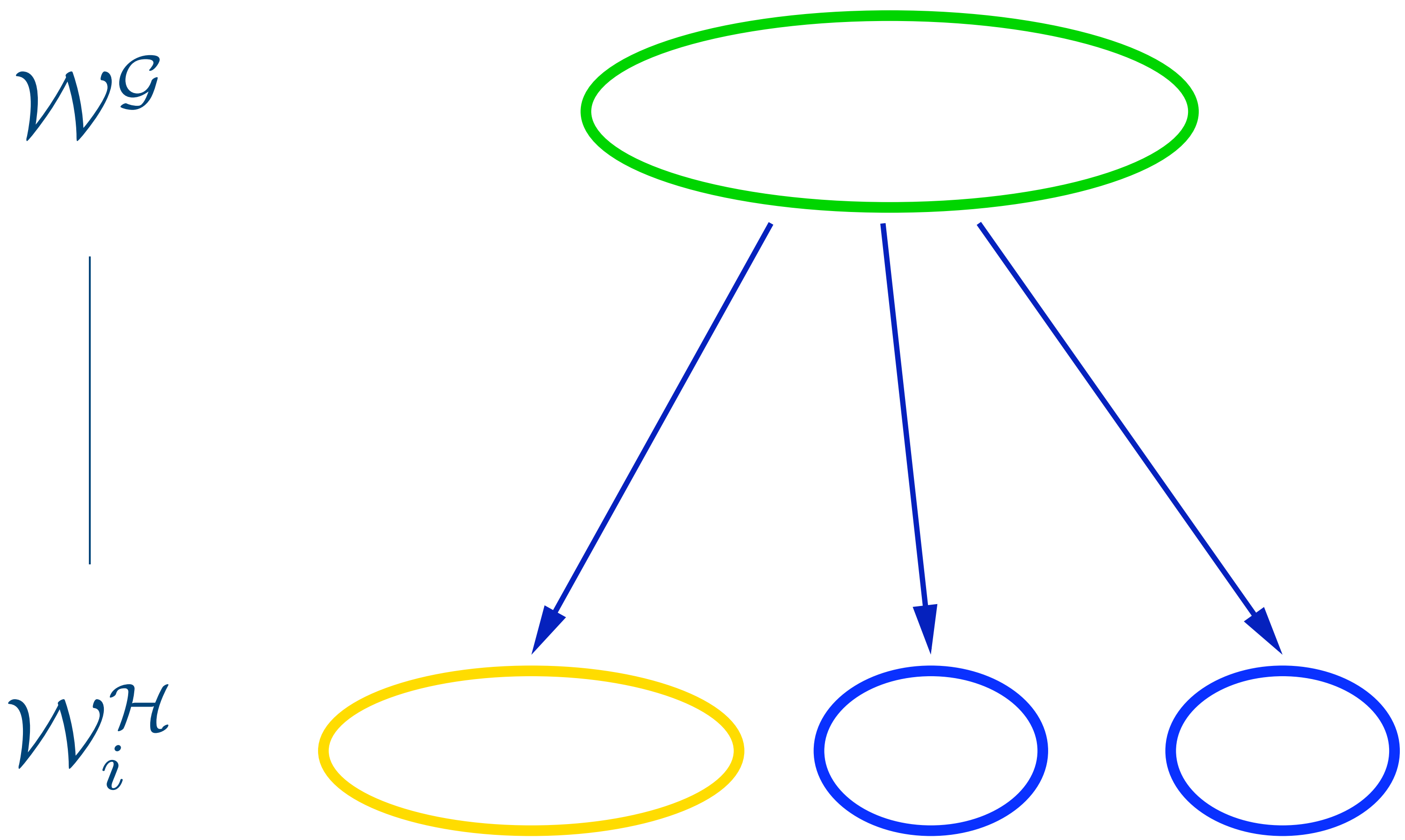
D_{4h}^{14} $P4_2/m2_1/n2/m$ No. 136 $P4_2/mnm$

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

Splittings of Wyckoff positions

General splitting rules

(Wondratschek 1993,1995)



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

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

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

WYCKSPLIT

GIVEN: Group-subgroup pair G>H
Transformation matrix (P,p)

PROCEDURE:

Step 1. Splitting of the general position X_o:

$$O_G(X_o) = \cup\, O_H(X_{o,k}) \Leftrightarrow G = \sum H g_k$$

Step 2. Splitting of the special positions X_i:

substitution $X_o \rightarrow X_i$
suborbits $O_H(X_{o,k}) \rightarrow O_H(X_{i,k})$

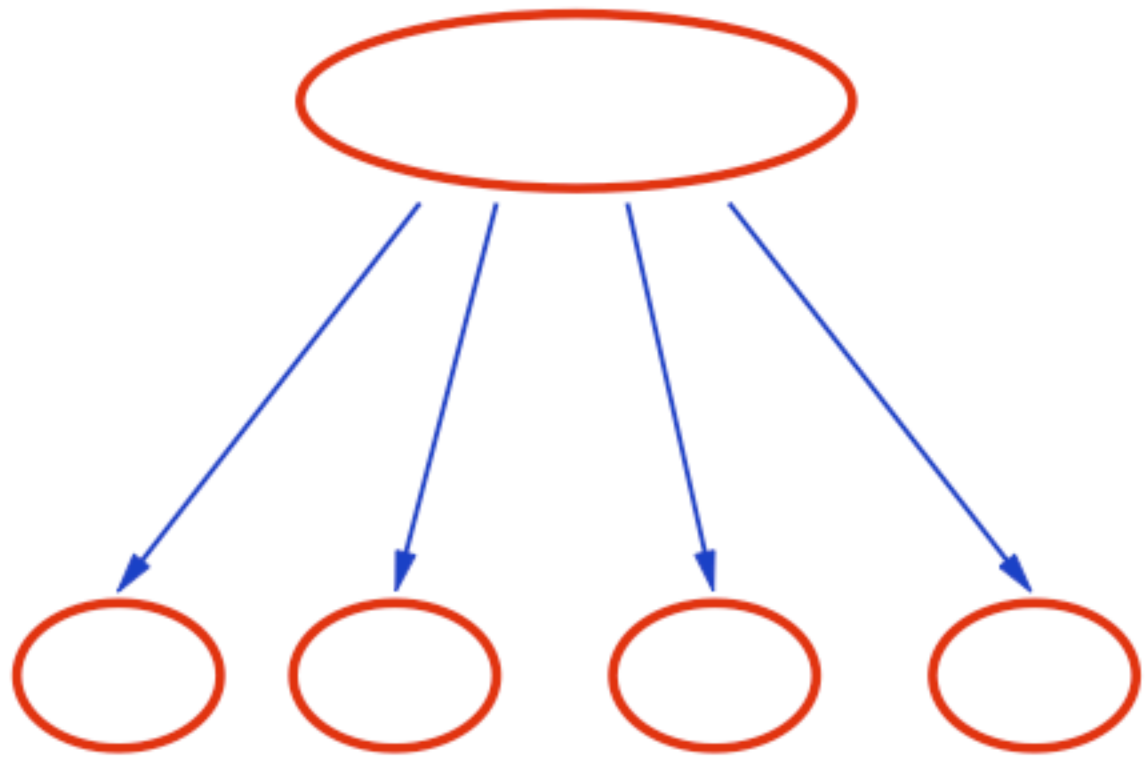
Step 3. Assignment of $O_H(X_{i,k})$ to W^P of H

relation between
representatives of W^P and $O_H(X_{i,k})$

SPLITTING OF THE GENERAL POSITION

TRANSFORM + COSETS

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



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

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

$$X = (x, y, z)$$
$$|\mathcal{S}_{\mathcal{G}}(X)| = 1$$

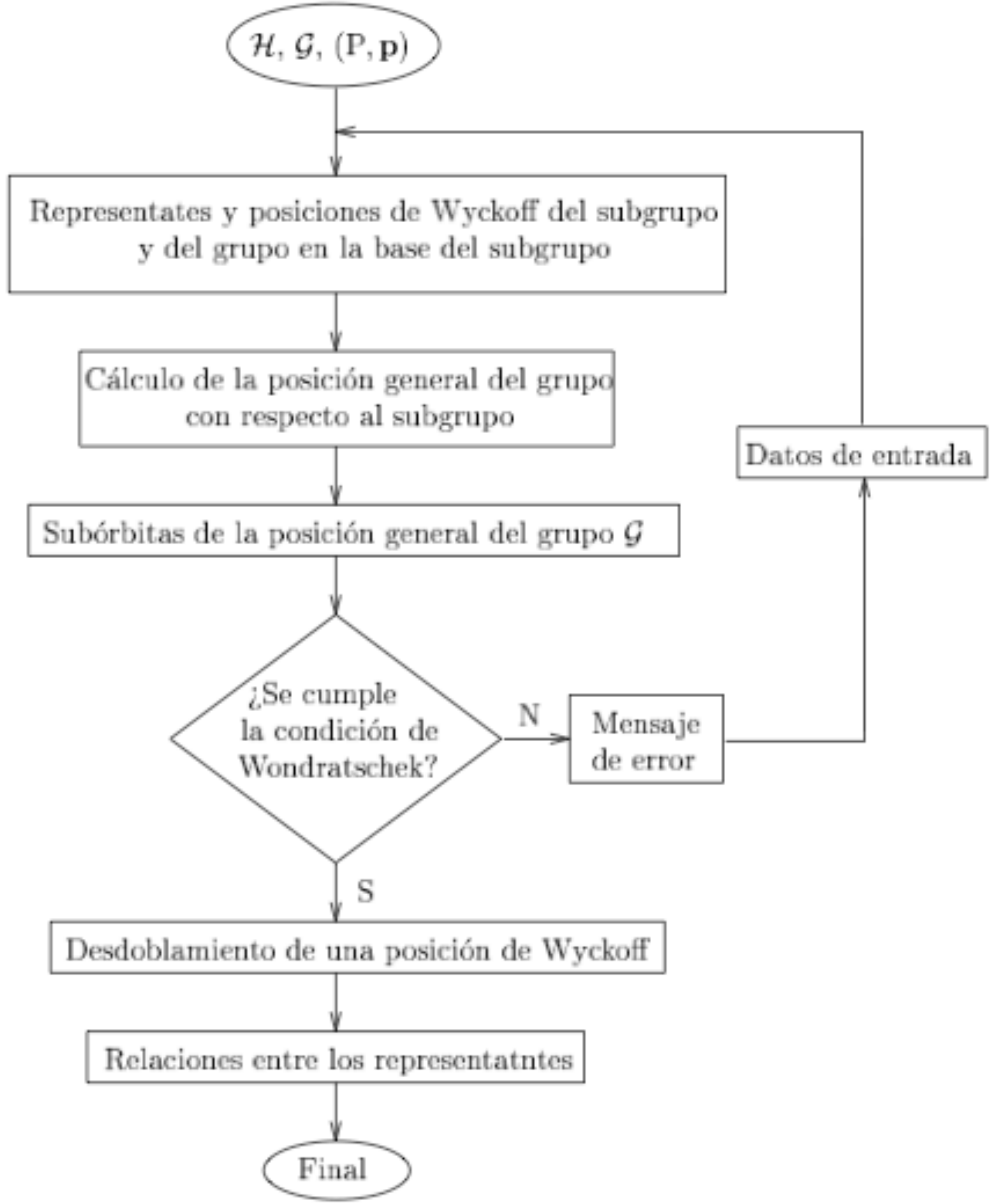
$$R_i = 1 \Rightarrow q = [i]$$

$$\mathcal{O}_{\mathcal{G}}(X_0) = \cup_{k=1}^{[i]} \mathcal{O}_{\mathcal{H}}(X_{0,k}) \Leftrightarrow \mathcal{G} = \sum_{k=1}^{[i]} \mathcal{H} g_k$$

FLOW-CHART

Wyckoff position splittings schemes

WYCKSPLIT



Eli Kroumova, PhD Thesis

EXAMPLE:

WYCKSPLIT: $P222 > P222_1$

$$(P,p) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$

Right coset decomposition

Coset 1

(x, y, z)
(-x, -y, z + 1/2)
(-x, y, -z + 1/2)
(x, -y, -z)

Coset 2

(x, y, z + 1/2)
(-x, -y, z)
(-x, y, -z)
(x, -y, -z + 1/2)

General position splitting

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, y, z)	(x, y, z)	$4e_1$	(x_1, y_1, z_1)
2	(-x, -y, z+1)	(-x, -y, z+1/2)		(-x_1, -y_1, z_1+1/2)
3	(-x, y, -z+1)	(-x, y, -z+1/2)		(-x_1, y_1, -z_1+1/2)
4	(x, -y, -z)	(x, -y, -z)		(x_1, -y_1, -z_1)
5	(-x, -y, z)	(-x, -y, z)	$4e_2$	(x_2, y_2, z_2)
6	(x, y, z+1)	(x, y, z+1/2)		(-x_2, -y_2, z_2+1/2)
7	(x, -y, -z+1)	(x, -y, -z+1/2)		(-x_2, y_2, -z_2+1/2)
8	(-x, y, -z)	(-x, y, -z)		(x_2, -y_2, -z_2)

EXAMPLE:

WYCKSPLIT: $P222 > P222_1$

Special position splitting

$(1a\ 000)_{P222} \longrightarrow (2a\ x00)_{P222_1}$

General position splitting

Coset 1

(*x*, *y*, *z*)
(-*x*, -*y*, *z* + 1/2)
(-*x*, *y*, -*z* + 1/2)
(*x*, -*y*, -*z*)

Coset 2

(*x*, *y*, *z* + 1/2)
(-*x*, -*y*, *z*)
(-*x*, *y*, -*z*)
(*x*, -*y*, -*z* + 1/2)

Substitution x=y=z=0

0,0,0
0,0,1/2
0,0,1/2
0,0,0

0,0,1/2
0,0,0
0,0,0
0,0,1/2

→

0,0,0
0,0,1/2

Assignment mult=2

4e (x, y, z)
2d (1/2 , y, 1/4
2c (0, y, 1/4)
2b (x, 1/2 , 0)
2a (x, 0, 0)

EXAMPLE: WYCKSPLIT: $P222 > P222_1$

Special position splitting

$$(2k\ x,½,0)_{P222} \longrightarrow 2*(2b\ x,½,0)_{P222_1}$$

General position splitting	Substitution y=1/2, z=0		Assignment mult=2

Coset 1

(*x*, *y*, *z*)
(-*x*, -*y*, *z* + 1/2)
(-*x*, *y*, -*z* + 1/2)
(*x*, -*y*, -*z*)

x,1/2,0	
-x,1/2,1/2	
-x,1/2,1/2	
x,1/2,0	

→

x,1/2,0	
-x,1/2,1/2	

Coset 2

(*x*, *y*, *z* + 1/2)
(-*x*, -*y*, *z*)
(-*x*, *y*, -*z*)
(*x*, -*y*, -*z* + 1/2)

x,1/2,1/2	
-x,1/2,0	
-x,1/2,0	
x,1/2,1/2	

→

-x,1/2,0	
x,1/2,1/2	

Assignment:

4e (x, y, z)
2d (1/2 , y, 1/4
2c (0, y, 1/4)
2b (x, 1/2 , 0)
2a (x, 0, 0)

EXAMPLE: WYCKSPLIT: $P222 > P222_1$

Output WYCKSPLIT

$(1a\ 000)_{P222} \longrightarrow (2a\ x00)_{P222_1}$

Group Wyckoff position **1*a*** representatives		Subgroup	
Group basis	Subgroup basis	Wyckoff position multiplicity and letter	Coordinate triplets
0, 0, 0	0, 0, 0	**2*a***	x_1, 0, 0
0, 0, 1	0, 0, 1/2		$-x_1$, 0, 1/2

$(2k\ x,½,0)_{P222} \longrightarrow 2*(2b\ x,½,0)_{P222_1}$

Group Wyckoff position **2*k*** representatives		Subgroup	
Group basis	Subgroup basis	Wyckoff position multiplicity and letter	Coordinate triplets
x, 1/2, 0	*x*, 1/2, 0	**2*b***	x_1, 1/2, 0
-*x*, 1/2, 1	-*x*, 1/2, 1/2		$-x_1$, 1/2, 1/2
x, 1/2, 1	*x*, 1/2, 1/2	**2*b***	$-x_2$, 1/2, 1/2
-*x*, 1/2, 0	-*x*, 1/2, 0		x_2, 1/2, 0

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≥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)

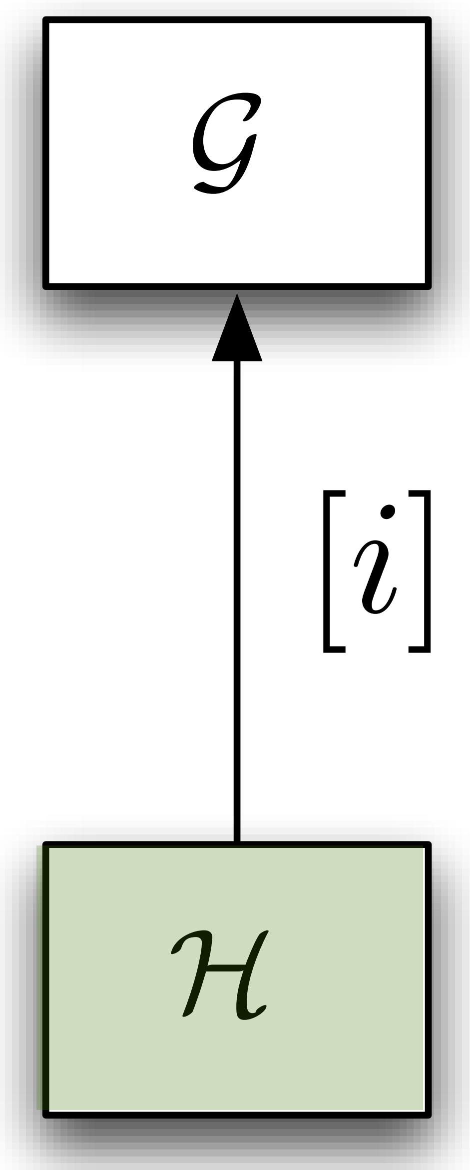
klassengleiche (k-type)

non-isomorphic   isomorphic

ITA1 data:

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

Group-supergroup relations



Applications

- ◇ Possible high-symmetry structures
- ◇ Prediction of phase transitions
- ◇ Prototype structures

AIM

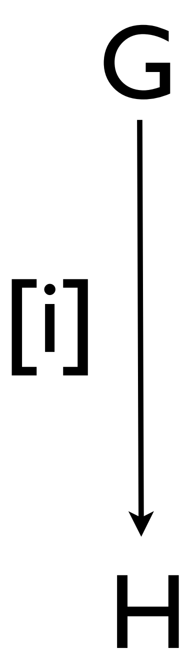
$$\mathcal{G} > \mathcal{H},\ [i]$$

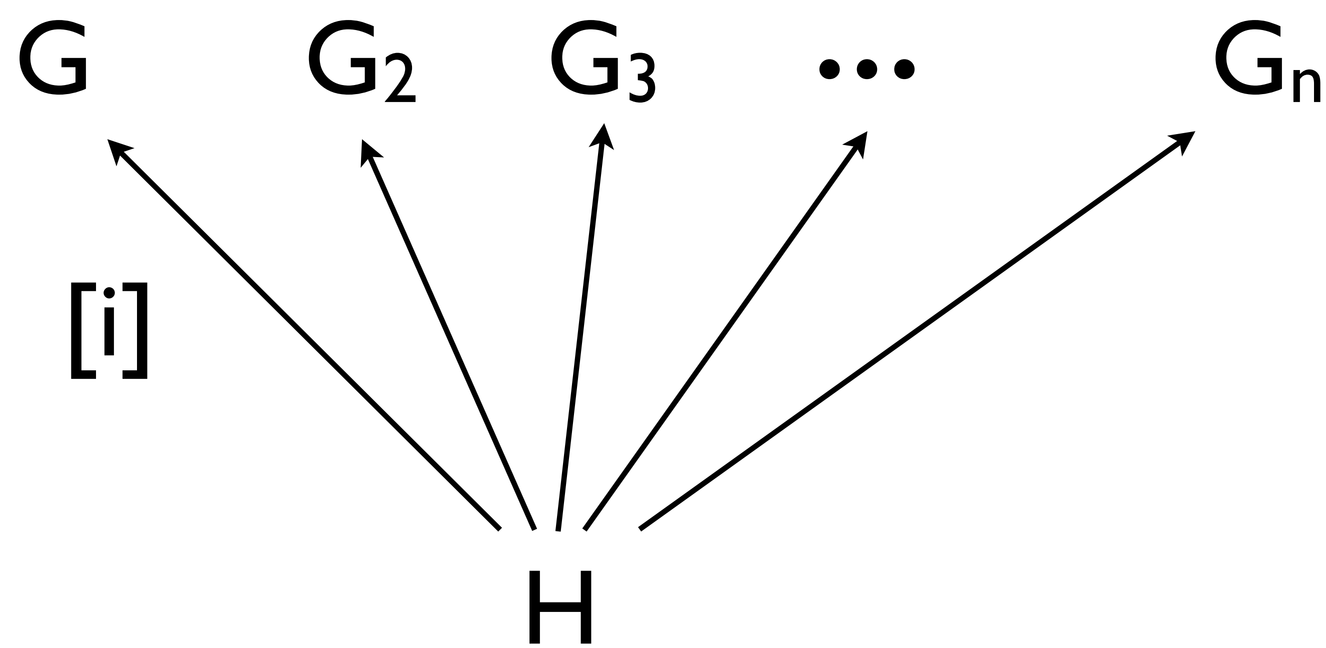
to obtain the $\mathcal{G}_k \overset{[i]}{\sim} \mathcal{G}$

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

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

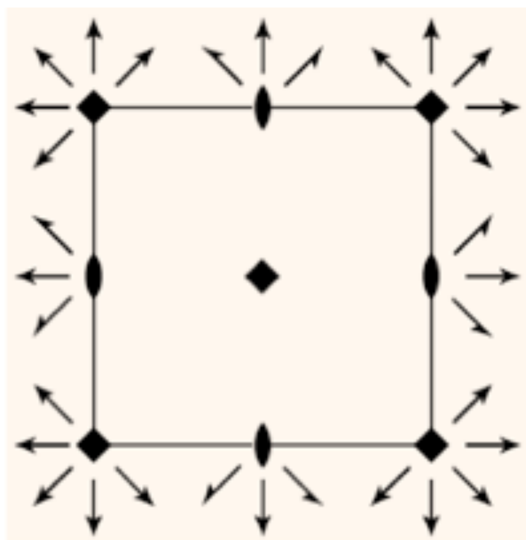
Example: Supergroup problem

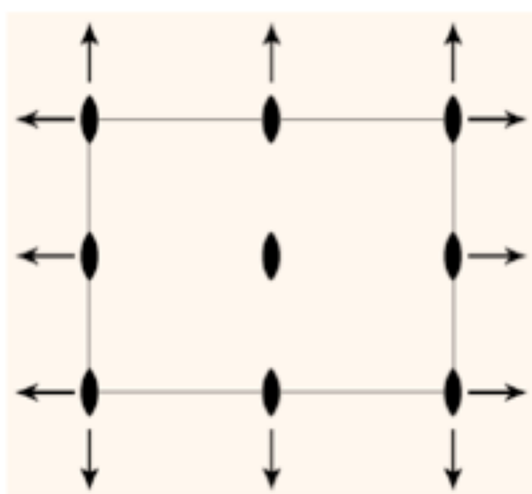
Group-subgroup pair P422>P222

P422

[2]

P222





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

Supergroups P422 of the group P222

$P4_z22$ $P4_x22$ $P4_y22$

[2]

P222

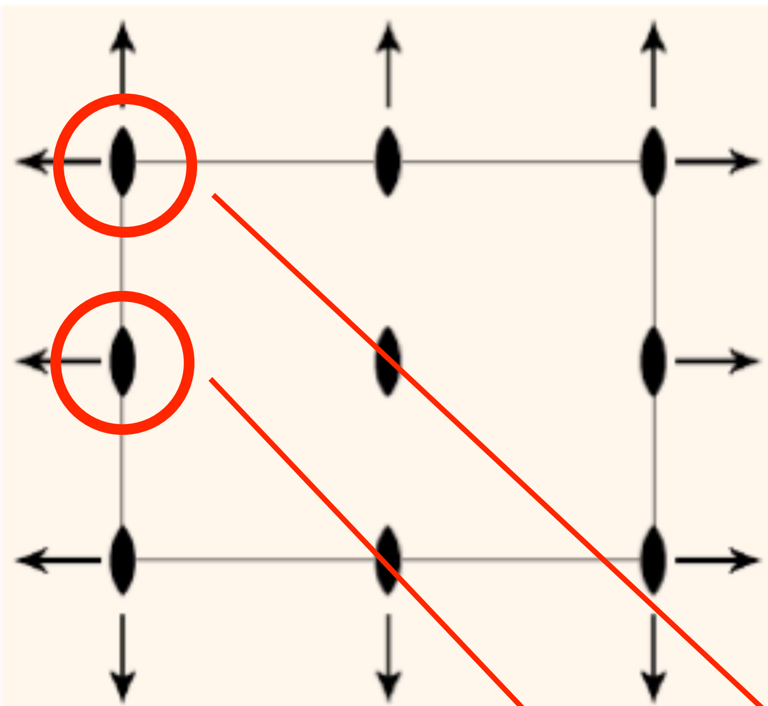
$P4_z22 = 222 + (222)(4_z,0)$

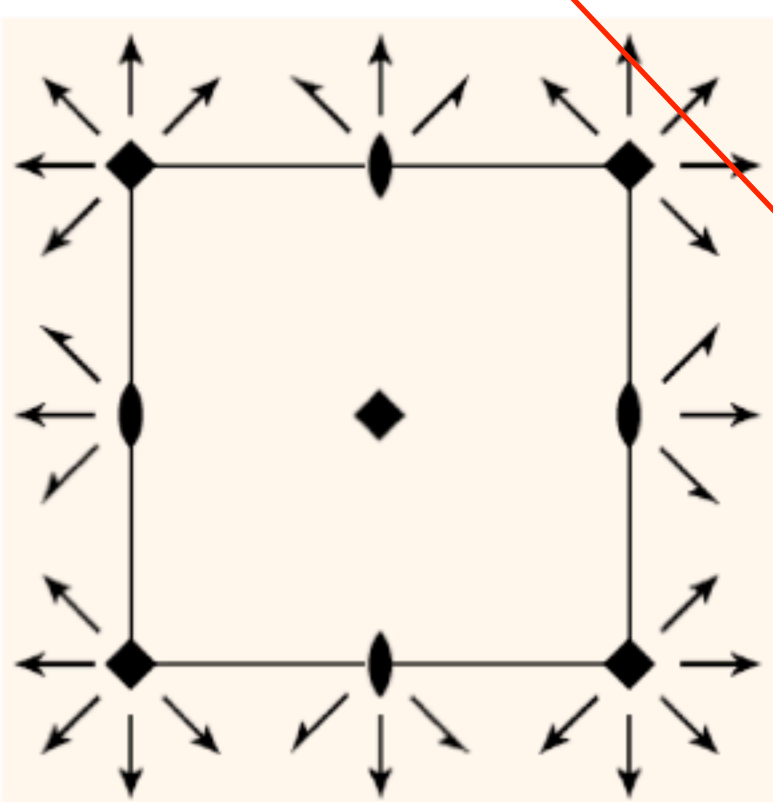
$P4_x22 = 222 + (222)(4_x,0)$

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

Are there more supergroups P422 of P222?

Example: Supergroups P422 of P222





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

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

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

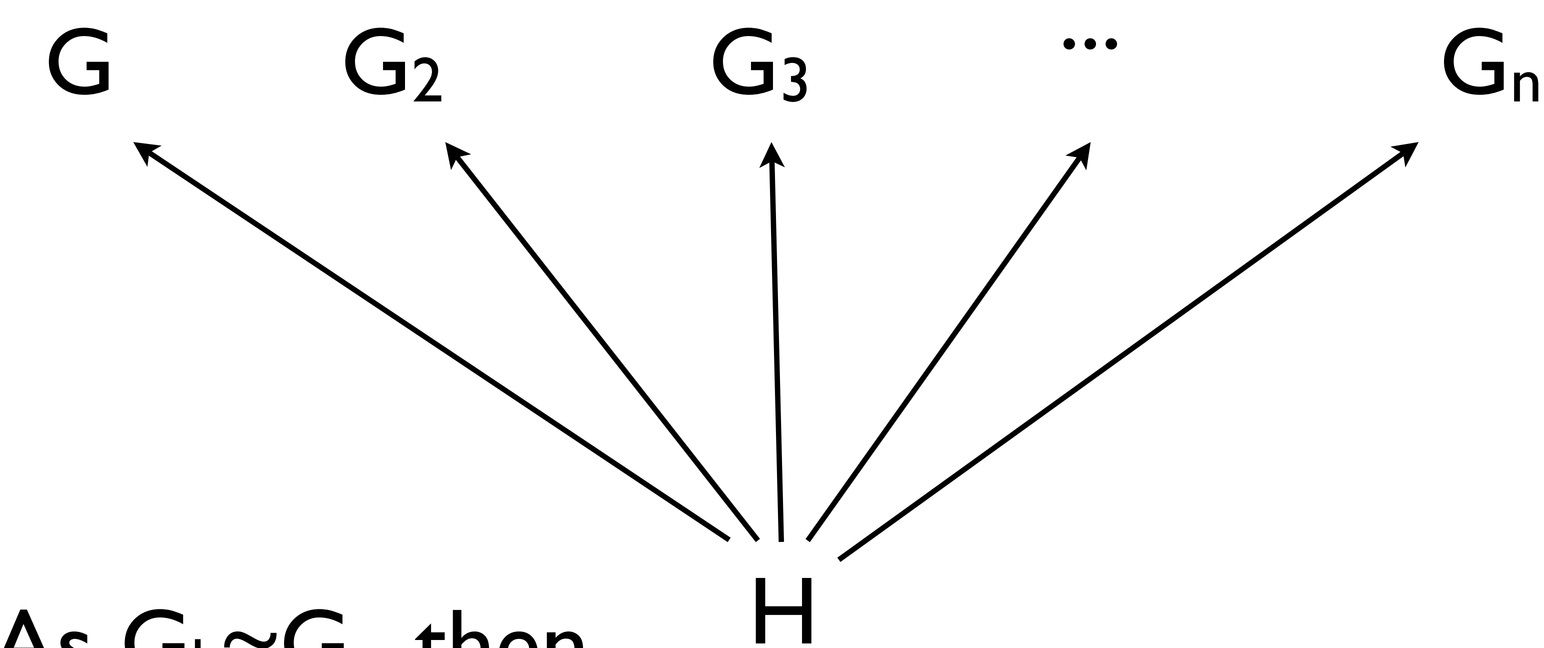
4 en		ω	$\mathcal{G}$
4_z	$(0,0,0)$	$(0,0,0)$	$(P422)_1$
4_y	$(0,0,0)$	$(0,0,0)$	$(P422)_2$
4_x	$(0,0,0)$	$(0,0,0)$	$(P422)_3$
4_z	$(\frac{1}{2},0,0)$	$(\frac{\bar{1}}{2},\frac{\bar{1}}{2},0)$	$(P422)'_1$
4_y	$(\frac{1}{2},0,0)$	$(\frac{1}{2},0,\frac{\bar{1}}{2})$	$(P422)'_2$
4_x	$(0,\frac{1}{2},0)$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

The Supergroup Problem

Group-subgroup pair $G>H$, (P,p)

H: general subgroup of G of index $[i]=n$

To determine: all $G_k>H$ of index $[i]=n$, $G_k \simeq G$



As $G_k \simeq G$, then

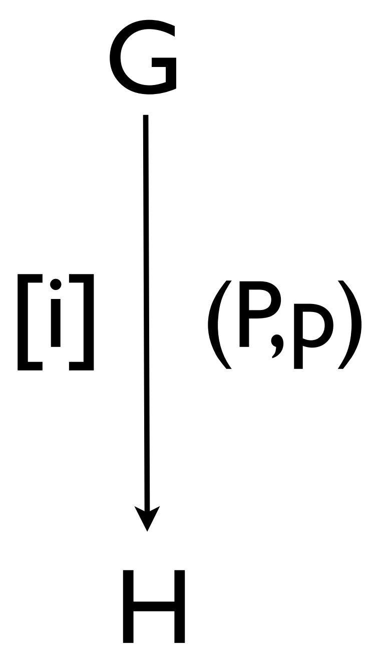
$G_k=a_k^{-1}Ga_k$ with $a_k \in \mathcal{A}$(affine)

How to determine the affine transformations a_k ?

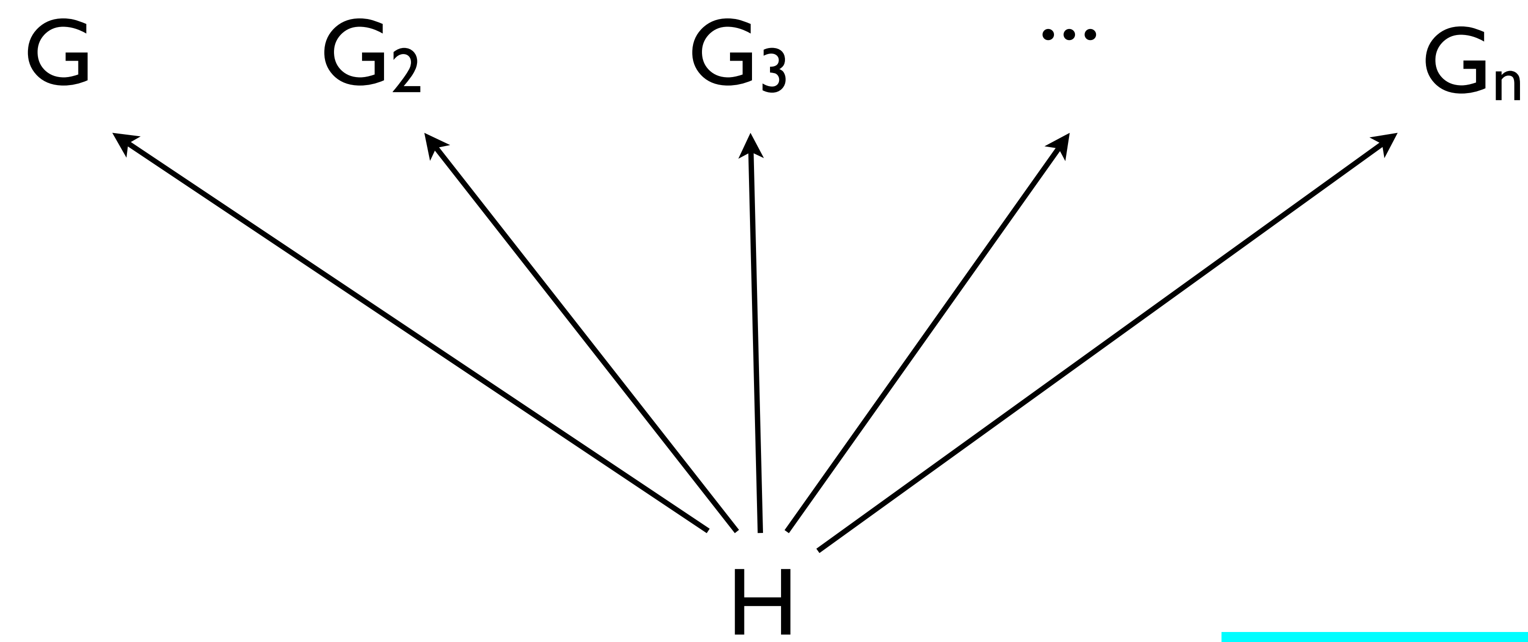
Case 1: $G_k = a_k^{-1} G a_k$ with $a_k \in \mathcal{N}(H)$ (normalizer procedure)

The Supergroup Problem

Given



To get:



(i) all $G_k > H$, that contain H as subgroup: $a_k \in N(H)$

(ii) different $G_k > H$: $a_k \notin N(G)$
a_k: coset representatives $[N(H):N(H) \cap N(G)]$

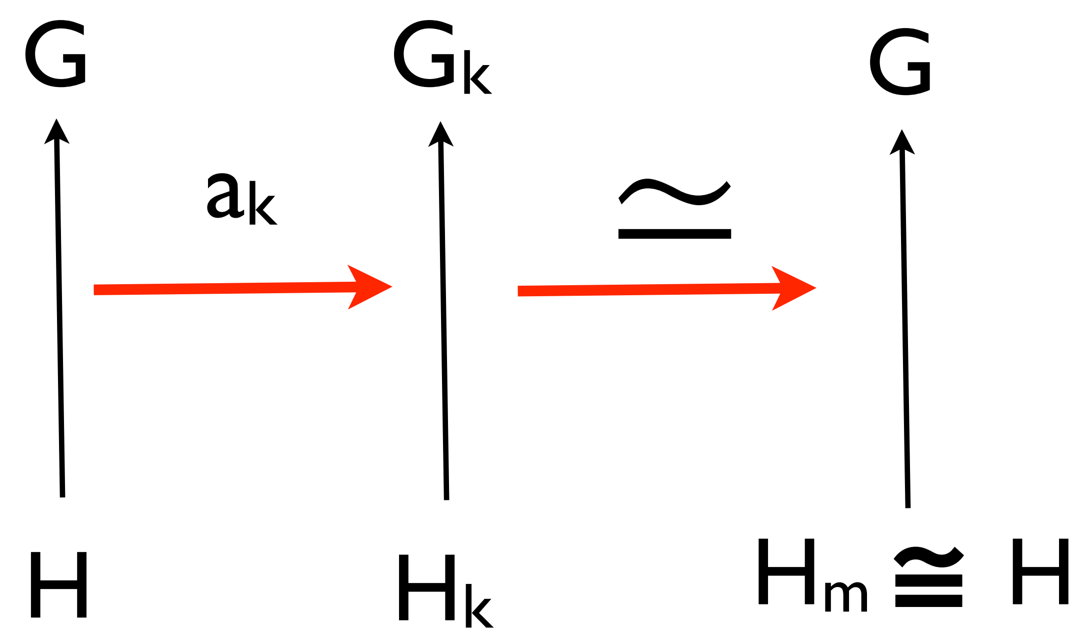
TRANSFORM

COSETS

$G>H: (P,p) \longrightarrow G_k>H: (P,p)\, a_k$

Case 2: $G_k=a_k^{-1}Ga_k$ with $a_k \notin \mathcal{N}(H)$

Given: G, H, index i



different $G_k>H$:

normalizer procedure
over different $H_m<G$, $(P,p)_m$

Supergroups calculation: SUPERGROUPS

ITA1: $\mathcal{G}$, $\mathcal{H}$, $(\mathrm{P}, \mathbf{p})$

$\downarrow$

Normalizer method

$\downarrow$

Different supergroups $\mathcal{G}_k \overset{[i]}{\sim} \mathcal{G} > \mathcal{H}$

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

Special cases

Polar groups:

Infinite number of supergroups $\mathcal{G}_k \overset{[i]}{\sim} \mathcal{G}$

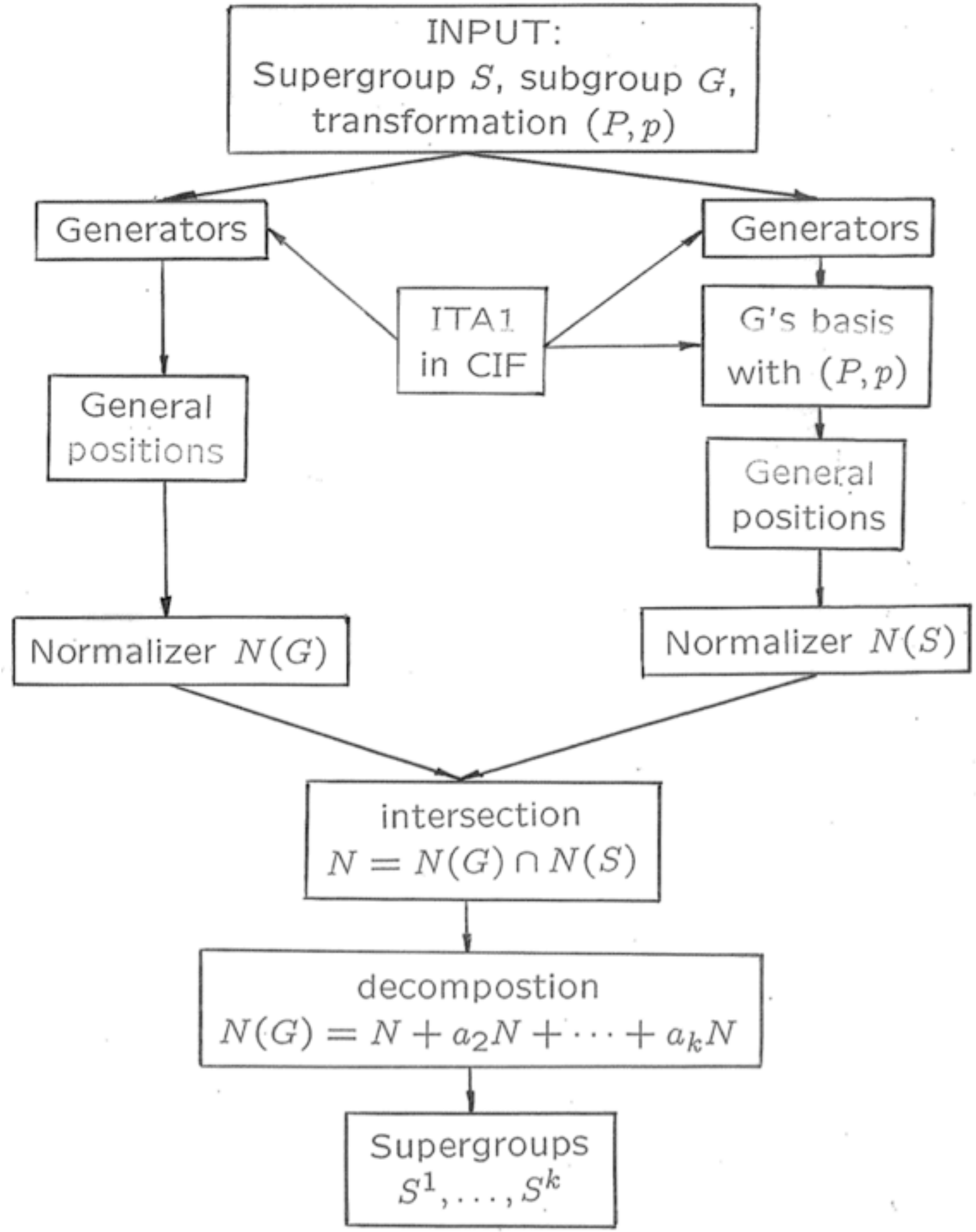
Monoclinic groups and triclinic:

normalizers ''enhanced''

FLOW-CHART

Calculation of Supergroups

Normalizer method



Eli Kroumova, PhD Thesis

Problem: Common supergroups COMMONSUPER

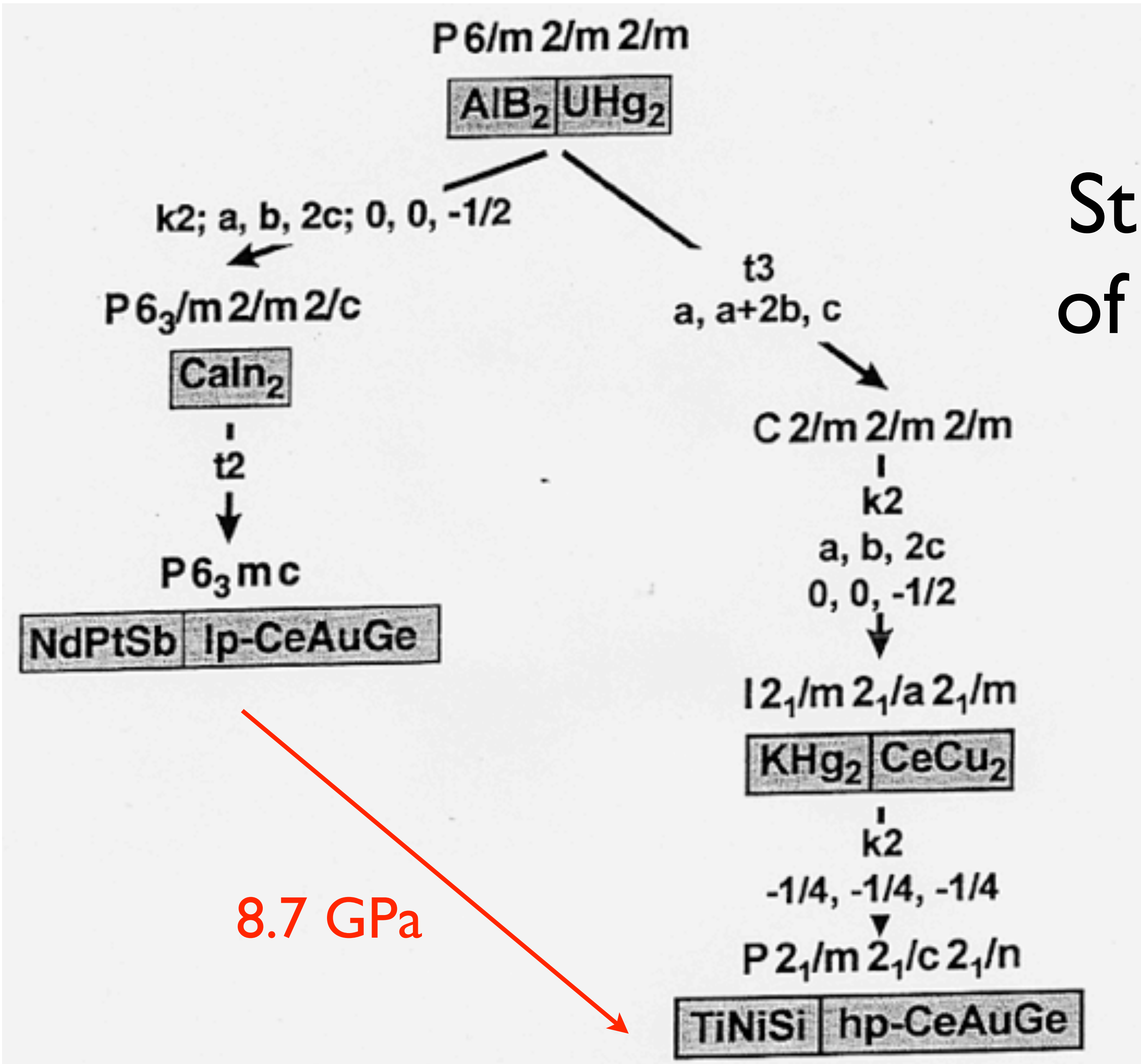


Fig. 7. *Bärnighausen* tree of the group-subgroup relationship [17] of the AlB_2-type and the distorted low-pressure (lp) and high-pressure (hp) modifications of CeAuGe (excerpt of Fig. 3. in Ref. [1]). The indices of the *klassengleiche* (*k*) and *translationengleiche* (*t*) transitions, as well as the unit cell transformations and origin shifts are given.

Structural phase transitions of CeAuGe at high pressure

Brouskov *et al.*

Z. Kristallogr. 220(2005) 122

Transition-path candidates

Common Subgroup H					Branch $G_1 > H$			Branch $G_2 > H$		
N	HM Symbol	P_H	Z_H	ITA	i_1	it_1	ik_1	i_2	it_2	ik_2
1	$Pna2_1$	mm2	4	033	6	3	2	2	2	1
2	$Pmn2_1$	mm2	4	031	6	3	2	2	2	1
3	$Pmc2_1$	mm2	4	026	6	3	2	2	2	1
4	Pc	m	4	007	12	6	2	4	4	1
5	Pm	m	4	006	12	6	2	4	4	1
6	$P2_1$	2	4	004	12	6	2	4	4	1
7	$P1$	1	4	001	24	12	2	8	8	1