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INTRODUCTION TO THE BILBAO CRYSTALLOGRAPHIC SERVER

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FCT/ZTF

bilbao crystallographic server

UPV/EHU

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

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

Sections

Retrieval Tools
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Representations
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New programs and updates:

- **COMMONSUPER**
  5-2006: New program for obtaining common supergroups of two space groups
- **SETSTRU**
  4-2006: Alternative settings for a given crystal structure.
- **WYCKPOS**
  4-2006: Space Group ITA Settings available for WYCKPOS program.

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 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.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

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Crystallographic databases and computing programs

Structural utilities

Solid-state applications

Representation theory applications

Phase-transition problems

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

Generators and General Positions

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 button [`choose it`].

To see the data in a non conventional setting click on [`Non conventional Setting`]. Otherwise, click on [`Conventional Setting`].

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

choose it 15

Show:

Generators only

All General Positions

Conventional Setting | Non Conventional Setting | ITA Settings

[Bilbao Crystallographic Server Main Menu]

International Tables for Crystallography

- Generators
- Wyckoff Positions
- Wyckoff Sets
- Normalizers
- Maximal subgroups
- Series of maximal isomorphic subgroups
- Minimal supegroups
- Relation between Wyckoff positions
- Generators
- Wyckoff Positions
- Wyckoff Sets
- Normalizers
- Maximal subgroups

$I4/mmm$ No. 139 $I4/m2/m2/m$ D_{4h}^{17}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32 o 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
	(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
	(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

GENPOS

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2m$ (121)	$(1;\ 2;\ 5;\ 6;\ 11;\ 12;\ 15;\ 16)+$	
[2] $I\bar{4}m2$ (119)	$(1;\ 2;\ 7;\ 8;\ 11;\ 12;\ 13;\ 14)+$	
[2] $I4mm$ (107)	$(1;\ 2;\ 3;\ 4;\ 13;\ 14;\ 15;\ 16)+$	
[2] $I422$ (97)	$(1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8)+$	
[2] $I4/m11$ (87, $I4/m$)	$(1;\ 2;\ 3;\ 4;\ 9;\ 10;\ 11;\ 12)+$	
[2] $I2/m2/m1$ (71, $Immm$)	$(1;\ 2;\ 5;\ 6;\ 9;\ 10;\ 13;\ 14)+$	
[2] $I2/m12/m$ (69, $Fmmm$)	$(1;\ 2;\ 7;\ 8;\ 9;\ 10;\ 15;\ 16)+$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2/nmc$ (137)	$1;\ 2;\ 7;\ 8;\ 11;\ 12;\ 13;\ 14;\ (3;\ 4;\ 5;\ 6;\ 9;\ 10;\ 15;\ 16)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,3/4,1/4$
[2] $P4_2/mnm$ (136)	$1;\ 2;\ 7;\ 8;\ 9;\ 10;\ 15;\ 16;\ (3;\ 4;\ 5;\ 6;\ 11;\ 12;\ 13;\ 14)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
[2] $P4_2/nnm$ (134)	$1;\ 2;\ 5;\ 6;\ 11;\ 12;\ 15;\ 16;\ (3;\ 4;\ 7;\ 8;\ 9;\ 10;\ 13;\ 14)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,3/4,1/4$
[2] $P4_2/mmc$ (131)	$1;\ 2;\ 5;\ 6;\ 9;\ 10;\ 13;\ 14;\ (3;\ 4;\ 7;\ 8;\ 11;\ 12;\ 15;\ 16)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$0,1/2,0$
[2] $P4/nmm$ (129)	$1;\ 2;\ 3;\ 4;\ 13;\ 14;\ 15;\ 16;\ (5;\ 6;\ 7;\ 8;\ 9;\ 10;\ 11;\ 12)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[2] $P4/mnc$ (128)	$1;\ 2;\ 3;\ 4;\ 9;\ 10;\ 11;\ 12;\ (5;\ 6;\ 7;\ 8;\ 13;\ 14;\ 15;\ 16)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
[2] $P4/nnc$ (126)	$1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8;\ (9;\ 10;\ 11;\ 12;\ 13;\ 14;\ 15;\ 16)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[2] $P4/mmm$ (123)	$1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8;\ 9;\ 10;\ 11;\ 12;\ 13;\ 14;\ 15;\ 16$	

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4/mmm$ (139)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

MAXSUB

- **Series of maximal isomorphic subgroups**

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

$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

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

$I4/mmm$ (139)	$\langle(2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

SERIES

I Minimal *translationengleiche* supergroups

[3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4/mmm$ (123, $P4/mmm$)

MINSUP

ITA space group *P4mm*

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

GENPOS

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

WYCKPOS

Reflection conditions	
General:	
no conditions	
Special:	
no extra conditions	
no extra conditions	
no extra conditions	
hkl : $h+k=2n$	
no extra conditions	
no extra conditions	

Symmetry of special projections

Along [001] *p*4*mm*
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] *p*1*m*1
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

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

MAXSUB

Maximal non-isomorphic subgroups

I [2]*P*4 1 1 (*P*4, 75) 1; 2; 3; 4
[2]*P*2 1*m* (*Cmm*2, 35) 1; 2; 7; 8
[2]*P*2*m*1 (*Pmm*2, 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]$C4md(\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b})$(*P*4*bm*, 100); [2]$F4mc(\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c})$(*I*4*cm*, 108); [2]$F4mm(\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c})$(*I*4*mm*, 107)

SERIES

Maximal isomorphic subgroups of lowest index

IIc [2]$P4mm(\mathbf{c}'=2\mathbf{c})$(99); [2]$C4mm(\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b})$(*P*4*mm*, 99)

MINSUP

Minimal non-isomorphic supergroups

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

II [2]*I*4*mm*(107)

NEW DATABASES

- Monoclinic and orthorhombic ITA Settings — GENPOS WYCKPOS SETSTRU
- Series of maximal isomorphic subgroups — SERIES
- Normalizers and Wyckoff Sets — NORMALIZER WYCKSETS
- Reflection conditions — HKLCOND
- Subperiodic group data: generators, general positions, Wyckoff positions and Maximal subgroups — GENPOS WYCKPOS MAXSUB

530 non-conventional settings of orthorhombic and monoclinic groups

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

Table 4.3.1 (*cont.*)

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						Unique axis *b* Unique axis *c* Unique axis *a*
			ab**c**	c**b̄**a	ab**c̄**	ba**c̄**	**a**bc	**ā**cb	
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$	$A121$	$A112$	$B112$	$B211$	$C211$	Cell choice 1
			$A121$	$C121$	$B112$	$A112$	$C211$	$B211$	Cell choice 2
			$I121$	$I121$	$I112$	$I112$	$I211$	$I211$	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$	$A1m1$	$A11m$	$B11m$	$Bm11$	$Cm11$	Cell choice 1
			$A1m1$	$C1m1$	$B11m$	$A11m$	$Cm11$	$Bm11$	Cell choice 2
			$I1m1$	$I1m1$	$I11m$	$I11m$	$Im11$	$Im11$	Cell choice 3
9	C_s^4	Cc	$C1c1$	$A1a1$	$A11a$	$B11b$	$Bb11$	$Cc11$	Cell choice 1
			$A1n1$	$C1n1$	$B11n$	$A11n$	$Cn11$	$Bn11$	Cell choice 2
			$I1a1$	$I1c1$	$I11b$	$I11a$	$Ic11$	$Ib11$	Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	
12	C_{2h}^3	$C2/m$	$C1\frac{2}{m}1$	$A1\frac{2}{m}1$	$A11\frac{2}{m}$	$B11\frac{2}{m}$	$B\frac{2}{m}11$	$C\frac{2}{m}11$	Cell choice 1
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	
			$A1\frac{2}{m}1$	$C1\frac{2}{m}1$	$B11\frac{2}{m}$	$A11\frac{2}{m}$	$C\frac{2}{m}11$	$B\frac{2}{m}11$	Cell choice 2
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	

Settings for the Space Group 15

Note: The transformation matrices must be read by columns

ITA number	Setting	P	P^{-1}
15	*C* 1 2/*c* 1	a,b,c	a,b,c
15	*A* 1 2/*n* 1	a+c,b,-a	-c,b,a+c
15	*I* 1 2/*a* 1	c,b,-a+c	a-c,b,a
15	*A* 1 2/*a* 1	c,b,-a	-c,b,a
15	*C* 1 2/*n* 1	a-1/4,b+1/4,c	a+1/4,b-1/4,c
15	*I* 1 2/*c* 1	a+c,b,c	a-c,b,c
15	*A* 1 1 2/*a*	c,a,b	b,c,a
15	*B* 1 1 2/*n*	-a,a+c,b	-a,c,a+b
15	*I* 1 1 2/*b*	-a+c,c,b	-a+b,c,b
15	*B* 1 1 2/*b*	-a,c,b	-a,c,b
15	*A* 1 1 2/*n*	a+c,a,b	b,c,a-b
15	*I* 1 1 2/*a*	c,a+c,b	-a+b,c,a
15	*B* 2/*b* 1 1	b,c,a	c,a,b
15	*C* 2/*n* 1 1	b,-a,a+c	-b,a,b+c
15	*I* 2/*c* 1 1	b,-a+c,c	-b+c,a,c
15	*C* 2/*c* 1 1	b,-a,c	-b,a,c
15	*B* 2/*n* 1 1	b,a+c,a	c,a,b-c
15	*I* 2/*b* 1 1	b,c,a+c	-b+c,a,b

The program WYCKSETS

- Affine/Euclidean Normalizer generators
- Coset decomposition of the Euclidean/Affine Normalizers N(G) with respect to the space group G
- Sets of equivalent point configurations
- http://www.cryst.ehu.es/cryst/wycksets.html

Wyckoff Sets of Space Group 99 (*P4mm*)

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

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

[Show Wyckoff Positions]

Cosets representatives of the Affine Normalizer with respect to the Space Group 99 (*P4mm*)

The Affine normalizer coincides with the *Euclidean* one.

Transformation of the Wyckoff Positions of Space Group 99 (*P4mm*) under Affine Normalizer N(G):

Index: 4*(infinite)

Coset Representative		Transformed WP
x,y,z	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	a b c d e f g
x+1/2,y+1/2,z	[1 0 0] [1/2] [0 1 0] [1/2] [0 0 1] [0]	b a c d f e g
-x,-y,-z	[-1 0 0] [0] [0 -1 0] [0] [0 0 -1] [0]	a b c d e f g
-x+1/2,-y+1/2,-z	[-1 0 0] [1/2] [0 -1 0] [1/2] [0 0 -1] [0]	b a c d f e g
x,y,z+t	[1 0 0] [0] [0 1 0] [0] [0 0 1] [t]	a b c d e f g

NON CONVENTIONAL DATA (ITA SETTINGS)

Monoclinic descriptions

	Transf.	**abc**	**cb̄a**	**abc**	**ba$\bar{c}$**	**abc**	**ācb**	Monoclinic axis b Monoclinic axis c Monoclinic axis a
HM	$C2/c$	$C12/c1$ $A12/n1$ $I12/a1$	$A12/a1$ $C12/n1$ $I12/c1$	$A112/a$ $B112/n$ $I112/b$	$B112/b$ $A112/n$ $I112/a$	$B2/b11$ $C2/n11$ $I2/c11$	$C2/c11$ $B2/n11$ $I2/b11$	Cell type 1 Cell type 2 Cell type 3

Orthorhombic descriptions

No.	HM	**abc**	**ba$\bar{c}$**	**cab**	**c̄ba**	**bca**	**ac̄b**
33	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$

Example ITA1: Space group I4/mmm

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		
32	o 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
		(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
		(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
		(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

GENPOS

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+	
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+	
[2] $I4mm$ (107)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+	
[2] $I4/m11$ (87, $I4/m$)	(1; 2; 3; 4; 9; 10; 11; 12)+	
[2] $I2/m2/m1$ (71, $Immm$)	(1; 2; 5; 6; 9; 10; 13; 14)+	
[2] $I2/m12/m$ (69, $Fmmm$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$

MAXSUB

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2/nmc$ (137)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,3/4,1/4
[2] $P4_2/mnm$ (136)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4_2/nnm$ (134)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,3/4,1/4
[2] $P4_2/mmc$ (131)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		0,1/2,0
[2] $P4/nmm$ (129)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,1/4,1/4
[2] $P4/mnc$ (128)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4/nnc$ (126)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,1/4,1/4
[2] $P4/mmm$ (123)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16		

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4/mmm$ (139)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,1
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,2

- **Series of maximal isomorphic subgroups**

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

$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

SERIES

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

$I4/mmm$ (139)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

MINSUP

Series of Maximal subgroups of group 99 (*P4mm*)

Note: Only series with an index less equal 27 will be displayed

Serie 1

Subgroup: *P4mm* (99)

Index: p

Transformation:
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & p & 0 \end{bmatrix}$$

Condition(s): p > 1

Static Databases

N	Subgroup	HM Symbol	Index	Setting ...
1	99	*P4mm*	2	setting...
2	99	*P4mm*	3	setting...
3	99	*P4mm*	5	setting...
4	99	*P4mm*	7	setting...
5	99	*P4mm*	11	setting...
6	99	*P4mm*	13	setting...
7	99	*P4mm*	17	setting...
8	99	*P4mm*	19	setting...
9	99	*P4mm*	23	setting...

SERIES OF MAXIMAL ISOMORPHIC SUBGROUPS

Serie 1

Subgroup: *I*4/*m* (87)

Index: p

Transformation:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & p & u/2 \end{bmatrix}$$

Condition(s): $p > 2$
$0 <= u < p$

Infinite number of maximal isomorphic subgroups

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.

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 or

Maximum index:

Optional: only subgroups with the chosen index

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

NOTE: the maximum index available is 131.

Show series

Data generated online

[Bilbao Crystallographic Server Main Menu]

SERIES OF MAXIMAL ISOMORPHIC SUBGROUPS

N	Subgroup	HM Symbol	Index	Setting ...
1	87	*I*4/*m*	3	setting...
2	87	*I*4/*m*	5	setting...
3	87	*I*4/*m*	7	setting...
4	87	*I*4/*m*	11	setting...
5	87	*I*4/*m*	13	setting...
6	87	*I*4/*m*	17	setting...
7	87	*I*4/*m*	19	setting...
8	87	*I*4/*m*	23	setting...

Space group *I*4/*m* (87)

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

Representation Data

Representations of space and point groups

k-vector data

Brillouin zones
representation domains
parameter ranges

POINT

character tables
multiplication tables
symmetrized products

Databases

Retrieval tools

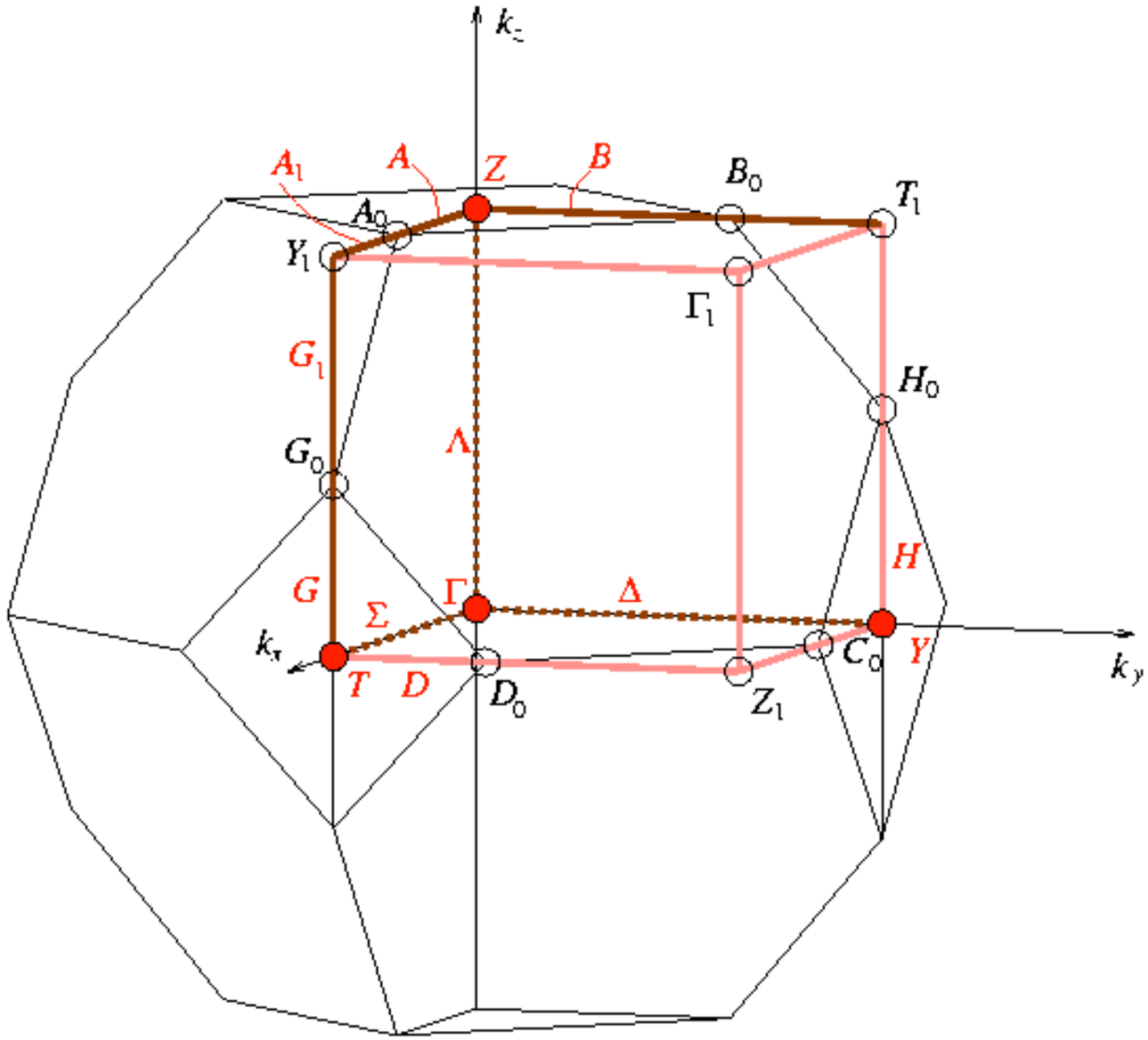
Brillouin zone

(Diagram for arithmetic crystal class 222F)

($a^{-2}<b^{-2}+c^{-2}$, $b^{-2}<c^{-2}+a^{-2}$, and $c^{-2}<a^{-2}+b^{-2}$) F222-D_2^7 (22)

Reciprocal-space group (I222)*, No. 23:(a*2<b*2+c*2, b*2<c*2+a*2 , and c*2<a*2+b*2)

The table with the k vectors.



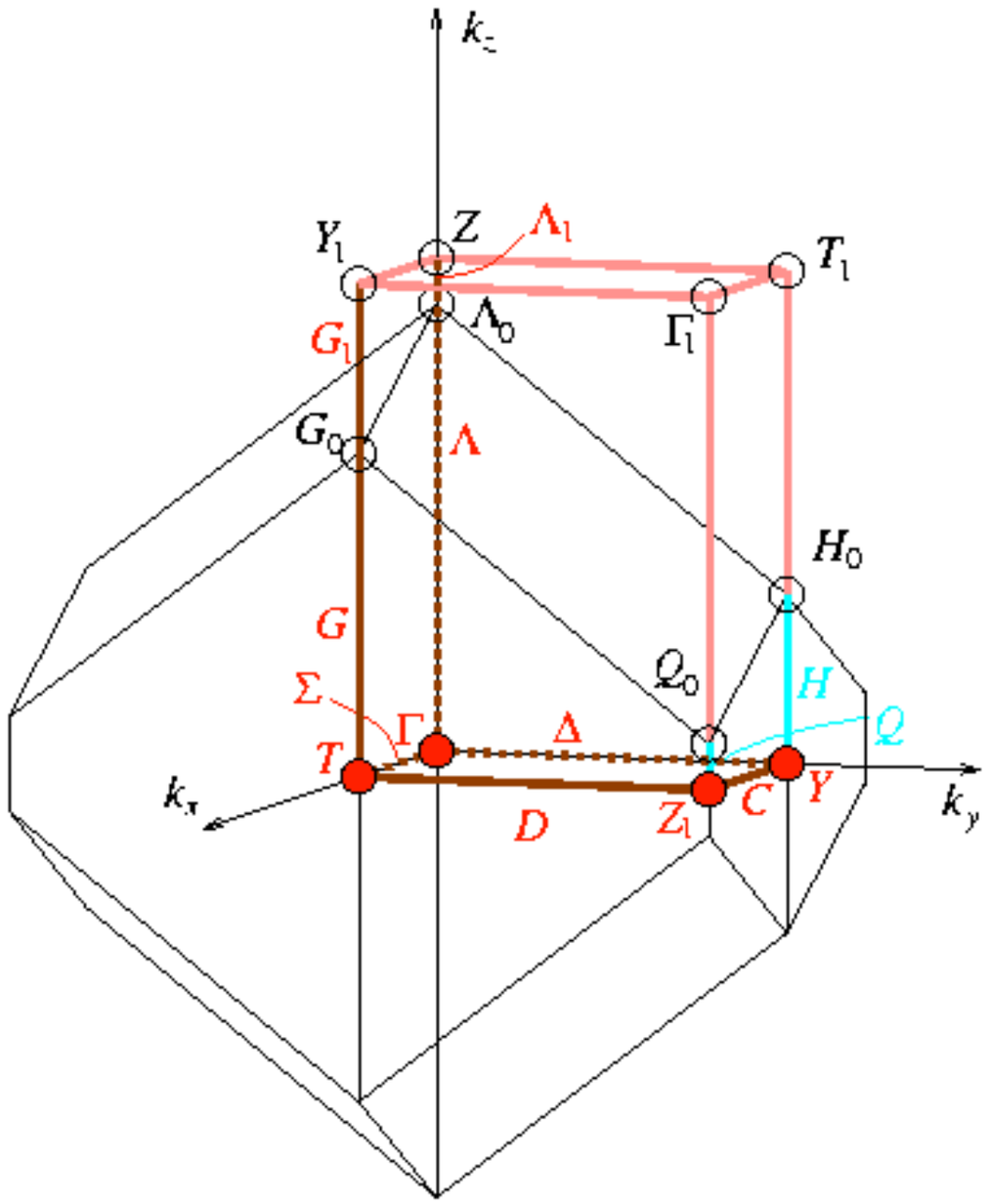
Brillouin zone

(Diagram for arithmetic crystal class 222F)

($c^{-2}>a^{-2}+b^{-2}$) F222-D_2^7 (22)

Reciprocal space group (I222)*, No.23: c*2>a*2+b*2

The table with the k vectors.



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

(Table for arithmetic crystal class 222F)

($a^{-2}<b^{-2}+c^{-2}$, $b^{-2}<c^{-2}+a^{-2}$, and $c^{-2}<a^{-2}+b^{-2}$) F222-D_2^7 (22)

Reciprocal space group (I222)*, No.23

Brillouin zone

k-vector label		Wyckoff position			Parameters
CDML		ITA			ITA
GM	0,0,0	2	a	222	0,0,0
T	0,1/2,1/2	2	b	222	1/2,0,0
Z	1/2,1/2 ,0	2	c	222	0,0,1/2
Y	1/2, 0, 1/2	2	d	222	0,1/2,0
SM	0, u, u	4	e	2..	x,0,0: 0<x<1/2
A	1/2, 1/2+u, u ex	4	f	2..	x,0,1/2 : 0<x<= a_0
C	1/2, u, 1/2+u ex	4	f	2..	x,1/2,0: 0<x<c_0
C ~ A_1 ex		4	f	2..	x,0,1/2 : a_0<x<1/2
A + A_1		4	f	2..	x,0,1/2 : 0<x<1/2

Brillouin-zone database

3-d Brillouin-zone figures for hexagonal and trigonal groups

The k-vector Types of Group 150 [*P*321]

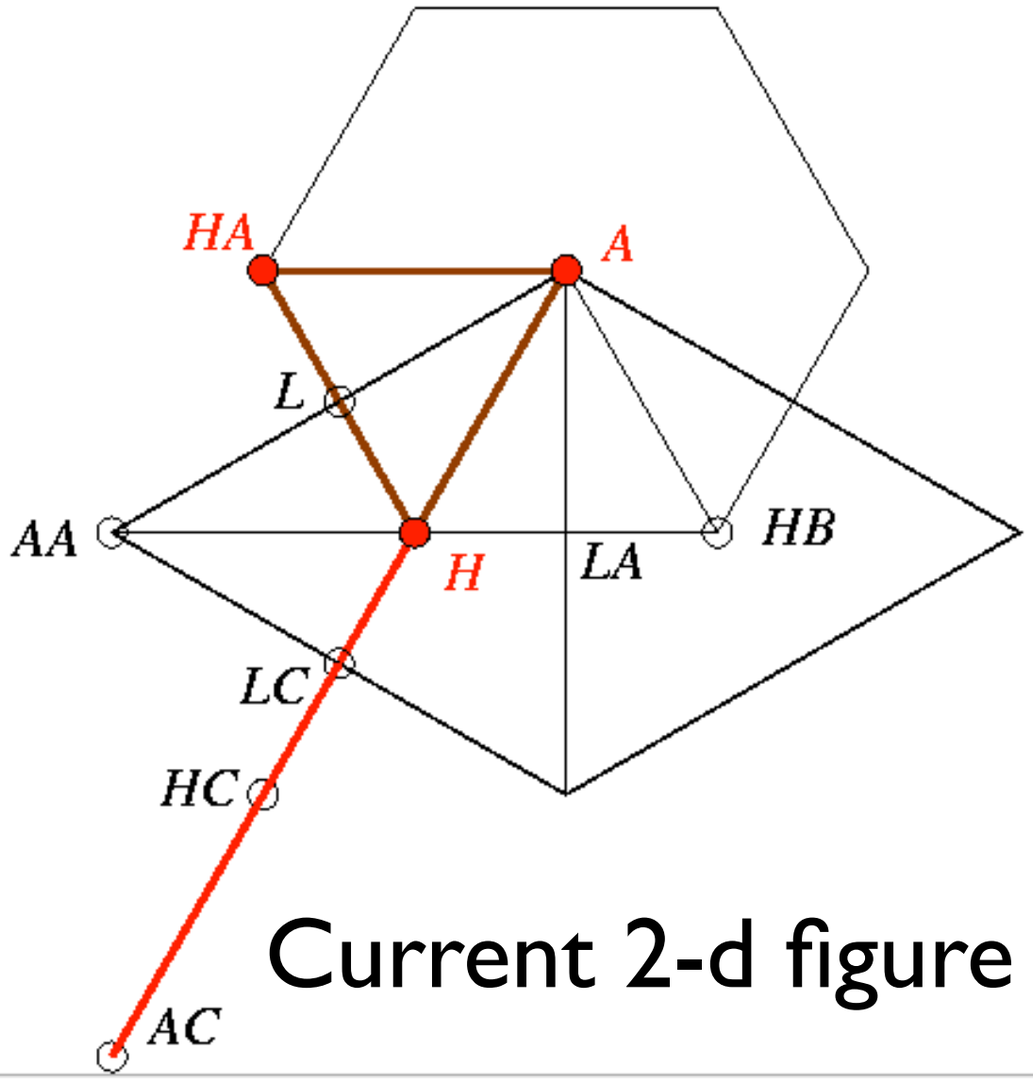
Brillouin zone

(Diagram for arithmetic crystal class 321P)

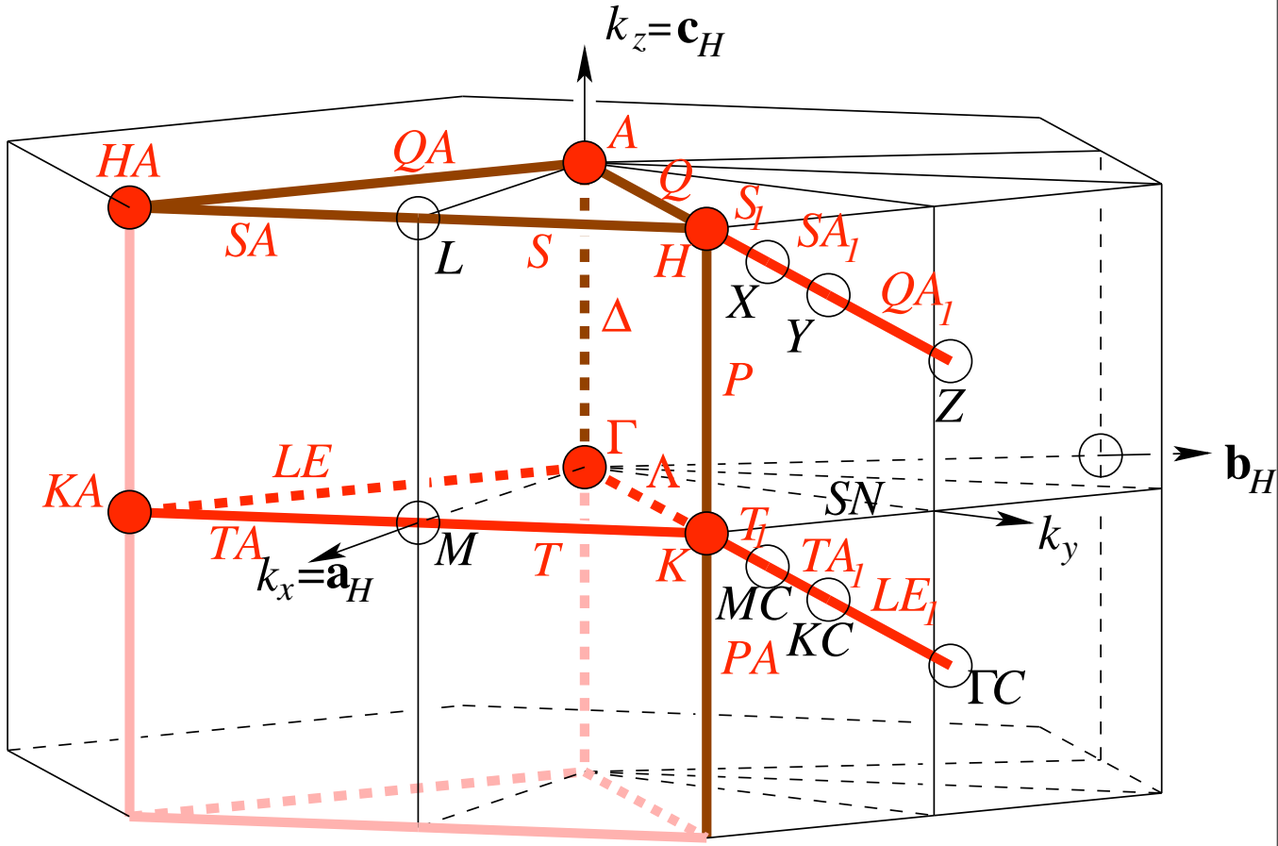
P321-D_3^2(150), P$3_1$21-D_3^4(152), P$3_2$21-D_3^6(154)

Reciprocal-space group (P312)*, No. 149

The table with the k vectors.



Current 2-d figure



New 3-d figure

EXERCISES

Bilbao Crystallographic Server
www.cryst.ehu.es

Bilbao Crystallographic Server - mirror site
http://158.227.0.68/

Problem 9.1.1, p.57

Problem 9.1.2

Databases and retrieval tools

Problem 9.1.1. Use the retrieval tools `GENPOS` (generators and general positions), `WYCKPOS` (Wyckoff positions, `NORMALISER` (normalizers of space groups), `WYCKSET`(equivalent sets of Wyckoff positions) and `HKLCOND` (reflection conditions) for accessing *IT*A and *IT*A1 data. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in *IT*A (*cf.* Table 4.3.2.1).

Problem 9.1.2. Consider the retrieval tool `KVEC` to the Brillouin-zone database: Compare the **k**-vector tables and Brillouin zones for the different sets of parameters for the space group *F*222, No.22.

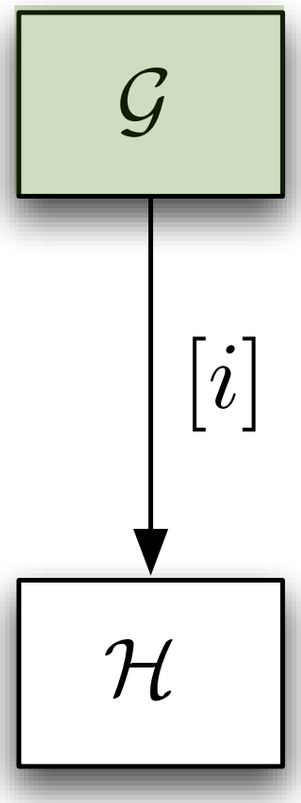
Problem 2.2.2, p. 16

Coordinate transformations of CaF_2 structure

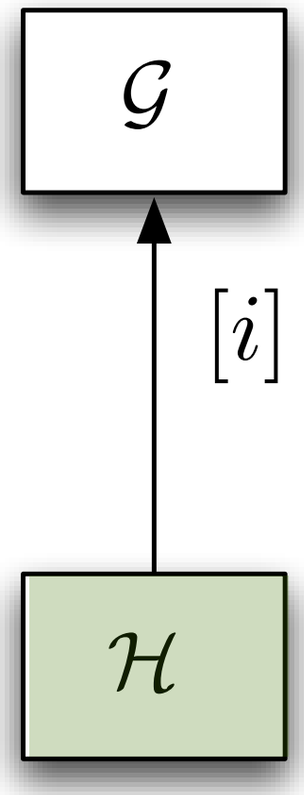
Crystallographic computing programs

- Group-subgroup relations
- Group-supergroup relations
- Relations between Wyckoff positions

GROUP-SUBGROUP RELATIONS



SUBGROUPGRAPH



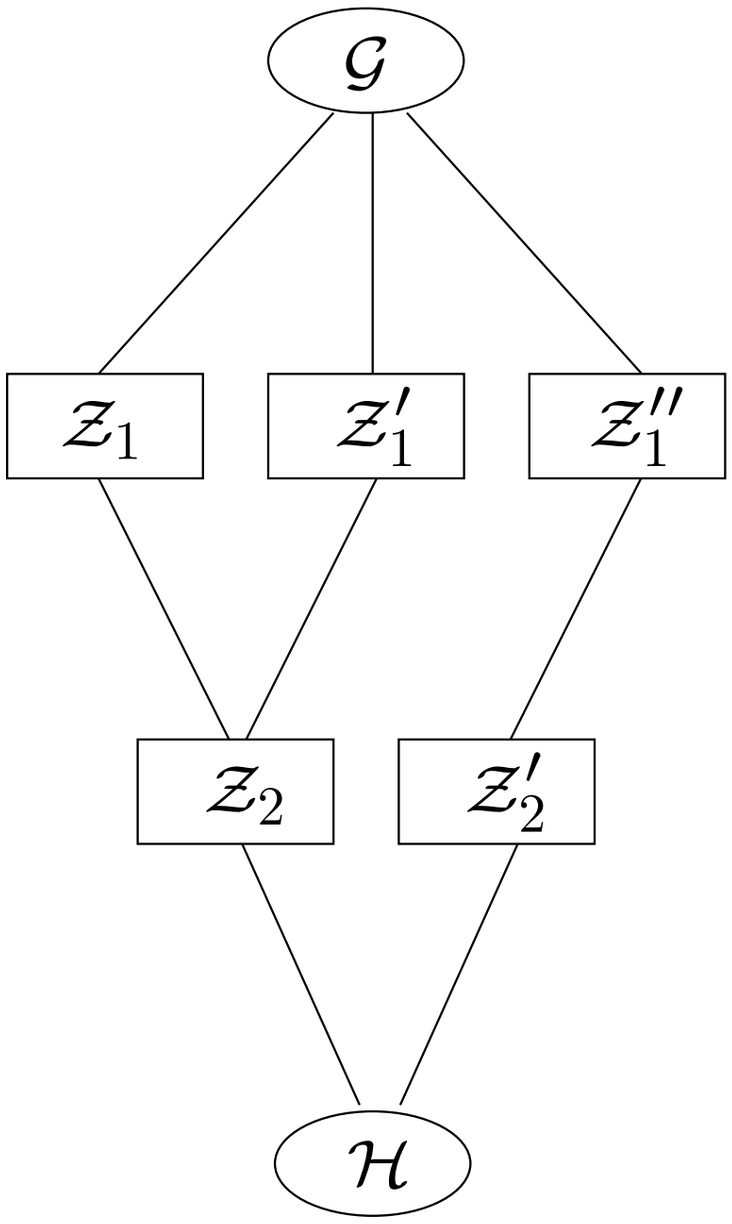
SUPERGROUPS

APPLICATIONS

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

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

Chains of maximal subgroups



Group-subgroup pair

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

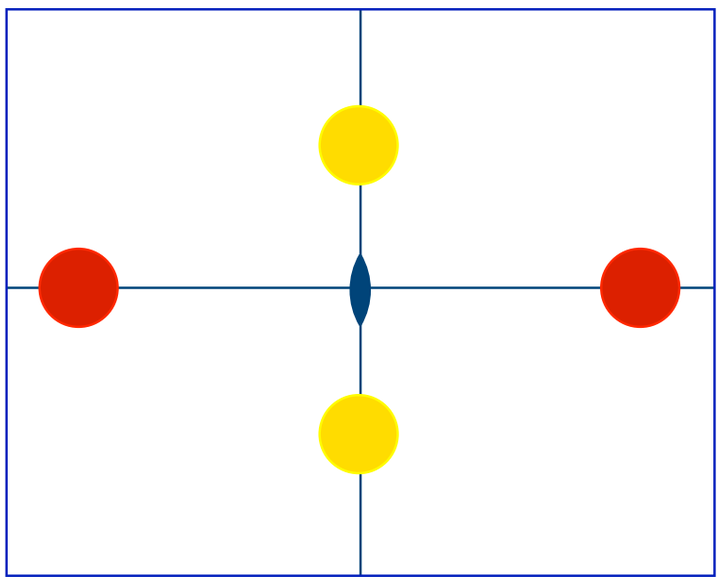
Pairs: group - maximal subgroup

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

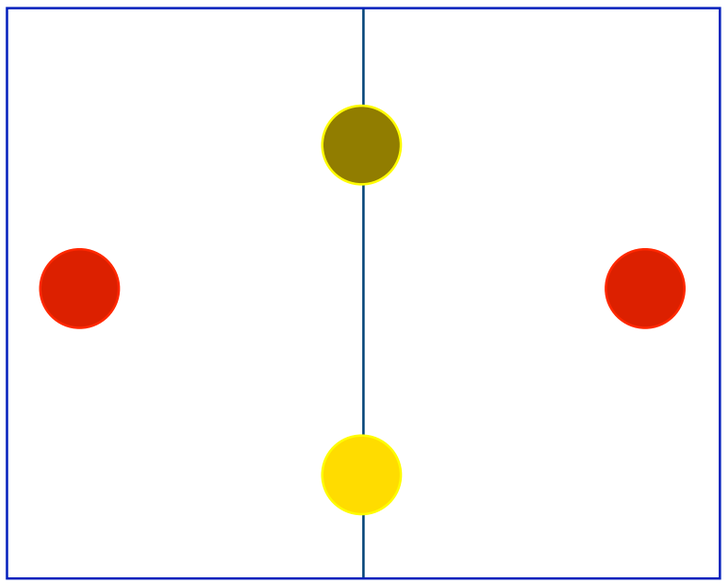
$$(\mathrm{P}, \mathbf{p}) = \prod_{k=1}^{n} (\mathrm{P}, \mathbf{p})_k$$

Different subgroups of the same type

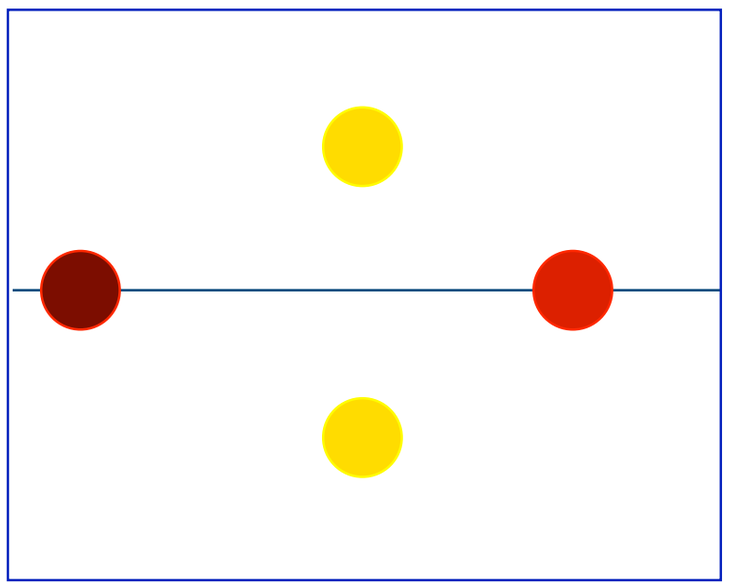
$$\mathcal{G} = \mathrm{P}mm2 > \mathcal{H} = \mathrm{P}m, \ [i] = 2$$



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



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



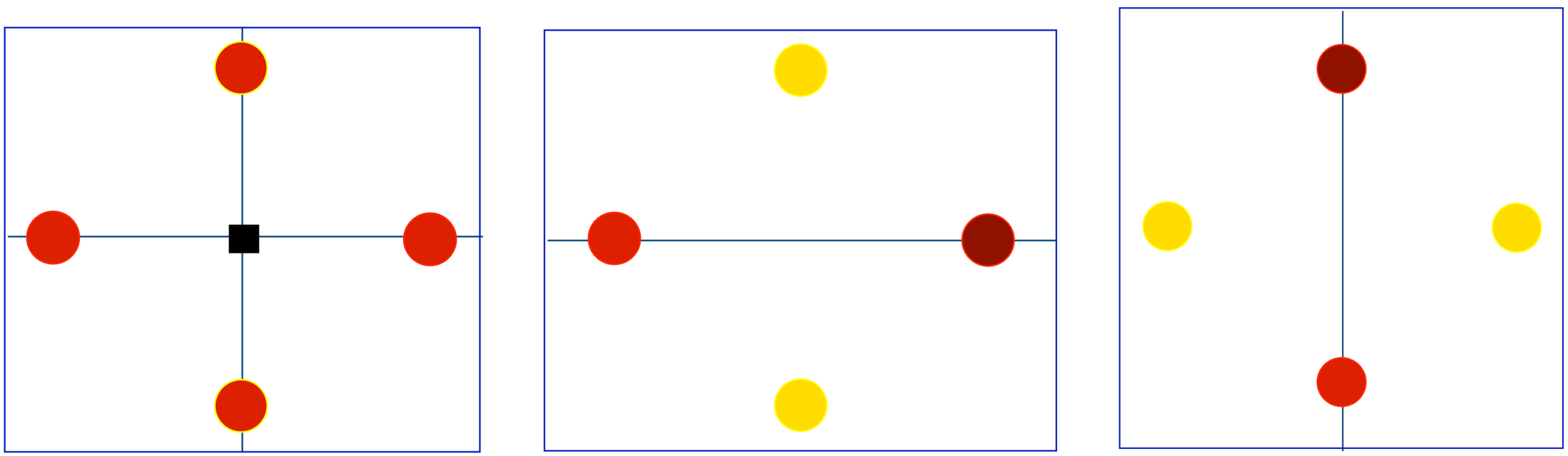
$S_2, \ \mathcal{H} = \mathrm{P}m11$

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

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

Different subgroups of the same type

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



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

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

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

THE GROUP-SUBGROUPS SUITE

HERMANN, COSETS, CELLSUB & COMMONSUBS

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

Subgroups calculation: SUBGROUPGRAPH

Chains of maximal subgroups

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

↓

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

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

↓

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

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

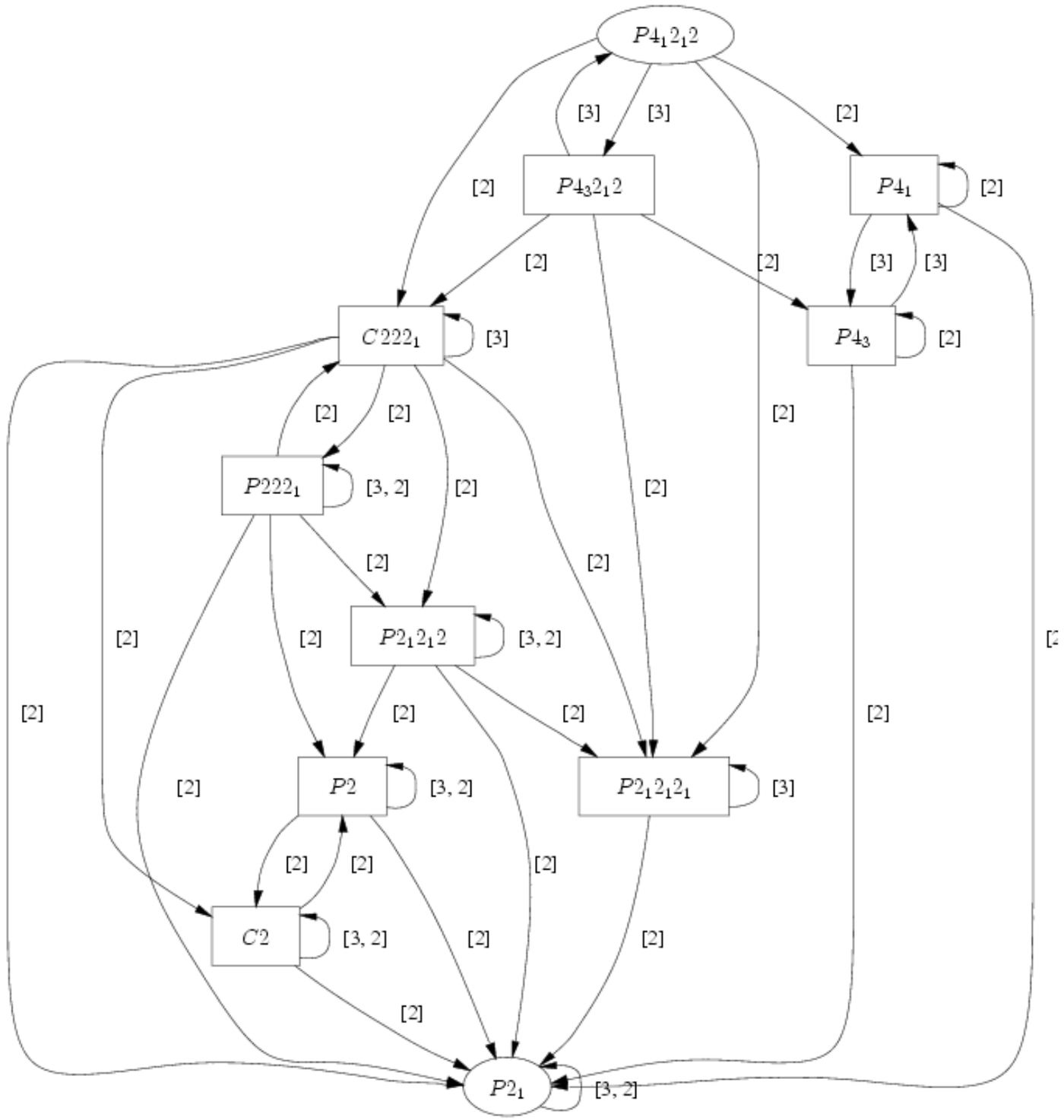
Comparison of the subgroup elements

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

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

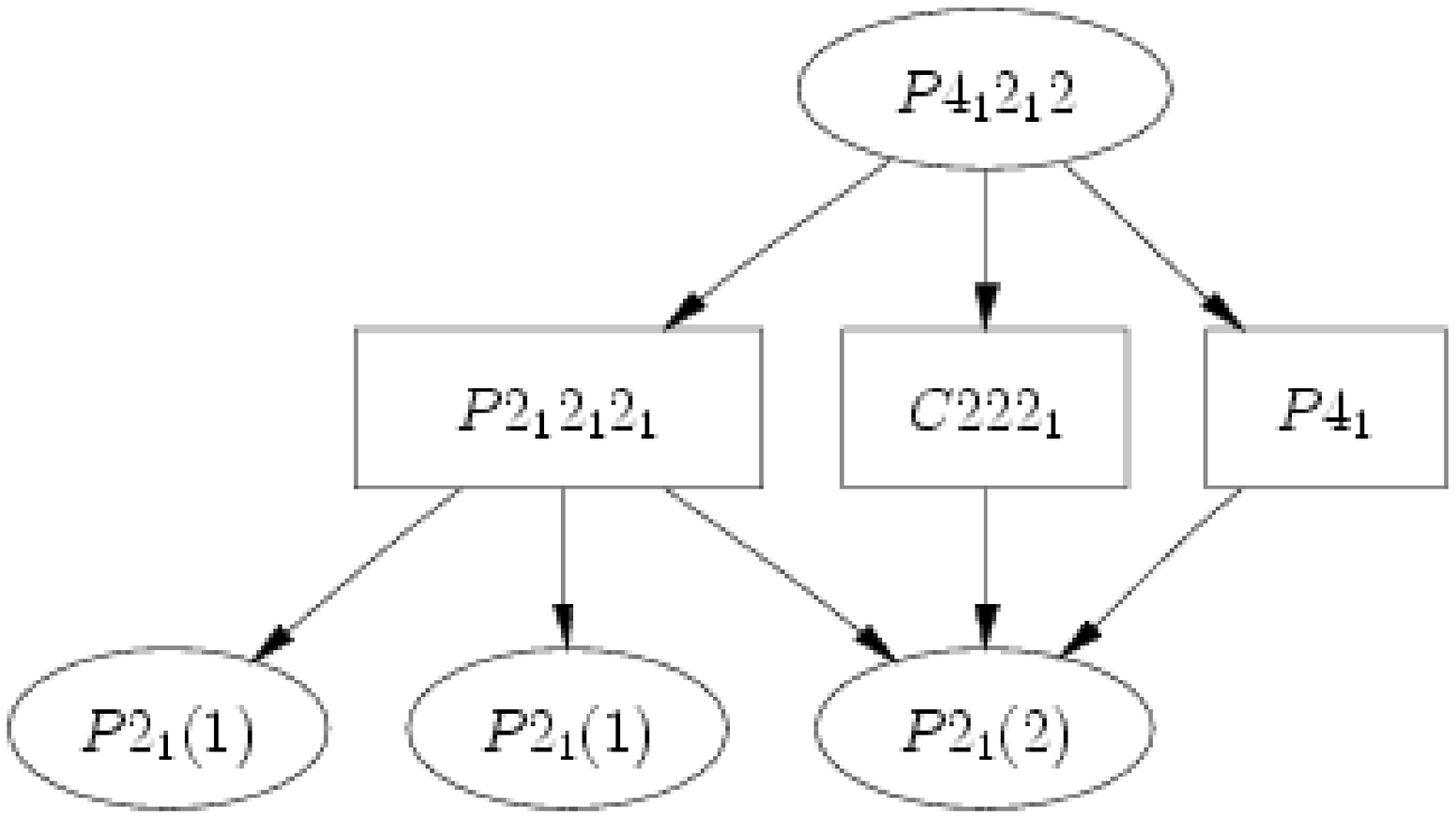
http://www.cryst.ehu.es/subgroupgraph.html

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

GROUP-SUBGROUP RELATIONS

PROBLEMS:

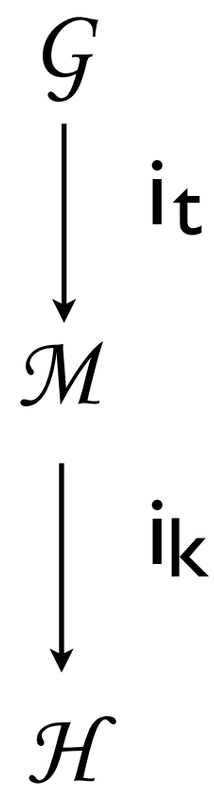
- No tools for space groups involving series of isomorphic subgroups
- High indices: Hermann group method

Hermann, 1929:

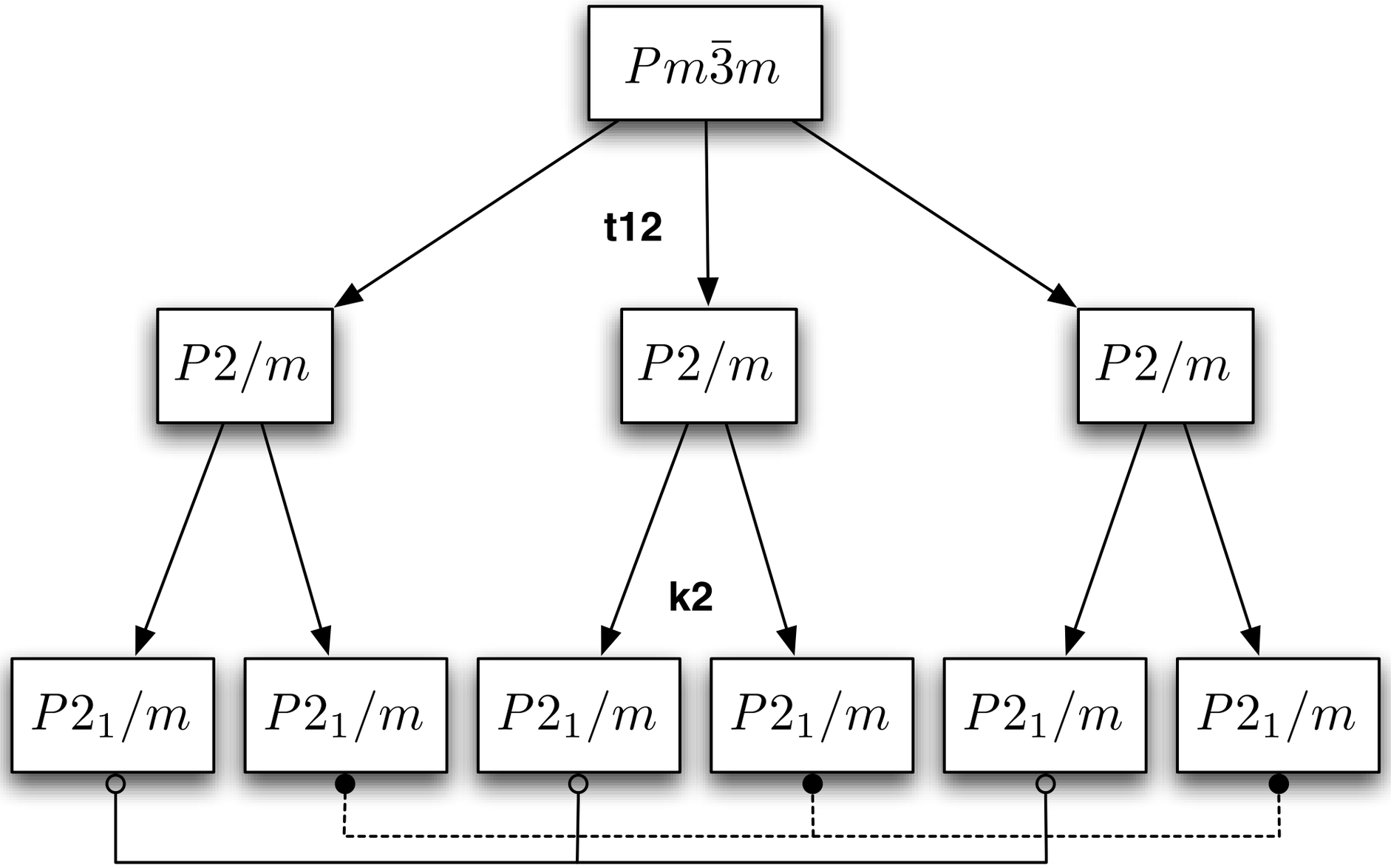
For each pair $\mathcal{G}>\mathcal{H}$, there exists a uniquely defined intermediate subgroup $\mathcal{M}$, $\mathcal{G} \geqq \mathcal{M} \geqq \mathcal{H}$, such that:

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

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



Example: *Pm*-3*m* > *P*2$_1$/*m* with index 24



Hermann Group M= *P*2/*m*

Classification of the subgroups of type 11 ($P2_1/m$) [unique axis b] of group 221 (Pm-3m) with index 24

Note: The group-subgroup relation is type *general*

Hermann Group: $P2/m$ (10) with $i_t = 12$ and $i_k = 2$

Classes representatives

Class #	Transformation Matrix	Matrix Representation	WP Splitting	Symmetry Modes	All subgroups
1	b,2c,a	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show
2	b,2c,a+1/2	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 1/2 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show

Hermann Group: $C2/m$ (12) with $i_t = 12$ and $i_k = 2$

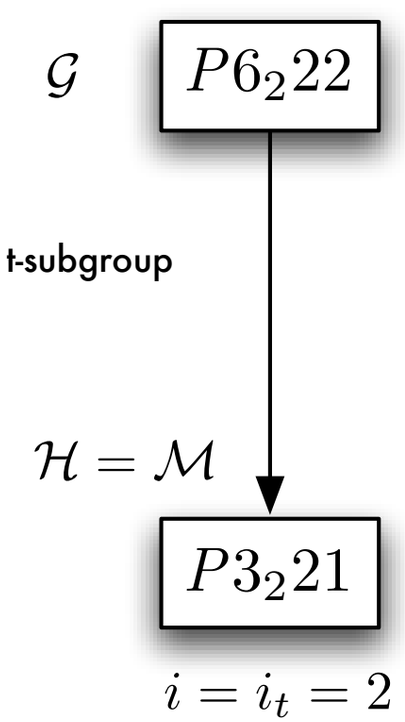
Classes representatives

Class #	Transformation Matrix	Matrix Representation	WP Splitting	Symmetry Modes	All subgroups
1	c+1/2,a+b,-a+b	$\begin{pmatrix} 0 & 1 & -1 & 1/2 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show

Problem: CLASSIFICATION OF DOMAINS

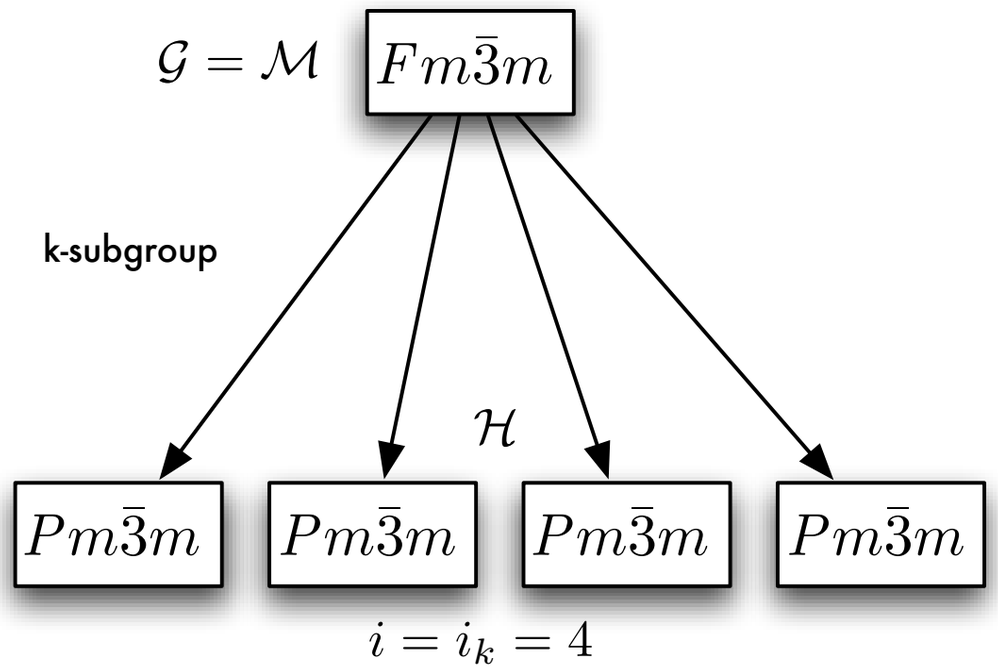
HERMANN

Quartz



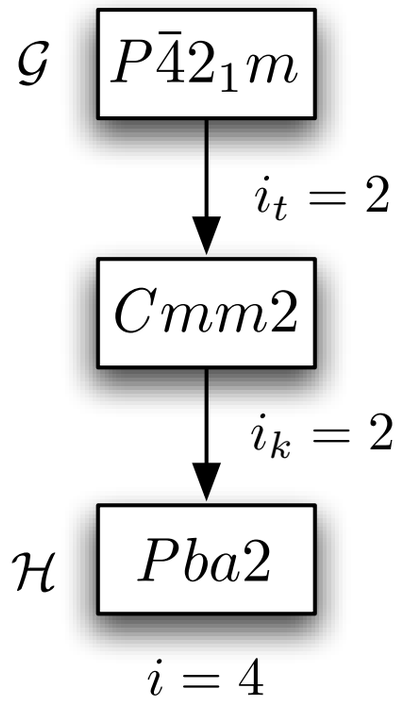
twin domains

Cu_3Au



antiphase domains

$Gd_2(MoO_4)_3$



twin and antiphase domains

Coset Decomposition

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:

Enter subgroup number (H) or choose it:

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

Enter transformation matrix :

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

Decomposition: left right

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

$\Delta=t_H$

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

$\Delta=V_2t_H$

Problem: LOW-SYMMETRY STRUCTURES FOR A GIVEN CELL MULTIPLICATION

CELLSUB

Example: $CsMgInF_6$

aristotype

↓

structure data: P lattice, orthorhombic

↓

unknown

Fd-3m

$[i_{k=2}]$

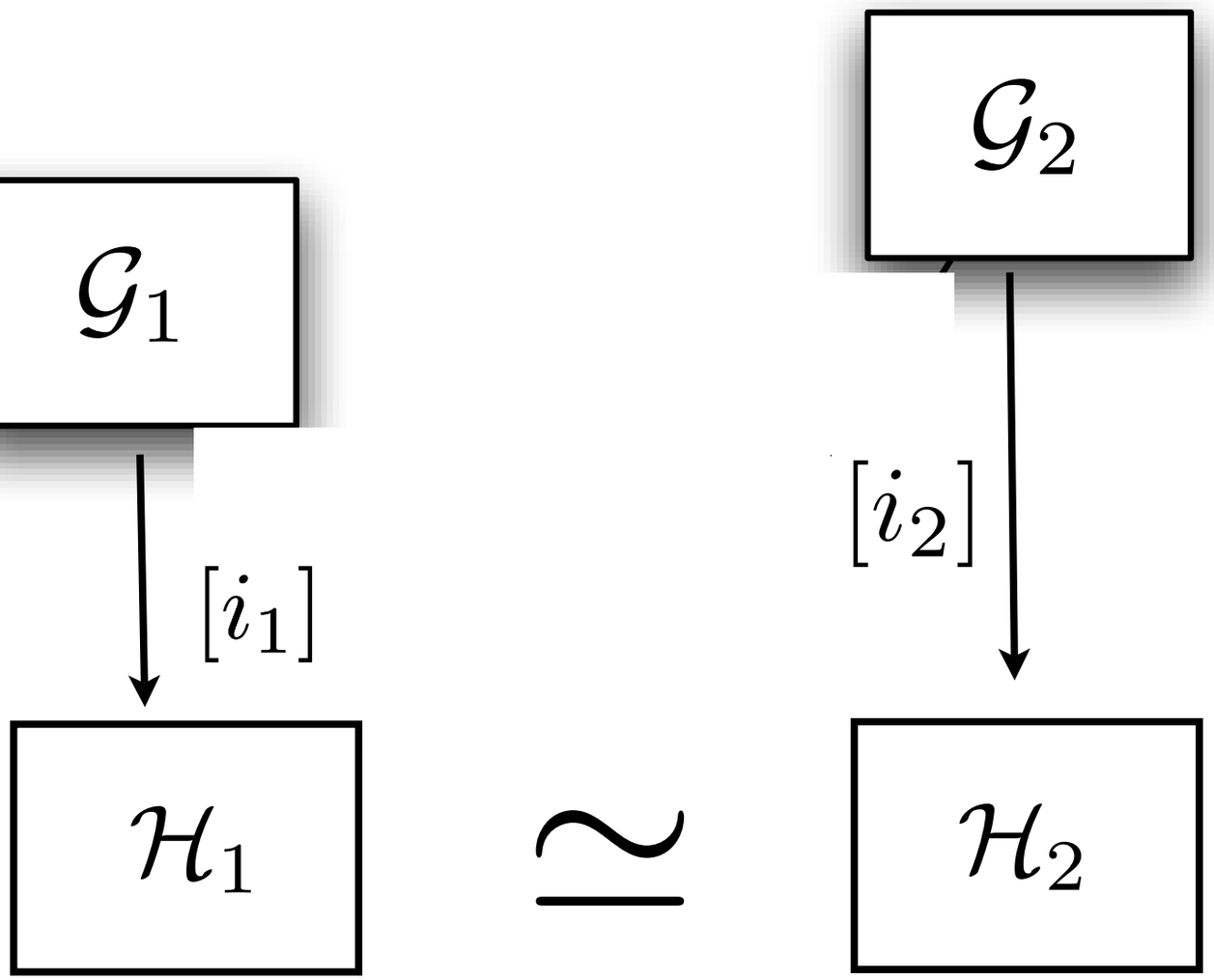
?

List of P-centred orthorhombic subgroups of Fd-3m(227) i_k=2

N	HM Symbol	ITA	index	t-index	k-index	More info
1	*Pnma*	062	12	6	2	show...
2	*Pmna*	053	12	6	2	show...
3	*Pnna*	052	12	6	2	show...
4	*Pmma*	051	12	6	2	show...
5	*Pnn2*	034	24	12	2	show...
6	$Pna2_1$	033	24	12	2	show...
7	$Pmn2_1$	031	24	12	2	show...
8	*Pnc2*	030	24	12	2	show...
9	*Pma2*	028	24	12	2	show...
10	$Pmc2_1$	026	24	12	2	show...
11	*Pmm2*	025	24	12	2	show...
12	$P2_12_12_1$	019	24	12	2	show...
13	$P222_1$	017	24	12	2	show...

Problem: PHASES WITH NO GROUP-SUBGROUP RELATIONS

COMMON SUBGROUPS



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

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

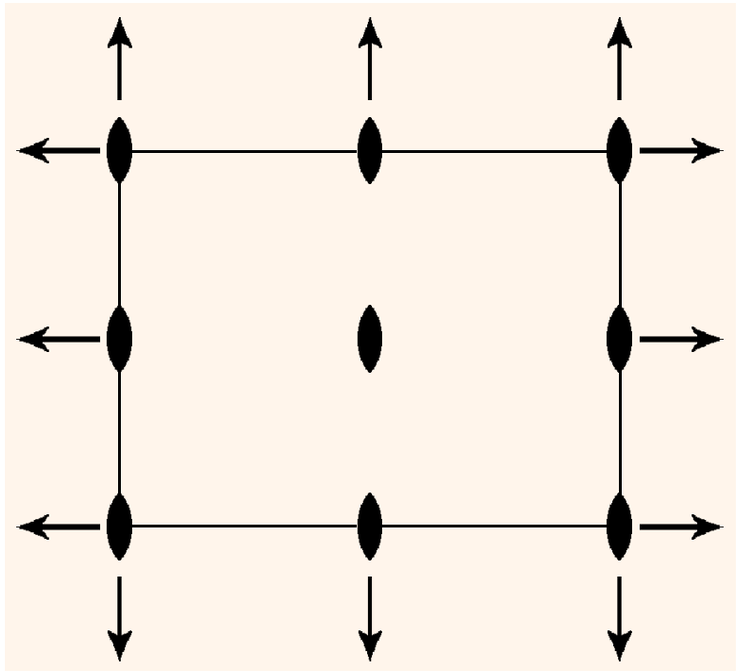
$$i_2 = \frac{|\mathcal{P}_{\mathcal{G}_2}|}{|\mathcal{P}_{\mathcal{H}_2}|} \cdot \frac{Z^p_{\mathcal{H}_2}}{Z^p_{\mathcal{G}_2}}$$

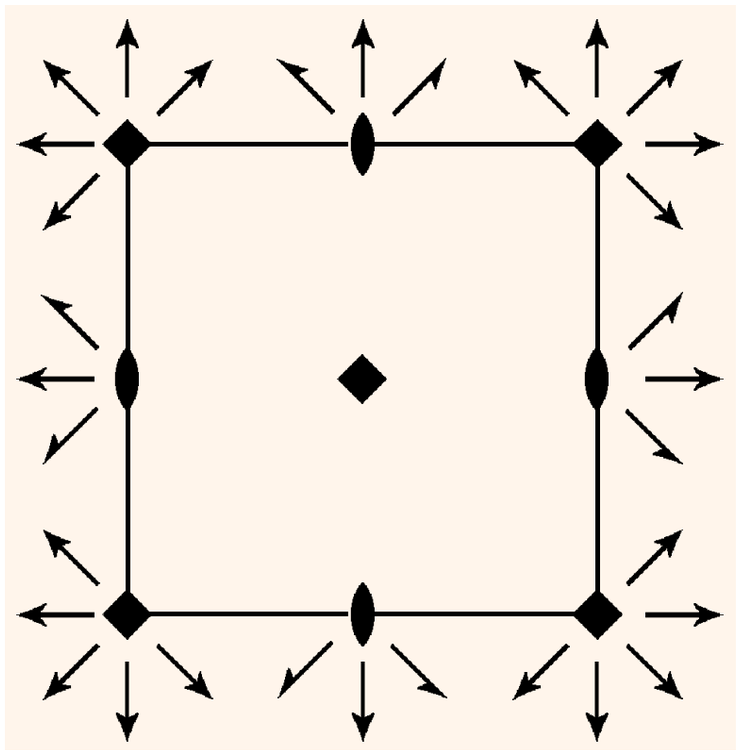
index condition

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

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

Supergroups of the same type





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

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

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

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

THE SUPERGROUPS SUITE

MINSUP, SUPERGROUPS, COSETS CELLSUPER & COMMONSUPER

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

Supergroups calculation: SUPERGROUPS

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

↓

Normalizer method

↓

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 super-groups $\mathcal{G}_k \overset{[i]}{\sim} \mathcal{G}$

Monoclinic groups and triclinic:

normalizers ''enhanced''

Common supergroups

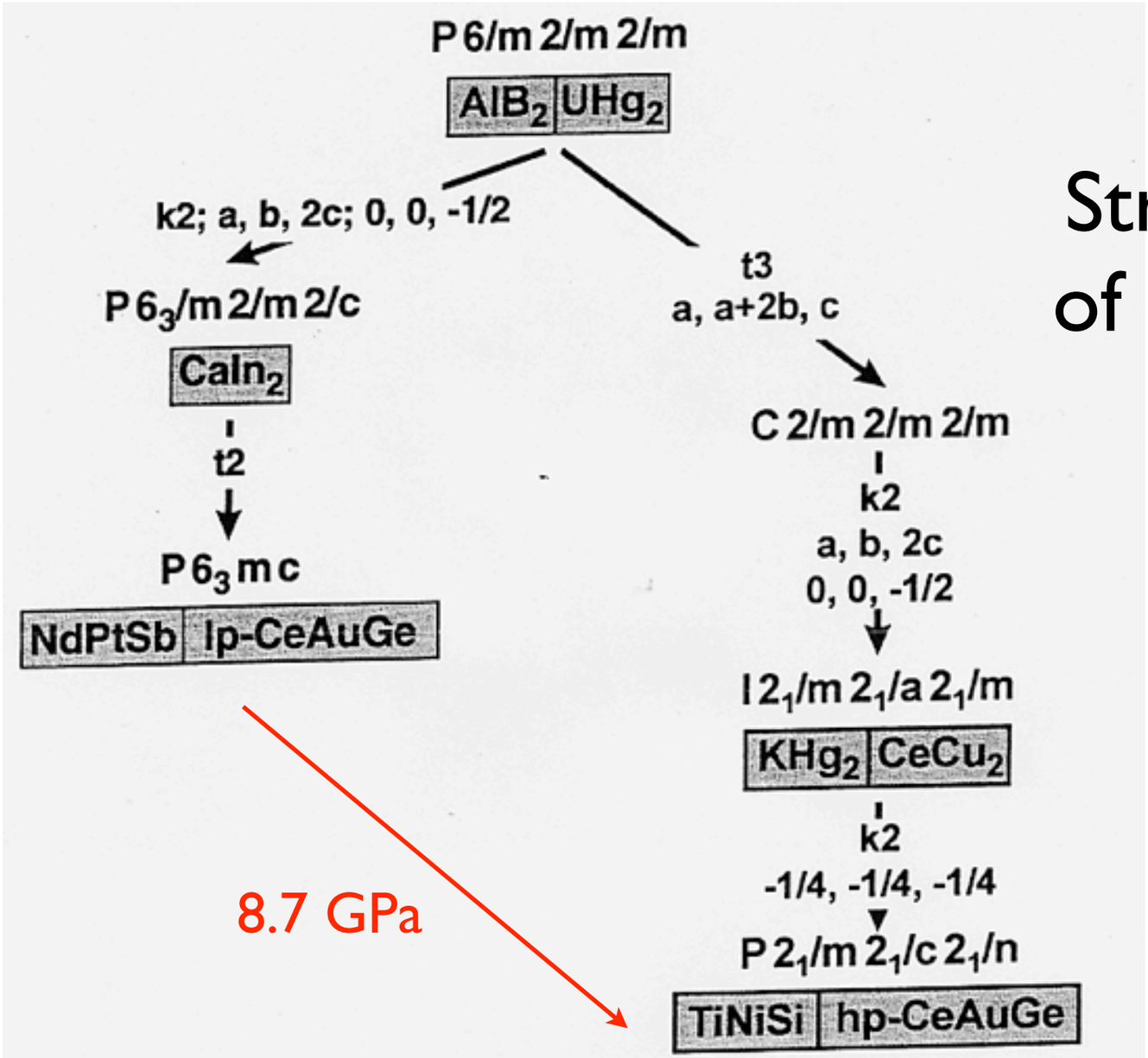


Fig. 7. *Bärnighausen* tree of the group-subgroup relationship [17] of the AlB_2-type and the distorted low-pressure (lp) and high-pressure (hp) modifications of CeAuGe (excerpt of Fig. 3. in Ref. [1]). The indices of the *klassengleiche* (*k*) and *translationengleiche* (*t*) transitions, as well as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

Splitting of Wyckoff positions

Applications

- Phase transitions
- Derivative structures
- Symmetry modes

AIM

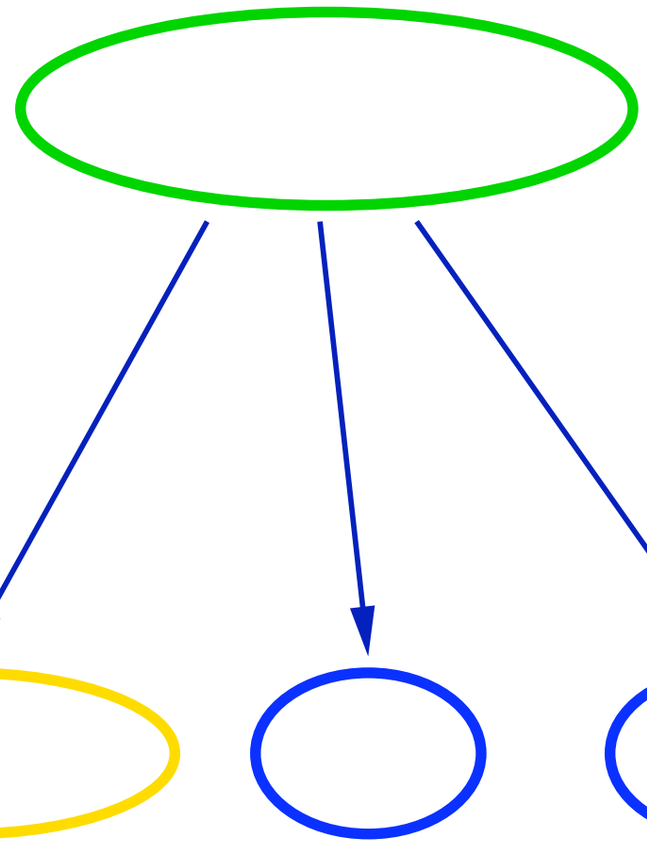
$$\mathcal{G} > \mathcal{H},\ (\mathrm{P}, \mathbf{p}),\ \mathcal{W}^{\mathcal{G}}$$

- splitting of $\mathcal{W}^{\mathcal{G}}$ in suborbits
- relation between the suborbits and $\mathcal{W}_i^{\mathcal{H}}$

General splitting rules

(Wondratschek 1993,1995)

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



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

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

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

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

Calculation of splitting: WYCKSPLIT

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

Special positions $\mathcal{O}_{\mathcal{G}}(X)$

substitute X_0 by X in $\mathcal{O}_{\mathcal{G}}(X_0) = \cup_{k=1}^{[i]} \mathcal{O}_{\mathcal{H}}(X_{0,k})$

$\Downarrow$

suborbits $\mathcal{O}_{\mathcal{H}}(X_i)$

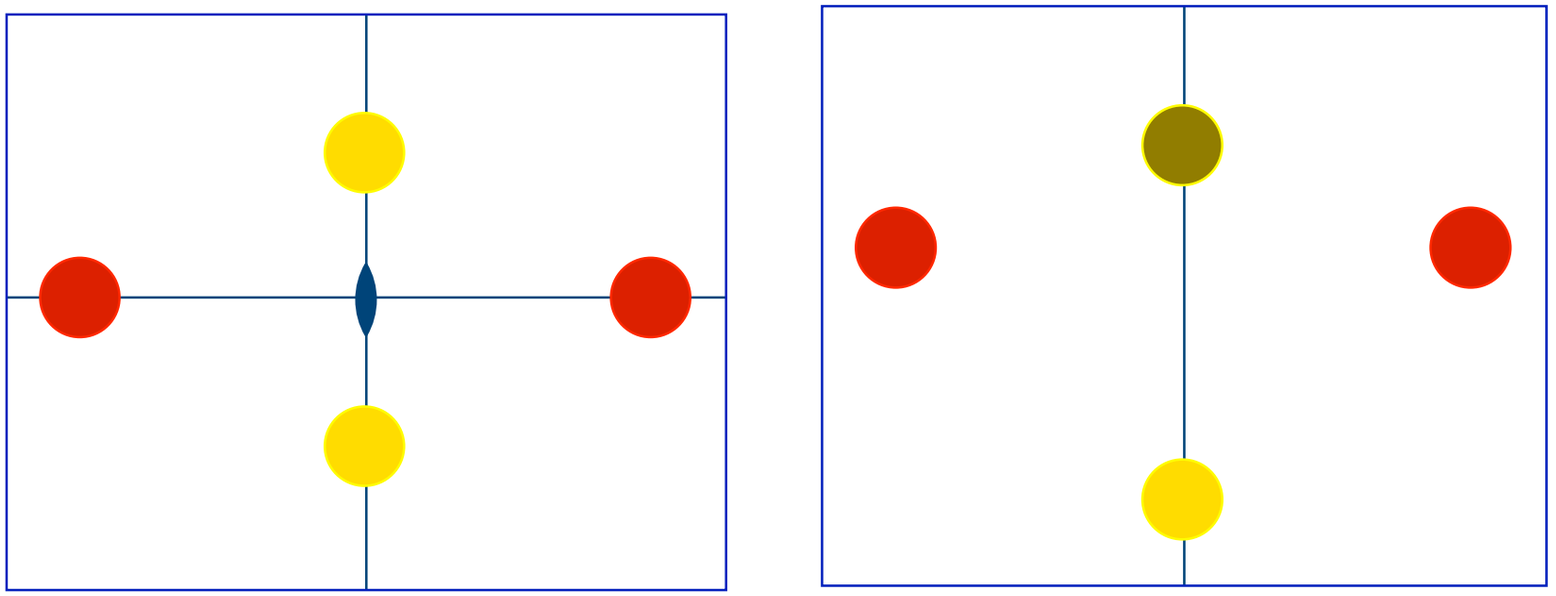
assign $\mathcal{W}^{\mathcal{H}}$ to any $\mathcal{O}_{\mathcal{H}}(X_i)$

relate the representatives of $\mathcal{W}^{\mathcal{H}}$
and the points of $\mathcal{O}_{\mathcal{H}}(X_i)$

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

SYMMETRY REDUCTION

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



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

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)

2*f* .m. (x,1/2,z) ⟶ 1*b* m (x_1,1/2,z_1)

Splitting of Wyckoff positions

*ITA*1 Space group $P4_2/mnm$ (selection)

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

	Axes	Coordinates	Wyckoff positions					
			2*a*	2*b*	4*c*	4*d*	4*e*	4*f*
				4*g*	8*h*	8*i*	8*j*	16*k*
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}n2$ (118)		$x+\frac{1}{2},y,z+\frac{1}{4}$	2*d*	2*c*	4*e*	2*a*;2*b*	4*h*	4*g*
				4*f*	2×4*e*	8*i*	8*i*	2×8*i*
[2] $P\bar{4}2_1m$ (113)		$x+\frac{1}{2},y,z+\frac{1}{4}$	2*c*	2*c*	4*d*	2*a*;2*b*	2×2*c*	4*e*
				4*e*	2×4*d*	8*f*	2×4*e*	2×8*f*
[2] $P4_2nm$ (102)			2*a*	2*a*	4*b*	4*b*	2×2*a*	4*c*
				4*c*	2×4*b*	8*d*	2×4*c*	2×8*d*
[2] $P4_22_12$ (94)			2*a*	2*b*	4*d*	4*d*	4*c*	4*e*
				4*f*	2×4*d*	8*g*	8*g*	2×8*g*
[2] $P4_2/m$ (84)		$x+\frac{1}{2},y,z$	2*d*	2*c*	2*a*;2*b*	2*e*;2*f*	4*i*	4*j*
				4*j*	4*g*;4*h*	2×4*j*	8*k*	2×8*k*
[2] *Pnnm* (58)			2*a*	2*b*	2*c*;2*d*	4*f*	4*e*	4*g*
				4*g*	2×4*f*	2×4*g*	8*h*	2×8*h*
[2] *Cmmm* (65)	**a−b**, **a+b**, **c**	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	2*a*;2*c*	2*b*;2*d*	4*e*;4*f*	8*m*	4*k*;4*l*	4*h*;4*i*
				4*g*;4*j*	2×8*m*	8*p*;8*q*	8*n*;8*o*	2×16*r*

Example

Example WYCKSPLIT: $P4_2/mnm$>$Cmmm$, index 2

Wyckoff Positions Splitting

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

Splitting of Wyckoff position 4g

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, -x, 0)	(x, 0, 0)	**$4g_1$**	(x_1, 0, 0)
2	(-x, x, 0)	(-x, 0, 0)		(-x_1, 0, 0)
3	(x+1, -x, 0)	(x+1/2, 1/2, 0)		(x_1+1/2, 1/2, 0)
4	(-x+1, x, 0)	(-x+1/2, 1/2, 0)		(-x_1+1/2, 1/2, 0)
5	(x+1/2, x+1/2, 1/2)	(0, x+1/2, 1/2)	**$4j_1$**	(0, y_2, 1/2)
6	(-x+1/2, -x+1/2, 1/2)	(0, -x+1/2, 1/2)		(0, -y_2, 1/2)
7	(x+1/2, x-1/2, 1/2)	(1/2, x, 1/2)		(1/2, y_2+1/2, 1/2)
8	(-x+1/2, -x-1/2, 1/2)	(1/2, -x, 1/2)		(1/2, -y_2+1/2, 1/2)

EXERCISES

Group-subgroup relations of space groups

Problem 9.1.3. Study the group–subgroup relations between the groups $\mathcal{G} = P4_12_12$, No. 92, and $\mathcal{H} = P2_1$, No. 4 using the program SUBGROUPGRAPH. Consider the cases with specified (*e.g.* $[i] = 4$) and not specified index of the group-subgroup pair. Compare the results with the data illustrated in Example 8.11, p. 49.

Problem 9.1.4. Explain the difference between the contracted and complete graphs of the t-subgroups of $P4mm$ (No. 99) obtained by the program SUBGROUPGRAPH. Compare the complete graph with the results of Problems 3.3.2 (p. 19) and 4.1.1 (p. 23). Explain why the t-subgroup graphs of all 8 space groups from No. 99 ($P4mm$) to No. 106 ($P4_2bc$) have the same 'topology' (*i. e.* the same type of 'family tree'), only the corresponding subgroup entries differ.

MAXSUBS, SUBGROUPGRAPH AND HERMANN

Problem 9.1.5. The retrieval tool `MAXSUB` gives an access to the database on maximal subgroups of space groups as listed in $ITA1$. Consider the maximal subgroups of the group $Pmna$, (No.53). Compare its k-subgroups obtained by doubling the b lattice parameter, *i. e.* $\mathbf{a}', \mathbf{b}', \mathbf{c}' = \mathbf{a}, 2\mathbf{b}, \mathbf{c}$ and compare with the list of subgroups derived in Problem 4.1.2, p. 23.

Problem 9.1.6. Consider the group–subgroup pair of the groups $\mathcal{G} = P422$, No. 89, and $\mathcal{H} = P2_1$, No. 4, of index $[i] = 8$. Using the programs `SUBGROUPGRAPH` and `HERMANN` determine the number of different subgroups, their distribution into conjugacy classes and the corresponding Hermann groups.

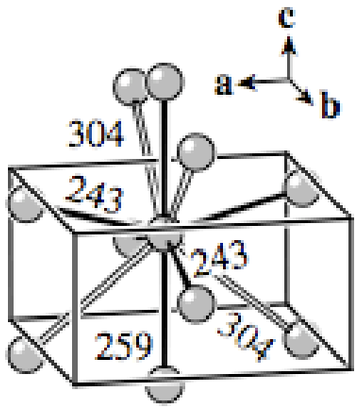
U. MÜLLER, p.34

11. At high temperatures, $BaTiO_3$ has the cubic perovskite structure, space group $Pm\bar{3}m$. Upon cooling, it distorts to the space group $P4mm$. Can we expect twinned crystals of the low-symmetry form? If so, with how many kinds of domains?

12. $SrTiO_3$ has the cubic perovskite structure ($Pm\bar{3}m$). Upon cooling below 105 K, the coordination octahedra are mutually rotated and the space group symmetry is reduced to $I4/mcm$; c is doubled and the unit cell is increased by a factor of four. Can we expect twinned crystals of the low-symmetry form? If so, with how many kinds of domains?

Input data: G_1=I4$_1$/amd, No. 141, Z_1=4

G_2=P6/mmm, No. 191, Z_2=1 i_k=2

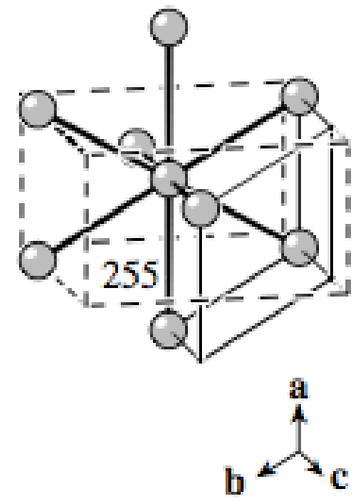


a_V = 254.9 pm
c_V = 238.3 pm
at 16.2 GPa

$P6/m2/m2/m$

Si-V

Si: 2*a*
6/*mmm*
0
0
0



t3
a, a+2b, c

$I4_1/a2/m2/d^{(2)}$

Si-II

Si: 4*a*
$\bar{4}m2$
0
$\frac{1}{4}$
$-\frac{1}{8}$

a_{II} = 466.5 pm
c_{II} = 256.5 pm
at 11.7 GPa

t2

$C2/m2/m2/m$

k2
b, 2c, a
$0, 0, -\frac{1}{2}$

2*a*
mmm
0
0
0

$y, \frac{1}{2}z+\frac{1}{4}, x$

$I2_1/m2_1/m2_1/a$

Si-XI

Si: 4*e*
*mm*2
0
$\frac{1}{4}$
−0.057

a_{XI} = 450.2 pm
b_{XI} = 473.7 pm
c_{XI} = 255.0 pm
at 15 GPa

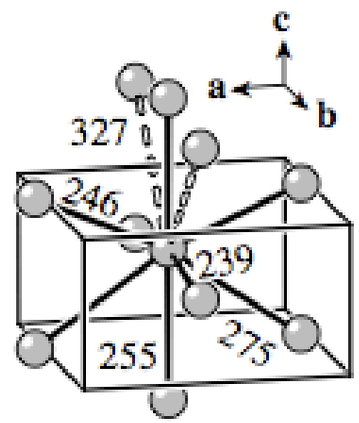


Figure 11: Symmetry relations among three high-pressure modifications of silicon.

Group-supergroup relations of space groups

Problem 9.1.8. Consider the group–supergroup pair $\mathcal{H} < \mathcal{G}$ with $\mathcal{H} = P222$, No. 16, and the supergroup $\mathcal{G} = P422$, No. 89, of index $[i] = 2$. Using the program `MINSUP` determine all supergroups $P422$ of $P222$ of index $[i] = 2$. How does the result depend on the normalizer of the supergroup and/or that of the subgroup. Compare with the results obtained in Example 5.12, p. 32.

Problem 9.1.9. Consider the minimal supergroups of $Pna2_1$ obtained by the program `MINSUP`. Explain the differences between the relations between the conventional bases for the group-subgroup pair $Pnma > Pna2_1$, $[i] = 2$ (*e.g.* accessed by the program `MAXSUB`), and the corresponding relations for the supergroup-group pair $Pnma > Pna2_1$, $[i] = 2$ (*e.g.* the program `MINSUP`).

Common supergroups: COMMONSUPER

U. MÜLLER, p.16

Input data: G_1=C12/c1, No. 15, Z_1=4

G_2=C12/m1, No. 12, Z_2=4

i_k=1

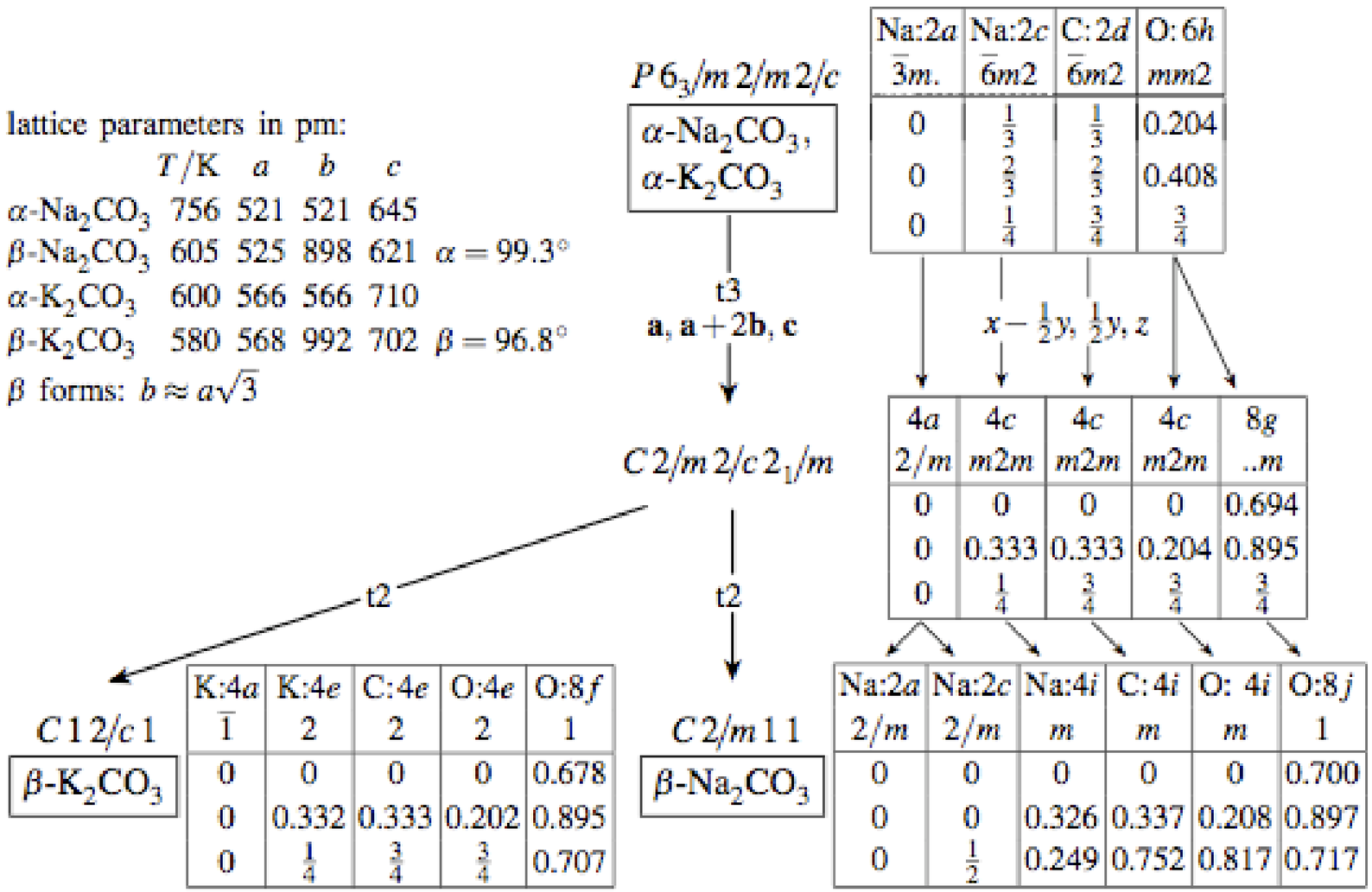


Figure 7: Group–subgroup relations among some modifications of the alkali metal carbonates [41]

Wyckoff-positions relations

Problem 9.1.10. Study the splittings of the Wyckoff positions for the group-subgroup pair $P4_2/mnm$ (No. 136)> $Cmmm$ (No. 65) of index 2 by the program `WYCKSPLIT`. Compare the results with the data obtained in Example 6.12, p. 35.

Problem 9.1.11. Study the splittings of the Wyckoff positions for the group-subgroup pair $P4mm$ (No. 99)> Cm (No. 4) of index 4 by the program `WYCKSPLIT`. Compare the results with the data obtained in Problem 6.1.1, p. 37.

U. MÜLLER, p.19

2. Die crystal data for *LT*-quartz are $a = 491\,\text{pm}$, $c = 541\,\text{pm}$; space group $P3_221$; atomic coordinates Si 0.470, 0, $\frac{1}{6}$ and O 0.414, 0.268, 0.286. Upon heating it is converted to *HT*-quartz, $a = 500\,\text{pm}$, $c = 546\,\text{pm}$; space group $P6_222$; coordinates Si $\frac{1}{2}$, 0, $\frac{1}{2}$ and O 0.416, 0.208, $\frac{2}{3}$. Set up the corresponding Bärnighausen tree. Which additional degrees of freedom are present in the lower symmetry form?

3. The crystal data for α-$AlPO_4$ are:

$P3_121$ $\quad a = 494\,\text{pm}$, $c = 1095\,\text{pm}$

	x	y	z		x	y	z
Al	0.466	0	$\frac{1}{3}$	O1	0.417	0.292	0.398
P	0.467	0	$\frac{5}{6}$	O2	0.417	0.257	0.883

What is its relation to quartz? (*cf.* exercise 8.2.)

Phase-transitions with a group-subgroup relation between the phases

Inverse Landau-problem

Symmetry-mode analysis

Pseudosymmetry Prediction of structural phase transitions

Example: Phase transitions in $SrBi_2Ta_2O_9$ (SBT)

Initial data:

High-temperature prototype

$\mathcal{G}$

*I*4/*mmm* (139)

Sr: 2a
Ta: 4e
Bi: 4e
O1: 2b
O2: 4e
O3: 4d
O4: 8g

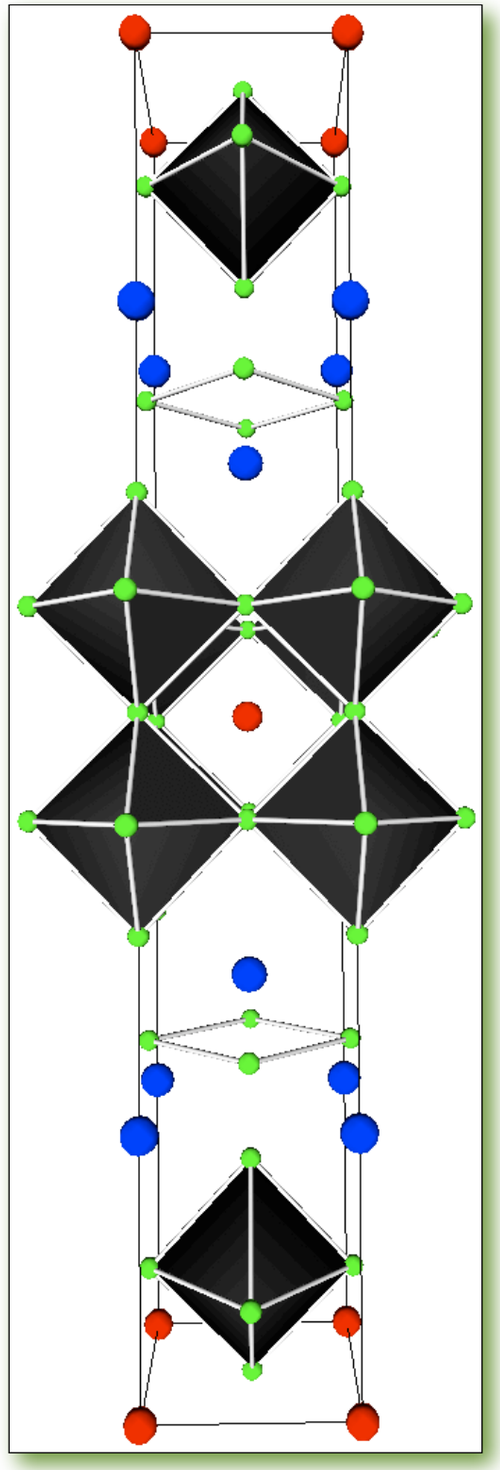
Group-theoretical analysis

[8]

Low-temperature ferroelectric

$\mathcal{H}$

$Cmc2_1$ (36)



Basis transformation: c, a-b, a+b

$$(\mathbf{a},\mathbf{b},\mathbf{c})_{\mathcal{H}} = (\mathbf{a},\mathbf{b},\mathbf{c})_{\mathcal{G}} \begin{pmatrix} 0 & 1 & 1 \\ 0 & -1 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

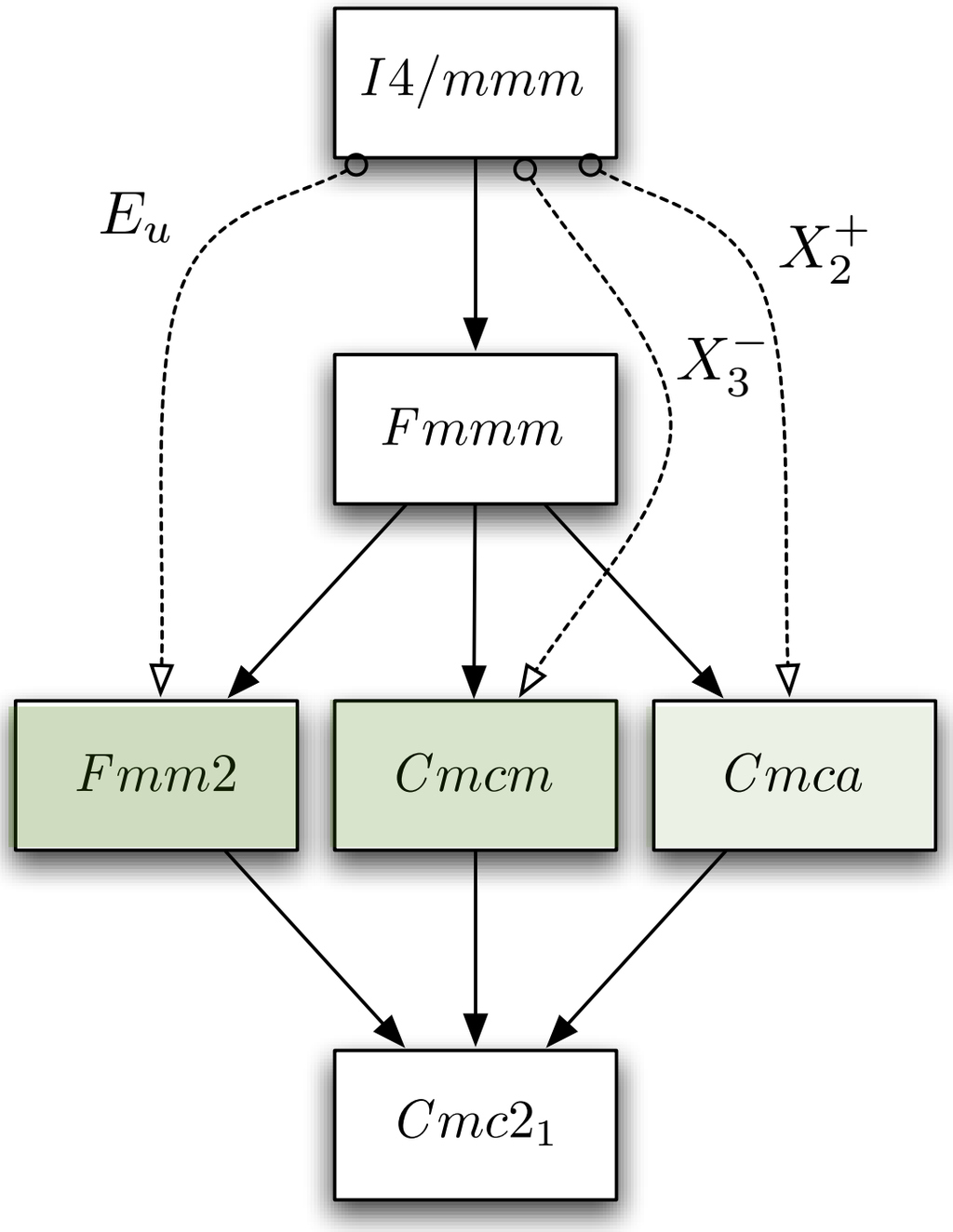
INVERSE LANDAU PROBLEM

SYMMODES

INPUT: $\mathcal{G} > \mathcal{H}, [i], W^{\mathcal{G}}$

- Group-subgroup graph — SUBGROUPGRAPH
- Classes of conjugate subgroups
- Wyckoff position splittings — WYCKSPLIT
- Primary and secondary modes — ISOTROPY
- Isotropy subgroups and irreps of G

Example: $SrBi_2Ta_2O_9$ (SBT)



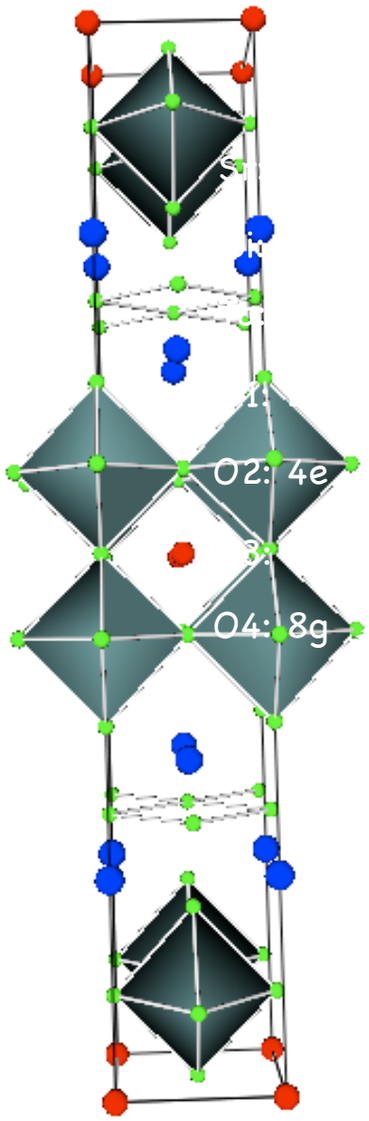
Coupled order parameters

$$\begin{cases} E_u \\ X_3^- \\ X_2^+ \end{cases}$$

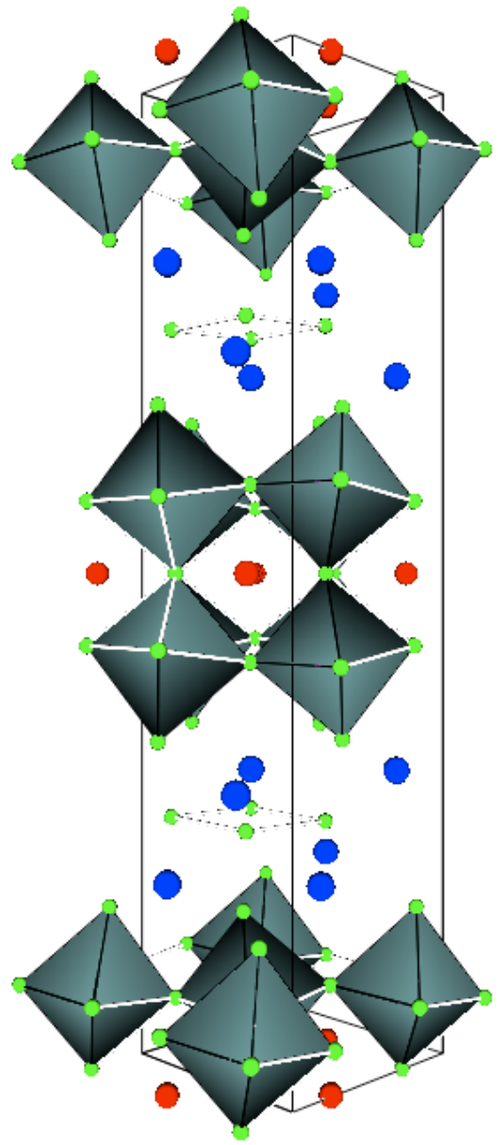
ISOTROPY SUBGROUPS

It is necessary at least two modes for breaking the symmetry until *Cmc*2_1

Example: $SrBi_2Ta_2O_9$ (SBT)



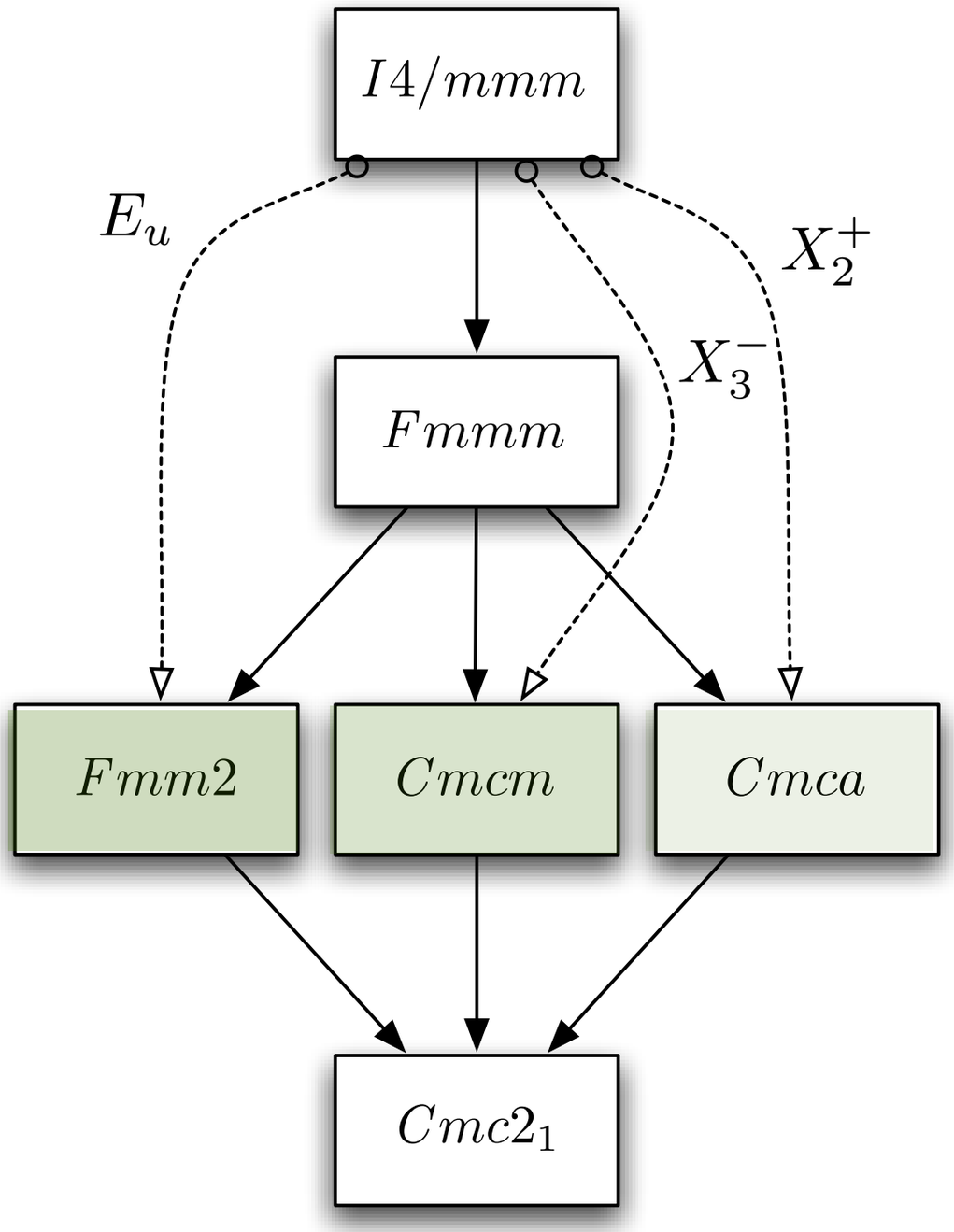
I4/mmm (139)		$Cmc2_1$ (36)
Sr: 2a	⟷	Sr: 4a
Ta: 4e	⟷	Ta: 8b
Bi: 4e	⟷	Bi: 8b
O1: 2b	⟷	O1: 4a
O2: 4e	⟷	O2: 8b
O3: 4d	⟷	O3: 8b
O4: 8g	⟷	O4: 8b
	⟷	O5: 8b



Structural data ⟶ Global distortion

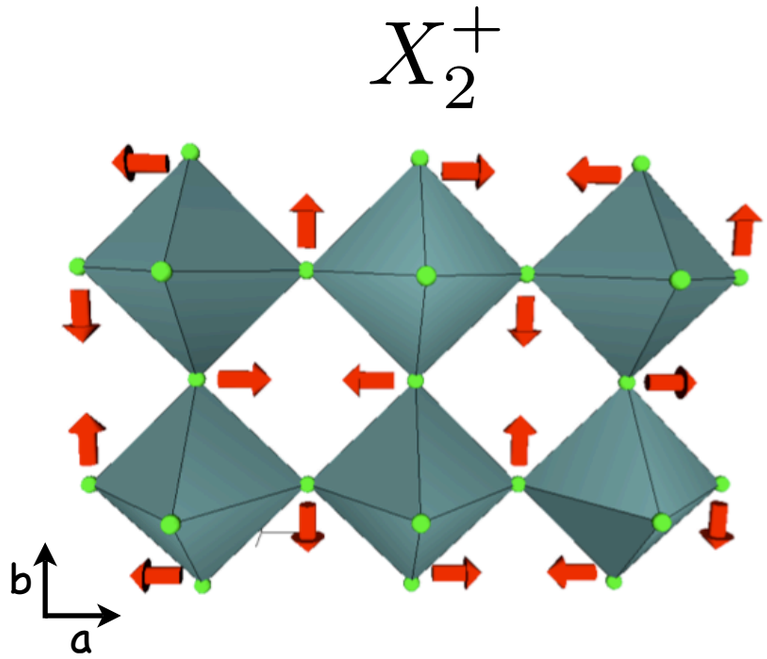
Problem: SYMMETRY-MODE ANALYSIS

AMPLIMODES



Three types of contributions to the global distortion

$$\begin{cases} E_u \\ X_3^- \\ X_2^+ \end{cases}$$



{Distortion} = $Q_{E_u}(E_u) + Q_{X_2^+}(X_2^+) + Q_{X_3^-}(X_3^-)$

Example: Modes for 8g position

E_u

WP 8g	Displacements	
(0,1/2,z)	(0,-1,0)	(1,0,0)
(-1/2,1,z+1/2)	(0,-1,0)	(1,0,0)
(0,-1/2,-z)	(0,-1,0)	(1,0,0)
(-1/2,0,-z+1/2)	(0,-1,0)	(1,0,0)
(-1/2,0,-z)	(1,0,0)	(0,-1,0)
(-1,1/2,-z+1/2)	(1,0,0)	(0,-1,0)
(-1/2,0,z)	(1,0,0)	(0,-1,0)
(-1,1/2,z+1/2)	(1,0,0)	(0,-1,0)

X_3^-

WP 8g	Displacements
(0,1/2,z)	(0,0,1)
(-1/2,1,z+1/2)	(0,0,-1)
(0,-1/2,-z)	(0,0,1)
(-1/2,0,-z+1/2)	(0,0,-1)
(-1/2,0,-z)	(0,0,1)
(-1,1/2,-z+1/2)	(0,0,-1)
(-1/2,0,z)	(0,0,-1)
(-1,1/2,z+1/2)	(0,0,1)

X_2^+

WP 8g	Displacements	
(0,1/2,z)	(0,1,0)	(1,0,0)
(-1/2,1,z+1/2)	(0,-1,0)	(-1,0,0)
(0,-1/2,-z)	(0,-1,0)	(-1,0,0)
(-1/2,0,-z+1/2)	(0,1,0)	(1,0,0)
(-1/2,0,-z)	(1,0,0)	(0,1,0)
(-1,1/2,-z+1/2)	(-1,0,0)	(0,-1,0)
(-1/2,0,z)	(1,0,0)	(0,1,0)
(-1,1/2,z+1/2)	(-1,0,0)	(0,-1,0)

$SrBi_2Ta_2O_9$ (SBT): Contributions to global distortion

$$Q_{X_3^-} = 0.8970\mathring{A} \longrightarrow Cmcm$$

O3 1	Sr1 1	Ta1 1	O4 1	O1 1	Bi1 1	O2 1
0.0446	-0.0471	-0.0271	-0.5278	0.3733	0.3306	-0.6840

$$Q_{X_2^+} = 0.2603\mathring{A} \longrightarrow Cmca$$

O4 2	O3 1	O4 1
0.0213	-0.3954	0.9183

$$Q_{E_u} = 0.6134\mathring{A} \longrightarrow Fmm2$$

O4 2	O3 1	Bi1 1	O2 1	Ta1 1	Sr1 1	O4 1	O1 1
-0.4657	-0.1745	0.0000	-0.4285	-0.3604	-0.1942	-0.5782	-0.2592

Pseudosymmetry search

Prediction of structural phase transitions

Pseudosymmetry Search

Initial Structure $\mathcal{H}$ low symmetry	**Structural Pseudosymmetry** $\Leftrightarrow$ *Distortion*	Prototype Structure $\mathcal{G}$ high symmetry

If the distortion is small enough, it can indicate a symmetry change at high temperature.

↓

Phase transition

PSEUDOSYMMETRY SEARCH

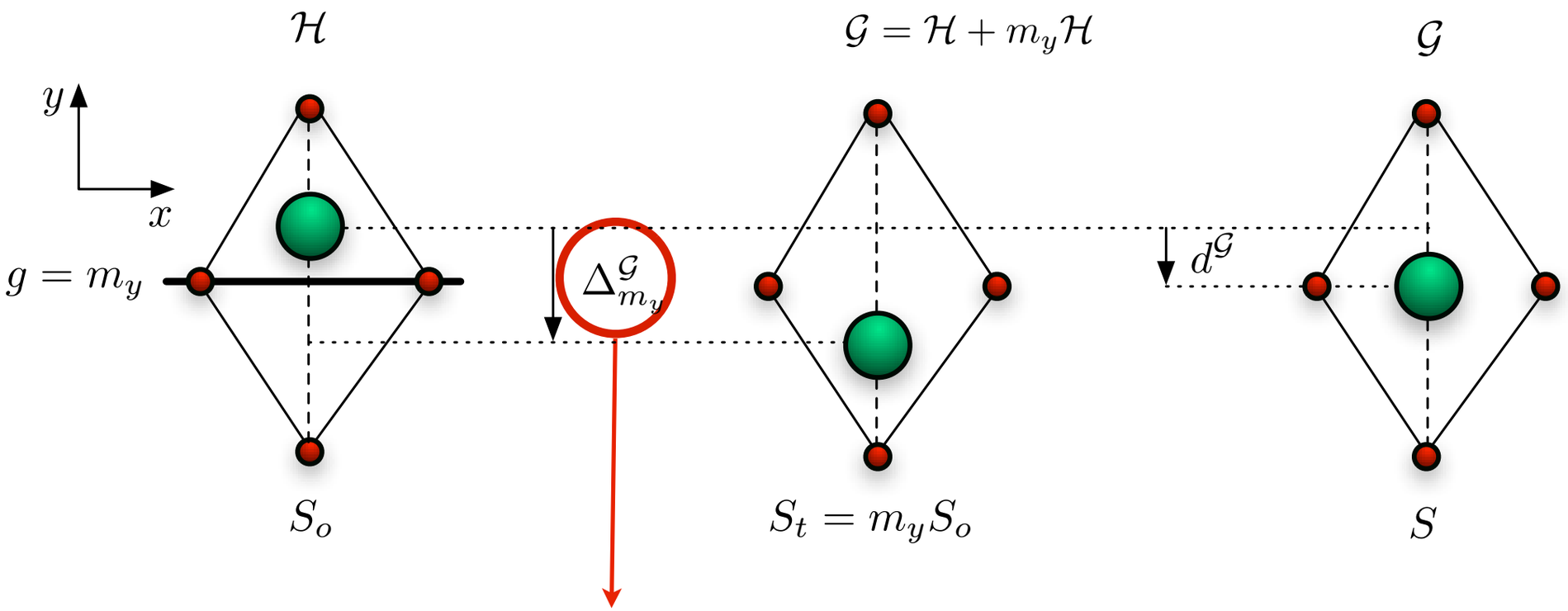
APPLICATIONS IN STRUCTURAL PHASE TRANSITIONS

- Systematic search for pseudosymmetry
- Prediction of displacive ferroelectrics
- Prediction of ferroelastics
- Overlooked symmetry

PSEUDOSYMMETRY SEARCH METHODS

- Atomic Displacement Method — PSEUDO
- Electron Density Method — DOPE
- KPLOT method — BPLOT

ATOMIC DISPLACEMENTS METHOD



Maximal distance between all compatible atom pairings

Asumption:
The high symmetry phase is described by a **supergroup** of the initial space group.

$$\mathcal{G} = \mathcal{H} + g_2\mathcal{H} + \cdots + g_m\mathcal{H}$$

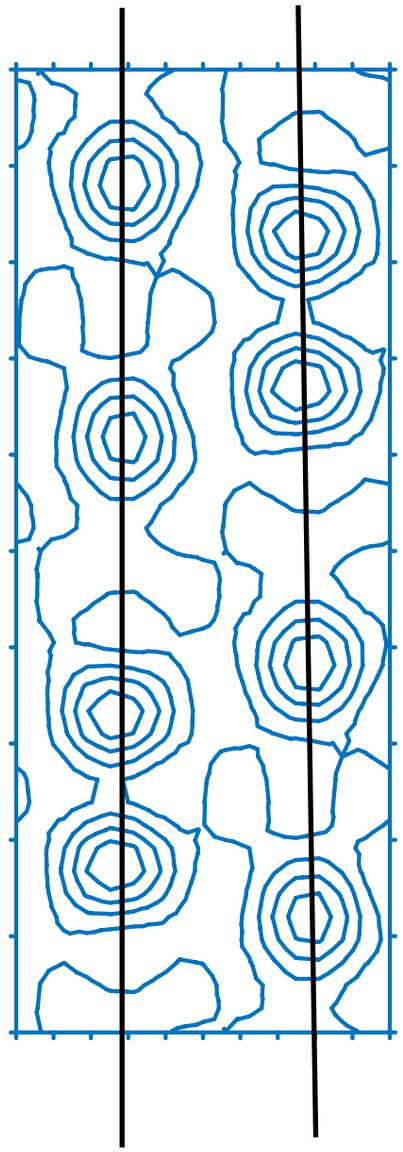
ELECTRON DENSITY METHOD

ELECTRON DENSITY

$$\rho(\mathbf{r}) = \rho_{\circ}^{\mathcal{G}}(\mathbf{r}) + \Delta\rho(\mathbf{r})$$

DEGREE OF DISSYMMETRY

$$\gamma = \frac{\int_V |\Delta\rho(\mathbf{r})|^2 dV}{\int_V |\rho(\mathbf{r})|^2 dV}$$



Asumption:
The high symmetry phase is described by a **supergroup** of the initial space group.

$$\mathcal{G} = \mathcal{H} + g_2\mathcal{H} + \cdots + g_m\mathcal{H}$$

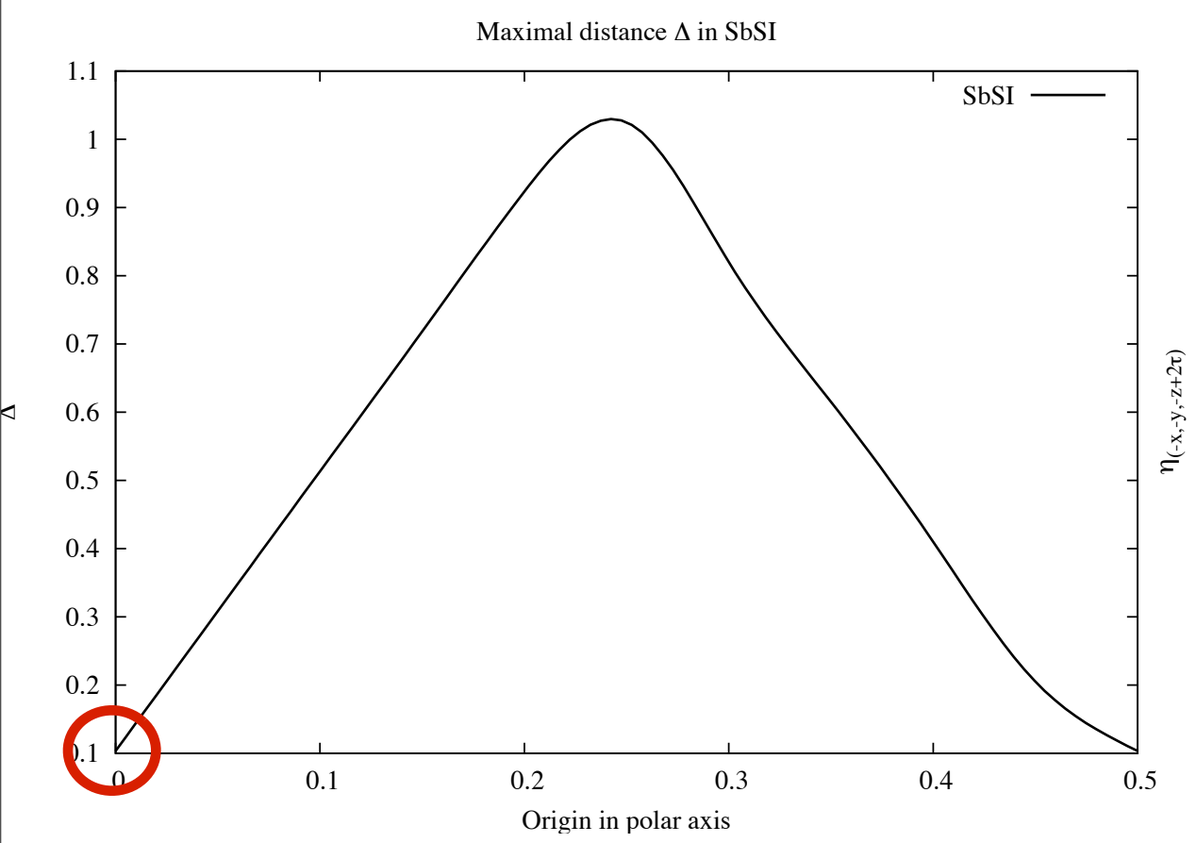
Comparison of the two methods

- PSEUDO: Geometric point of view: point like atoms whose displacements are restricted by the group-subgroup relations and the Wyckoff position splitting rules.
- DOPE : Crystallographic point of view based on the average of all atoms in the structure weighted by the atomic factors.

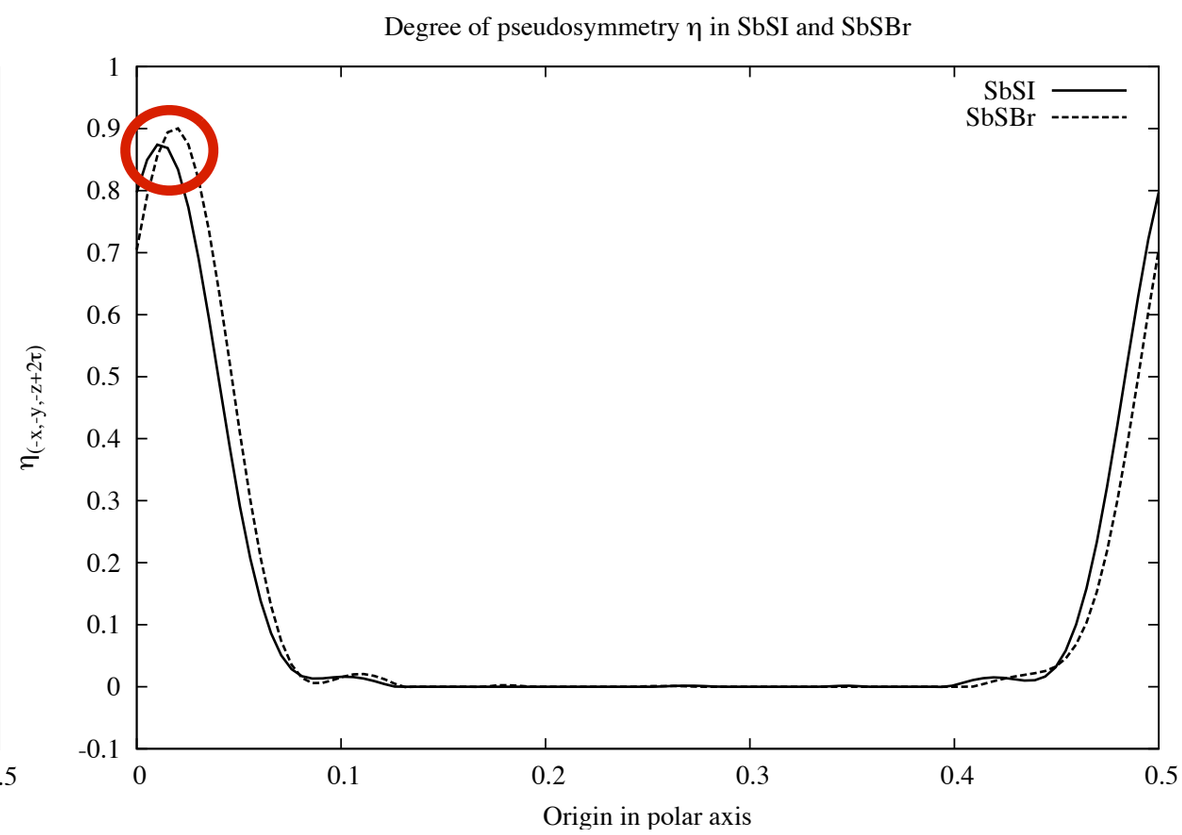
- Parameters:
  - PSEUDO: related to the maximal distance between all pairs of atoms of the initial and transformed structure.
  - DOPE : Related to the overlapping of electron clouds of the pair of atoms in the initial and the transformed structure.

THE FERROELECTRIC CASE: POLAR GROUPS

Δ



η



The origin in the polar axis is chosen for the minimum distance and maximum degree of pseudosymmetry

Problem: Prediction of *Pna2₁* ferroelectrics

PSEUDO DOPE

ICSD (Inorganic Crystal Structure Database)

	Binary	Ternary	Quaternary	Total
Entries	39	202	223	464
Compounds	26	125	161	312
Pseudo. Entries	20	100	40	160
Pseudo. Compounds	12	66	36	114
Overlooked Sym.	7	30	9	46
Known Ferro.	1	14	4	19
Candidates?	1	13	4	18

Known Ferroelectrics

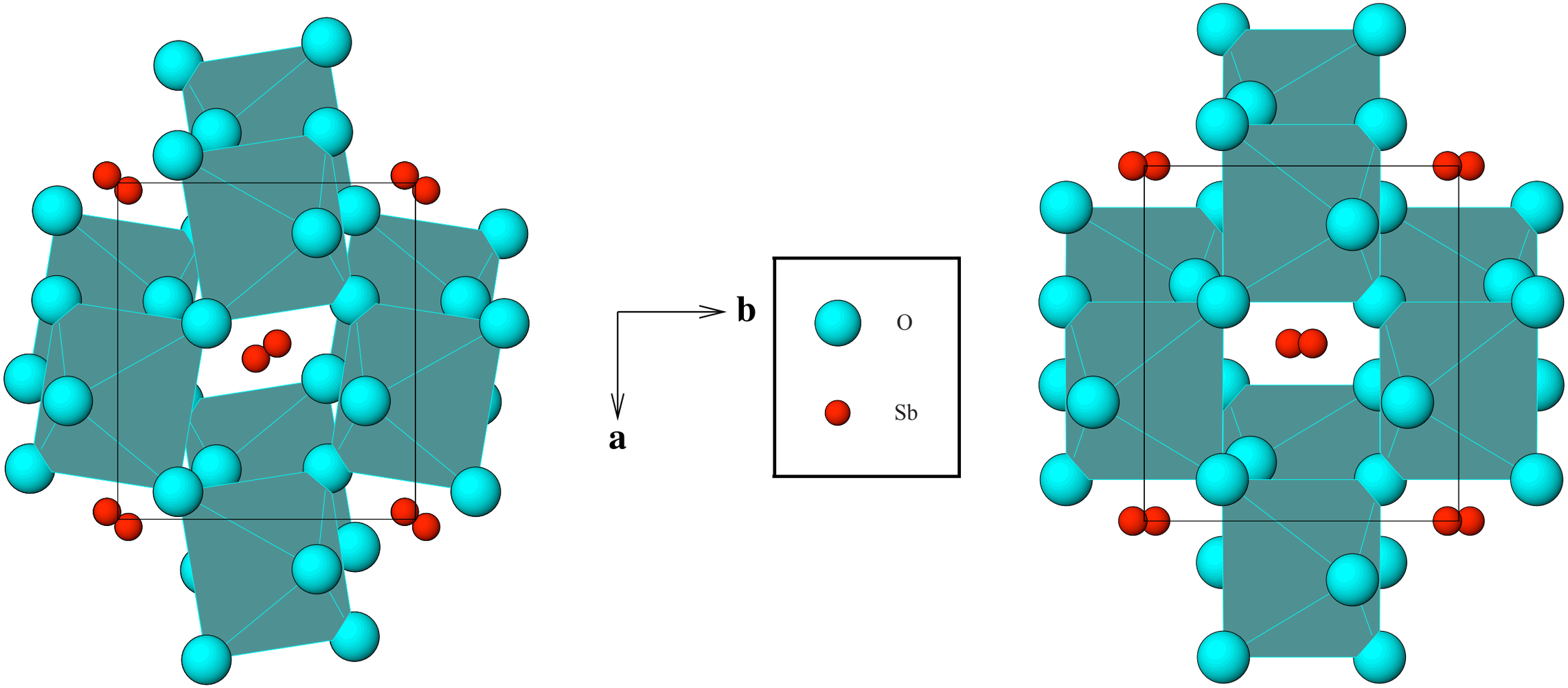
Compound	$\mathcal{G}$	$[i]$	$\Delta_{\max}$(Å)	η_g	γ	$T_c(K)$
Nb_6I_{11}	$Pccn$	2	0.547	0.623	0.189	274
$D_{0.45}Nb_6I_{11}$	$Pccn$	2	0.745	0.626	0.187	?
$NaTaO_3$	$Pnma$	2	0.232	0.988	0.006	753
$LaYbO_3$	$Pnma$	2	0.347	0.968	0.016	?
$RbGeBr_3$	$Pnma$	2	0.536	0.519	0.240	366
K_2SeO_4	$Pnma$	2	0.539	0.833	0.084	93
Cs_2BeF_4	$Pnma$	2	0.174	0.663	0.168	?
Rb_2BeF_4	$Pnma$	2	0.171	0.992	0.004	921
K_2BeF_4	$Pnma$	2	0.338	0.772	0.114	968
Rb_2ZnBr_4	$Pnma$	2	0.131	0.961	0.020	200
Rb_2ZnCl_4	$Pnma$	2	0.463	0.849	0.076	189
K_2ZnCl_4	$Pnma$	2	0.177	0.898	0.051	130
SbSI	$Pnma$	2	0.103	0.766	0.117	293
SbSBr	$Pnma$	2	0.109	0.821	0.089	23
$SbNbO_4$	$Pnna$	2	0.421	0.455	0.272	678
$(BiO)_4(NbO_4)Cl$	$Pbcn$	2	0.623	0.733	0.133	640
$CsTiO(AsO_4)$	$Pnna$	2	0.447	0.622	0.189	?
$KTiO(AsO_4)$	$Pnna$	2	0.610	0.997	0.002	?
$TlTiO(PO_4)$	$Pnna$	2	0.408	0.792	0.104	856

Candidates

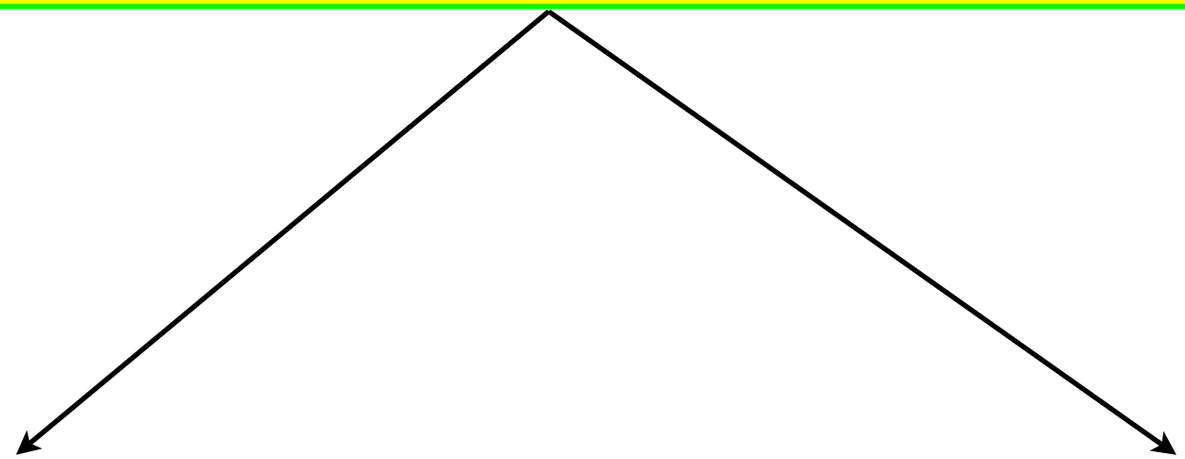
Compound	$\mathcal{G}$	$[i]$	$\Delta_{\max}$(Å)	η_g	γ
Sb_2O_4	$\mathrm{P}nna$	2	0.581	0.641	0.179
PbNCN	$\mathrm{P}nma$	2	0.193	0.996	0.002
$NaIO_3$	$\mathrm{P}nma$	2	0.194	0.977	0.012
$YScS_3$	$\mathrm{P}nma$	2	0.179	0.865	0.068
$CeSiP_3$	$\mathrm{P}nma$	2	0.648	0.935	0.032
$SmBeF_4$	$\mathrm{P}nma$	2	0.325	0.979	0.010
K_3AsS_4	$\mathrm{P}nma$	2	0.227	0.847	0.077
WPO_5	$\mathrm{P}nma$	2	0.457	0.986	0.007
$Sr_3Sb_4S_9$	$\mathrm{P}nma$	2	0.230	0.822	0.089
$Be_4Pr_9O_{20}$	$\mathrm{P}nma$	2	0.246	0.904	0.048
$Ca_{0.84}Sr_{1.16}SiO_4$	$\mathrm{P}nma$	2	0.580	0.747	0.127
$Tl_{1.1}AlSiO_4$	$\mathrm{P}nma$	2	0.590	0.953	0.024
$Na_2UO_2P_2O_7$	$\mathrm{P}nma$	2	0.559	0.991	0.040
$TlSnPS_4$	$\mathrm{P}nma$	2	0.488	0.734	0.133

Example: Sb_2O_4 ($Pna2_1 \overset{(2)}{\rightarrow} Pnna$)

$$\boldsymbol{\Delta = 0.581}\text{Å y } \boldsymbol{\eta_g = 0.641}\text{Å}$$



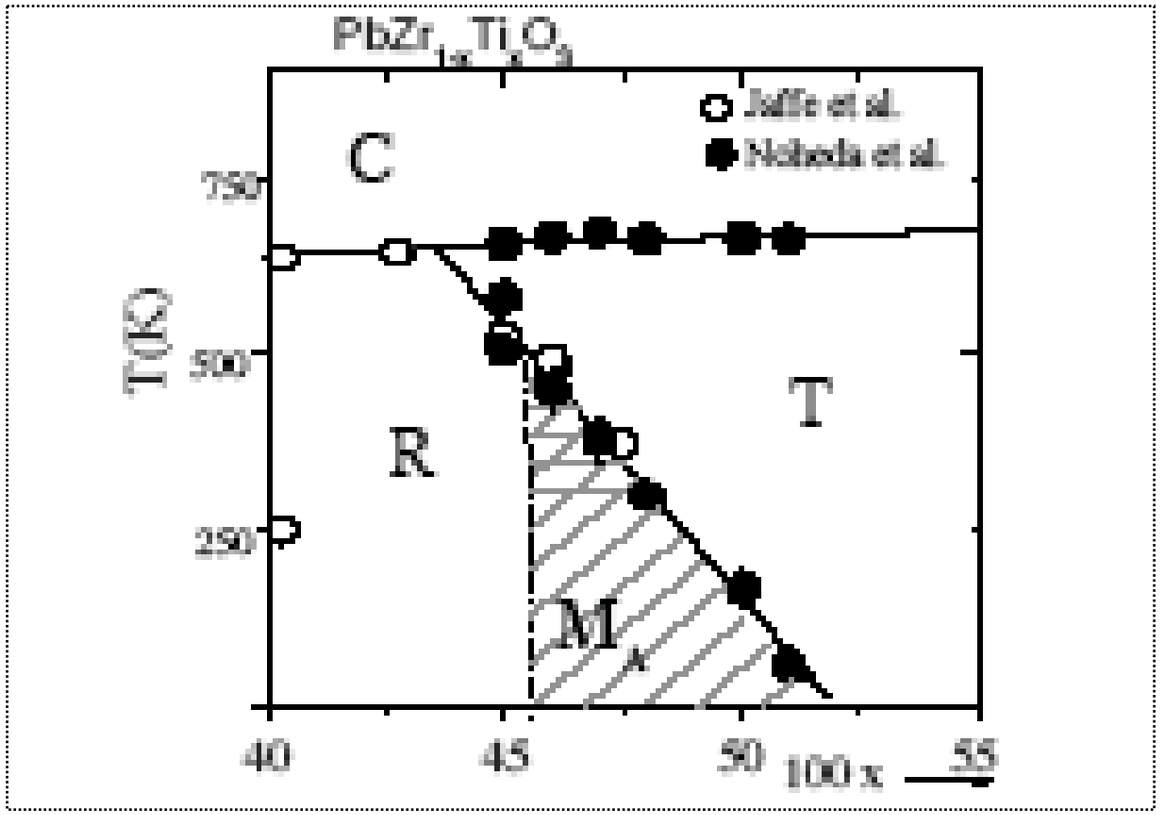
Group-NOT-Subgroup Related Phases



Structural relationship via a stable phase of common subgroup symmetry

Phase transitions with no group-subgroup relations between the phases

Example: Monoclinic phase of the system $PbZr_{1-x}Ti_xO_3$

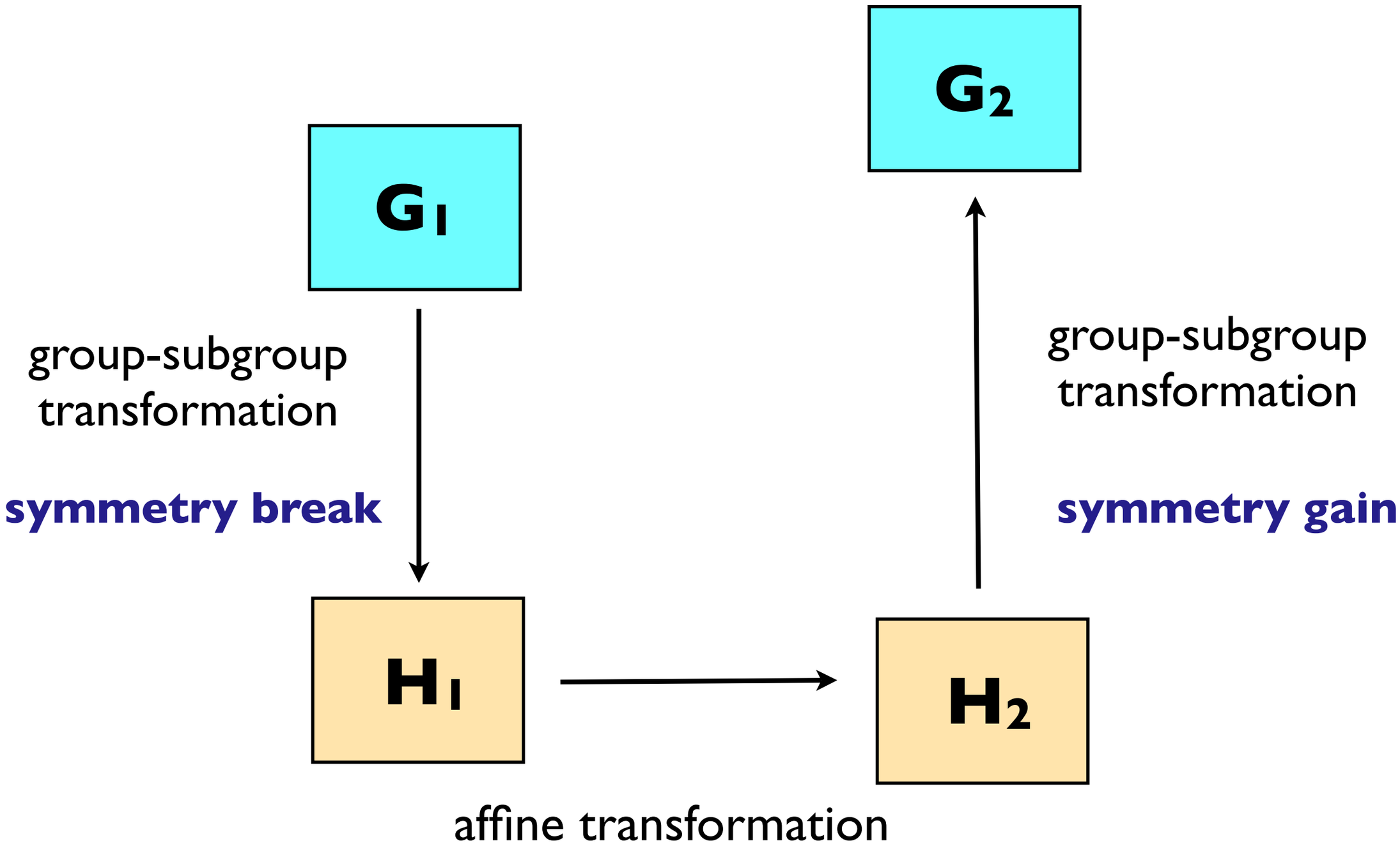


Phase diagram of PZT in the vicinity of its morphotropic phase boundary. C, R, and T represent cubic, rhombohedral and tetragonal regions. The diagonally-shaded M_A area represents the stability region of monoclinic phase.
(D.E. Cox et al. Condensed Matter, cond-mat/0102457, 2001.)

Symmetry arguments for the determination of the monoclinic phase ?

Problem: STRUCTURAL RELATIONSHIP

GROUP-THEORETICAL MODEL



Symmetry Conditions

- The description of the intermediate state involves a common subgroup pair (H_1, H_2) of the symmetry groups of the two phases such $G_1 > H_1$ and $G_2 > H_2$.
- The compatibility between the occupied Wyckoff orbits in the intermediate state.

Example PZT:COMMON SUBGROUPS

Branch 1

P4mm

$Z_1=1$

$i_1=4$

Cm

Branch 2

R3m

$Z_2=3$

$i_2=3$

Cm

index condition: $i_2=i_1\frac{Z_1\ f_2\ |P_2|}{f_1\ Z_2\ |P_1|}$

Example PZT: Wyckoff positions compatibility

Branch 1 | Branch 2

P4mm | *Cm* | *R3m*

Pb1 1a 4mm (00z_1)	→	2a m (x0z)	←	3a 3m (00z_1) Pb1
Ti/Zr 1b 4mm (1/2 1/2 z_2)	→	2a m (x0z)	←	3a 3m (00z_2) Ti/Zr
O1 1b 4mm (1/2 1/2 z_3)	→	2a m (x0z)	←	9b .m (x-xz_3) O1
O2 2c 2mm. (1/2 0 z_4)	→	4b 1 (xyz)		

Structural Conditions

- Minimum deformation strain in the transformation
- Minimum distance between the corresponding atoms in the initial structures described in the subgroup reference frame

FURTHER APPLICATIONS OF

GROUP-NOT-SUBGROUP RELATIONS:

-PHASE TRANSITIONS WITH NO GROUP-SUBGROUP RELATIONS

-FERROELECTRIC PHASES WITH DIFFERENT ORIENTATIONS OF POLARIZATIONS

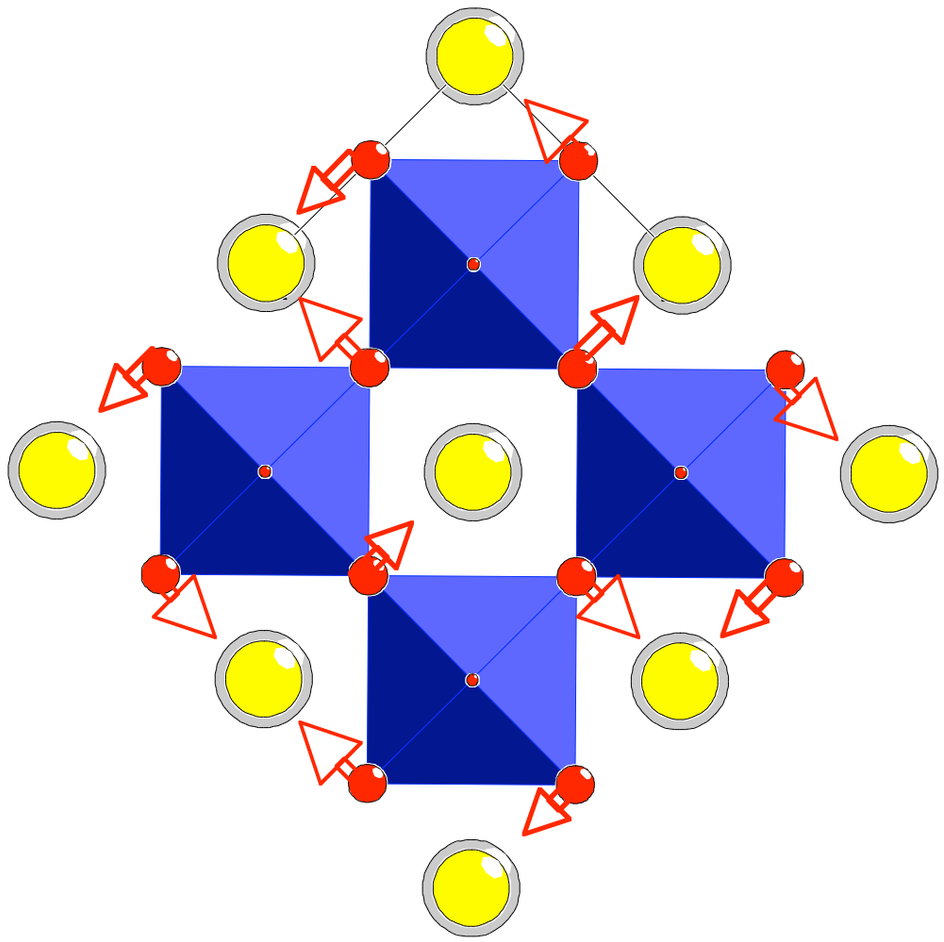
CRYSTALLOGRAPHIC SOFTWARE

Representation Theory Applications	
REPRES	Space Groups Representations
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations Between Representations
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure

Site-symmetry approach

-Relations between localized states
and crystal extended states



Strain Calculation

$$\mathbf{X_1} = R_1 \cdot \mathbf{x_1} \quad \mathbf{X_2} = R_2 \cdot \mathbf{x_2} \qquad R_i = \begin{pmatrix} a_i sin(\beta_i) sin(\gamma_i^*) & 0 & 0 \\ -a_i sin(\beta_i) cos(\gamma_i^*) & b_i sin(\alpha_i) & 0 \\ a_i cos(\beta_i) & b_i cos(\alpha_i) & c_i \end{pmatrix}$$

standard root tensor

Strain definition:

$$\mathbf{X_2} - \mathbf{X_1} = e \cdot \mathbf{X_1} \quad \text{with} \quad e = R_2^{-1} R_1 - I$$

$$M_i = \begin{pmatrix} \vec{a_i} \cdot \vec{a_i} & \vec{a_i} \cdot \vec{b_i} & \vec{a_i} \cdot \vec{c_i} \\ \vec{b_i} \cdot \vec{a_i} & \vec{b_i} \cdot \vec{b_i} & \vec{b_i} \cdot \vec{c_i} \\ \vec{c_i} \cdot \vec{a_i} & \vec{c_i} \cdot \vec{b_i} & \vec{c_i} \cdot \vec{c_i} \end{pmatrix}$$

metric tensor

$$\eta = \frac{1}{2}(e + e^T + e^T e) = \frac{1}{2} R_1^{-T} (M_1 - M_2) R_1^{-1}$$

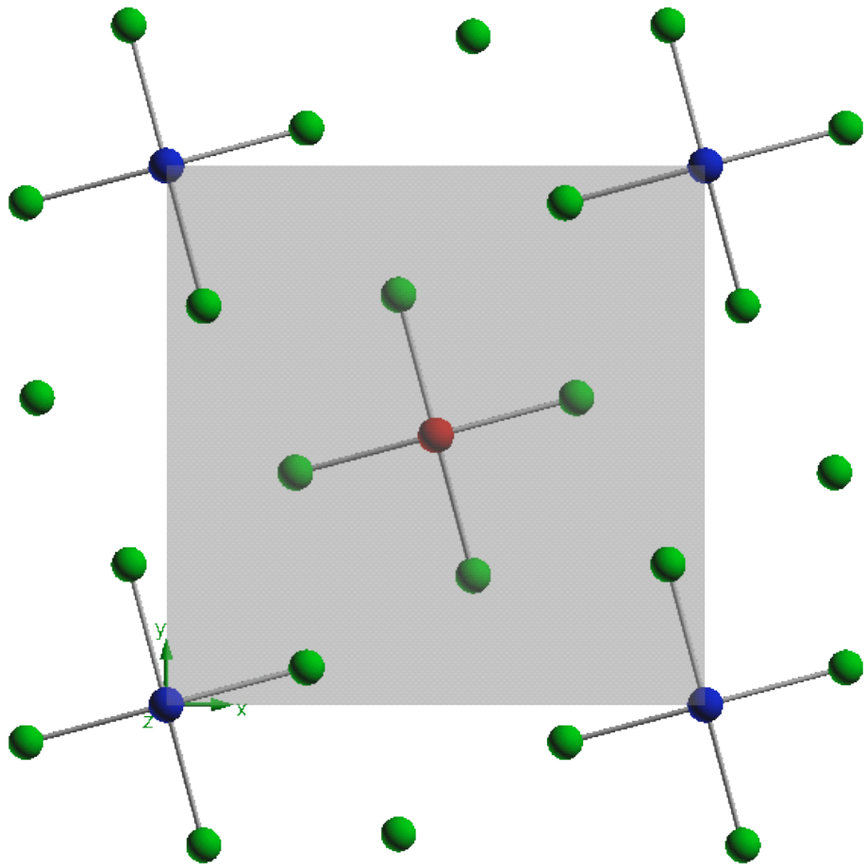
Degree of lattice distortion: $$\mathcal{S} = \frac{1}{3} \sqrt{\sum_{i=1}^{3} \eta_i^2}$$

Valid for linear and non-linear strains!

Problem: Equivalent descriptions

EQUIVSTRU

Example: $WOBr_4$



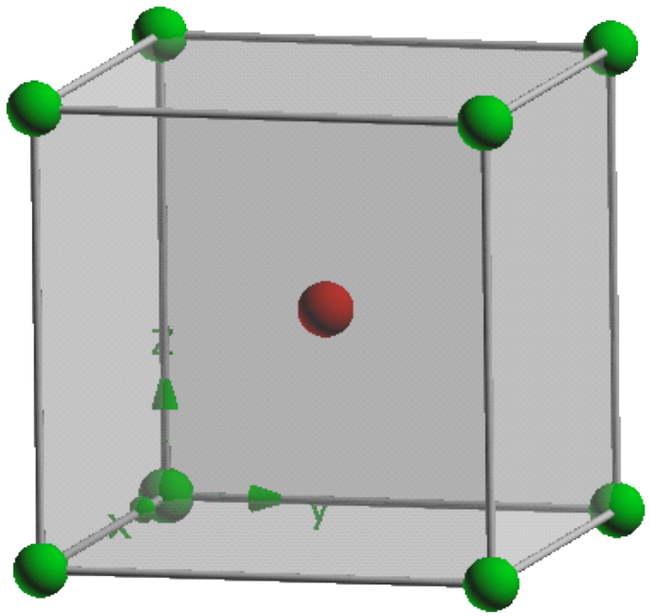
Space Group: $I4$

Euclidean Normalizer: $P^1 4/mmm$

Index: 4

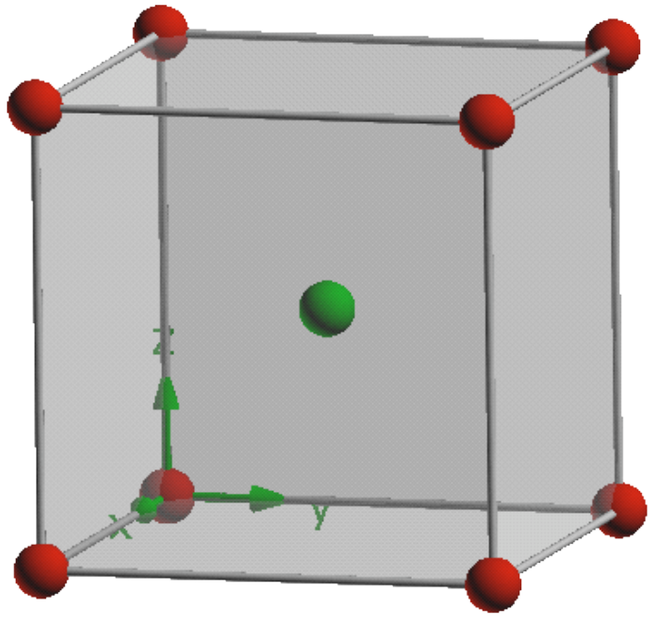
$$P4/mmm = I4 + (\bar{x}, \bar{y}, \bar{z})I4 + (y, x, z)I4 + (\bar{y}, \bar{x}, \bar{z})I4$$

EQUIVALENT DESCRIPTIONS



CsCl

Pm-3*m* (221)

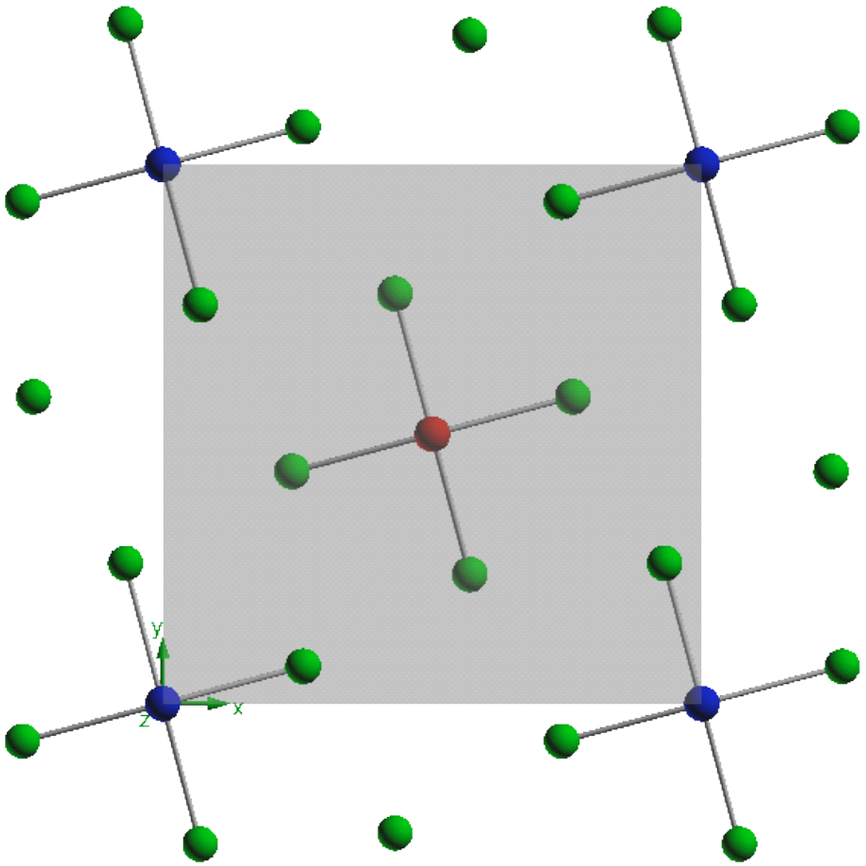


Normalizer operation: x+1/2, y+1/2, z+1/2

1a (0,0,0) ⟶ 1b (1/2,1/2,1/2)

1b (1/2,1/2,1/2) ⟶ 1a (0,0,0)

Example: $WOBr_4$



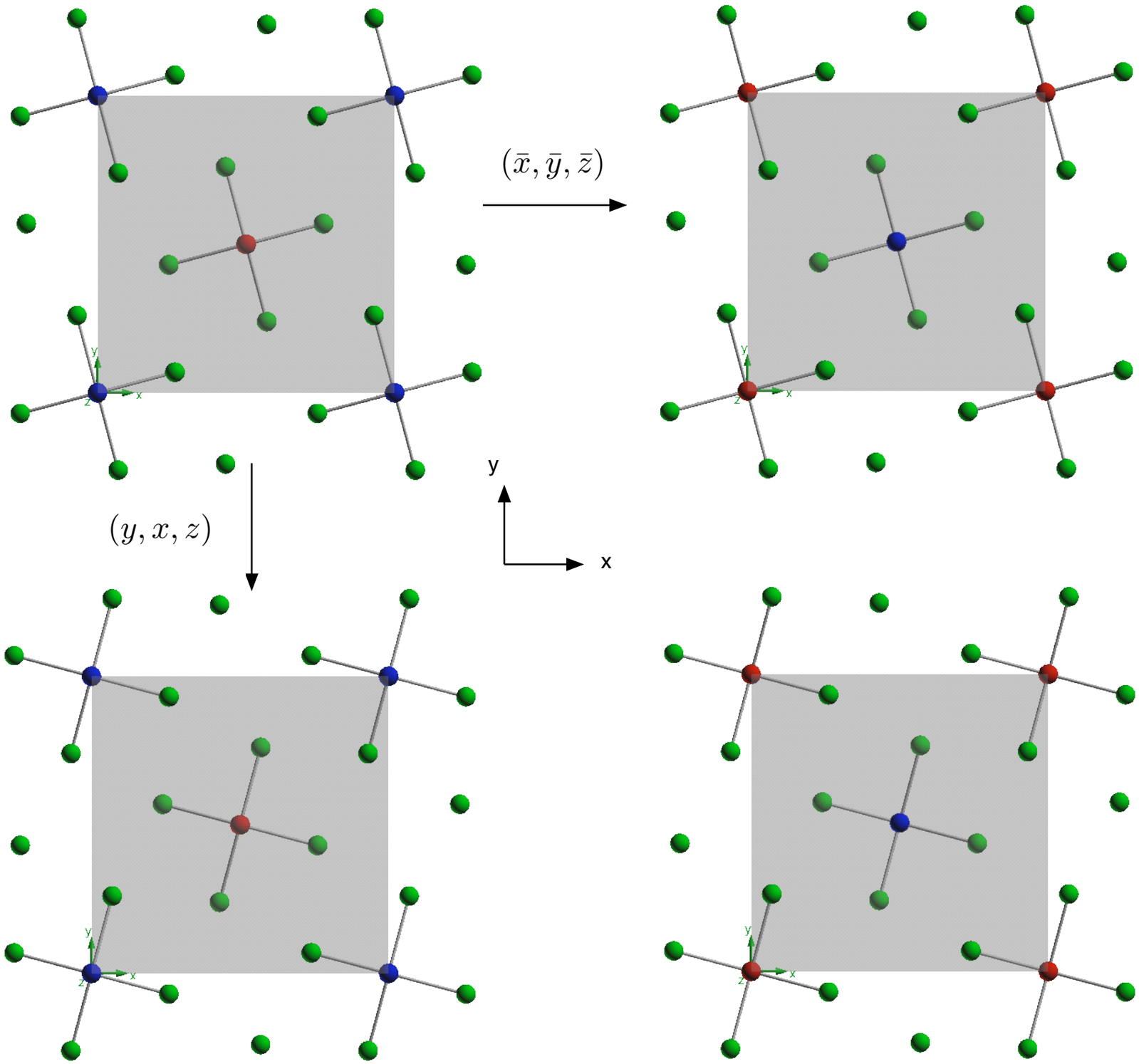
Space Group: $I4$

Euclidean Normalizer: $P^1 4/mmm$

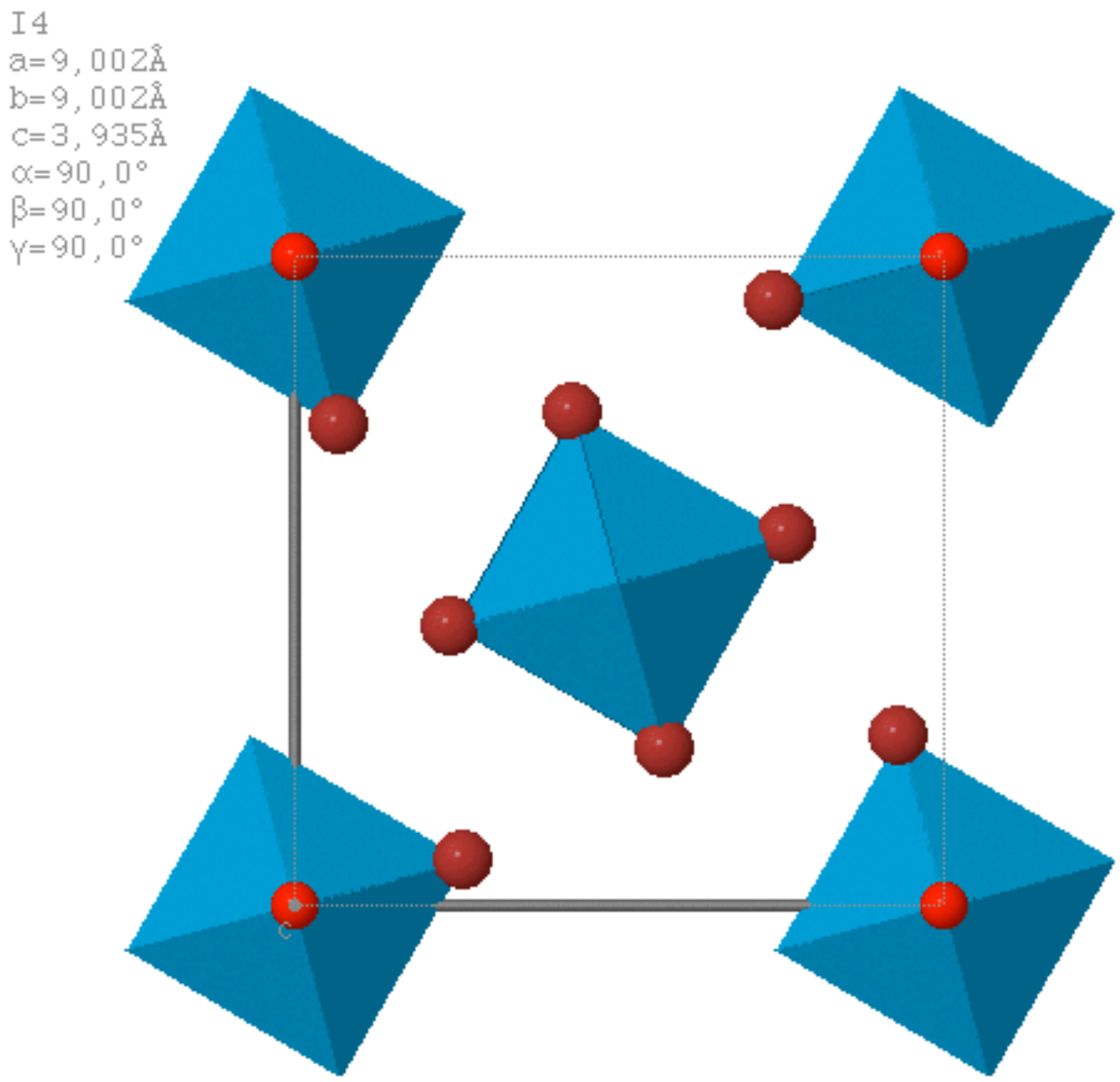
Index: 4

$$P4/mmm = I4 + (\bar{x}, \bar{y}, \bar{z})I4 + (y, x, z)I4 + (\bar{y}, \bar{x}, \bar{z})I4$$

EQUIVALENT DESCRIPTIONS



View Structure (with Jmol applet)



www.cryst.ehu.es Jmol

zoom +10% | zoom -10% | zoom 250% | C4x | top | perspective | stereo

select atoms | labels | atoms 20% | colour | bgcolor | polyhedra | bonds | wireframe 0.15

expand cell a: 1 b: 1 c: 1 bonds/polyhedra from 0.75 to 2.75 Å Reload Print

Note: If you can not visualize the structure you can download the CIF file and view it with some viewer as Jmol

Equivalent descriptions of crystal structures

EQUIVSTRU

U. MÜLLER, p.20

9. $P(C_6C_5)_4[MoNCl_4]$ is tetragonal, space group $P4/n$, with the following coordinates. How many equivalent sets of coordinates can be used to describe this structure? What are their coordinates?

	x	y	z		x	y	z
P	$\frac{1}{4}$	$\frac{3}{4}$	0	Mo	$\frac{1}{4}$	$\frac{1}{4}$	0.121
C 1	0.362	0.760	0.141	N	$\frac{1}{4}$	$\frac{1}{4}$	–0.093
C 2	0.437	0.836	0.117	Cl	0.400	0.347	0.191

(H atoms and C 3 to C 6 omitted)

For data input file:

www.cryst.ehu.es/html/gargnano.html

http://158.227.0.68/html/gargnano.html

Different setting description of crystal structures

SETSTRU

M. Aroyo, p.15

Structural data: Space group $I4_1/amd = D_{4h}^{19}$, No. 141;
lattice constants a = 6.60 Å; c = 5.88 Å.

The origin choice is not stated explicitly. However, Wyckoff's *Crystal Structures* started to appear in 1948, when there was one conventional origin only (the later ORIGIN CHOICE 1, *i. e.* **Origin** at $\bar{4}m2$).

$Zr : (a)$ $0,0,0;\ 0,\frac{1}{2},\frac{1}{4};\ \frac{1}{2},0,\frac{3}{4};\ \frac{1}{2},\frac{1}{2},\frac{1}{2};$
$Si : (b)$ $0,0,\frac{1}{2};\ 0,\frac{1}{2},\frac{3}{4};\ \frac{1}{2},0,\frac{1}{4};\ \frac{1}{2},\frac{1}{2},0;$
$O : (h)$ $(0,u,v;\ 0,\bar{u},v;\ u,0,\bar{v};\ \bar{u},0,\bar{v};\ 0,\frac{1}{2}+u,\frac{1}{4}-v;\ 0,\frac{1}{2}-u,\frac{1}{4}-v;$
$\bar{u},\frac{1}{2},v+\frac{1}{4};\ u,\frac{1}{2},v+\frac{1}{4};)$ [and the same with $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$].

The parameters u and v are listed with $u = 0.20$ and $v = 0.34$.

(b) In the *Structure Reports*, vol. **22**, (1958), p. 314 one finds:

'a = 6.6164(5) Å, c = 6.0150(5) Å'

'Atomic parameters. Origin at center $(2/m)$ at $0, \frac{\bar{1}}{4}, \frac{1}{8}$ from $\bar{4}m2$.'

'Oxygen: $(0, y, z)$ with $y = 0.067$, $z = 0.198$.'

In order to compare the different data, the parameters of Wyckoff's book are to be transformed to 'origin at center $2/m$', *i. e.* ORIGIN CHOICE 2.

Phase transitions

SYMMODES and AMPLIMODES

M. CATTI

Example: AgI: Fm-3m -->$P2_1/m$

For data input file:

www.cryst.ehu.es/html/gargnano.html

http://158.227.0.68/html/gargnano.html

URLs of the programs

Bilbao Crystallographic Server

http://www.cryst.ehu.es

Suggestions and comments

cryst@wm.lc.ehu.es