AIC Commission on Crystallographic Teaching

AIC International Crystallography School 2019

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www.cristallografia.org/aicschool2019

BILBAO CRYSTALLOGRAPHIC SERVER I

SPACE-GROUP SYMMETRY

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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

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ECM31-Oviedo Satellite

Crystallography online: workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20-21 August 2018

News:

- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305.
- **New program: BANDREP**
  04/2017: Band representations and Elementary Band representations of Double Space Groups.
- **New section: Double point and space groups**
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    04/2017: General positions of Double Space Groups
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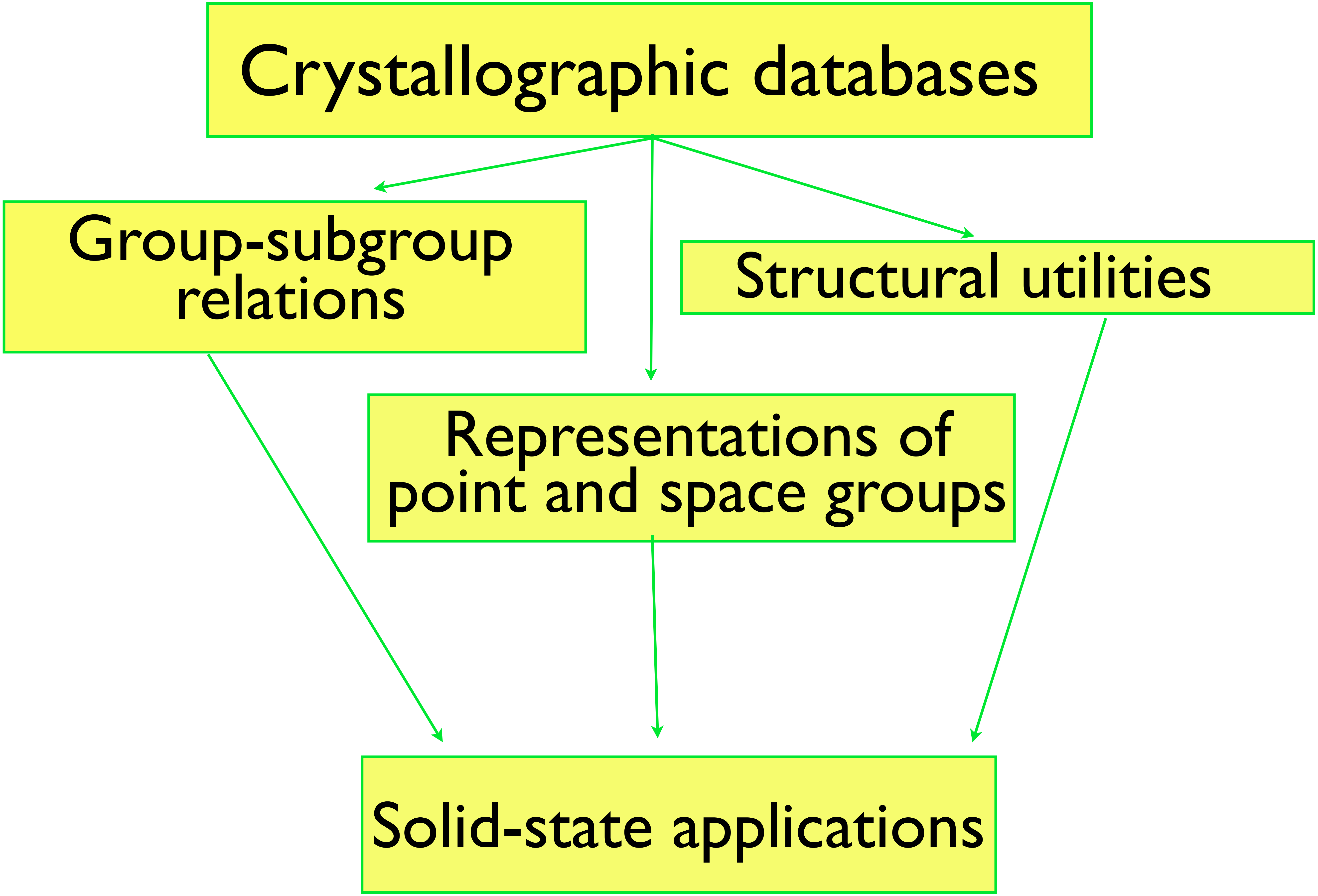
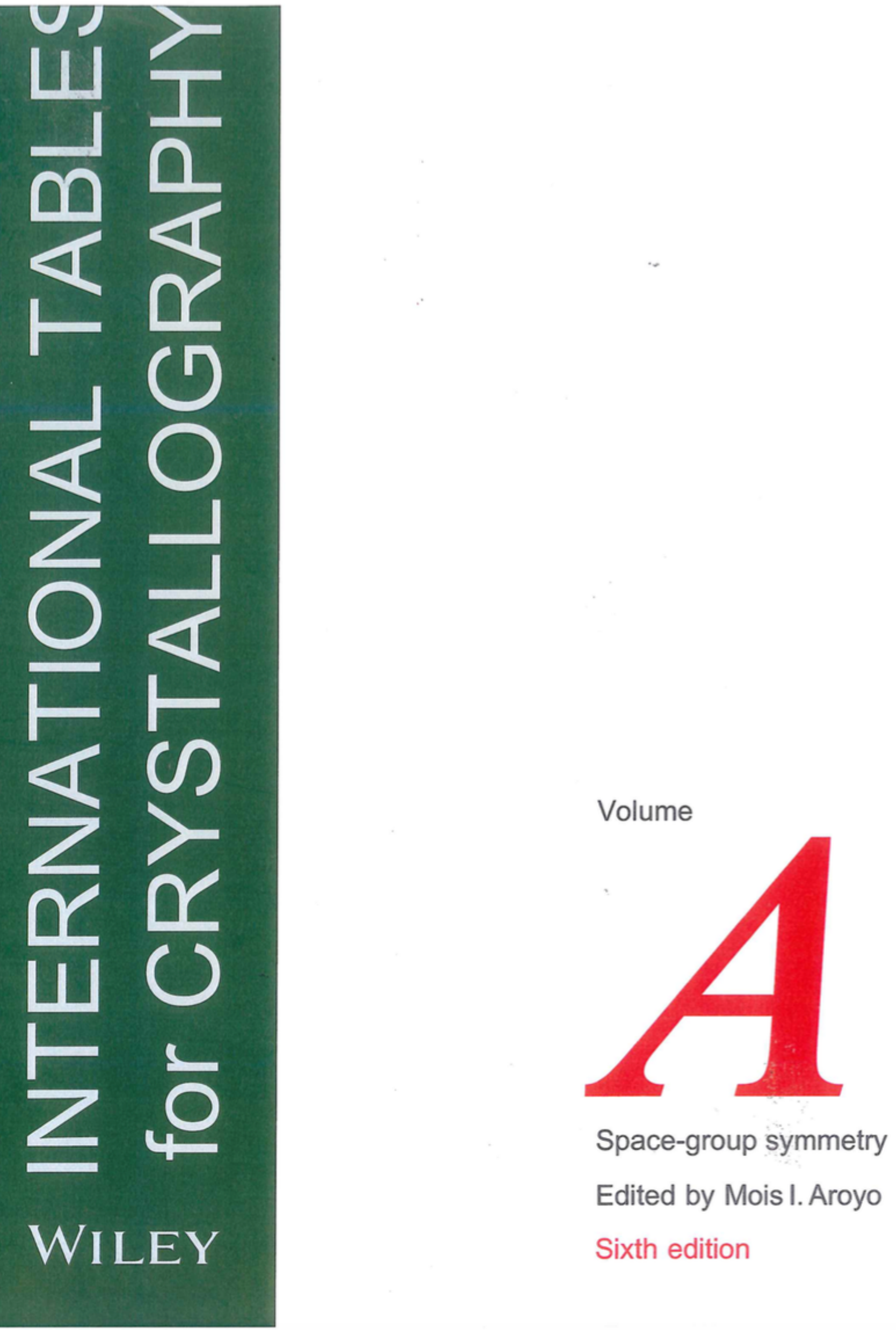
    04/2017: Irreducible representations of

Crystallographic Databases

International Tables for Crystallography


Crystallographic databases
Group-subgroup relations
Structural utilities
Representations of point and space groups
Solid-state applications

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY VOLUME A: SPACE-GROUP SYMMETRY



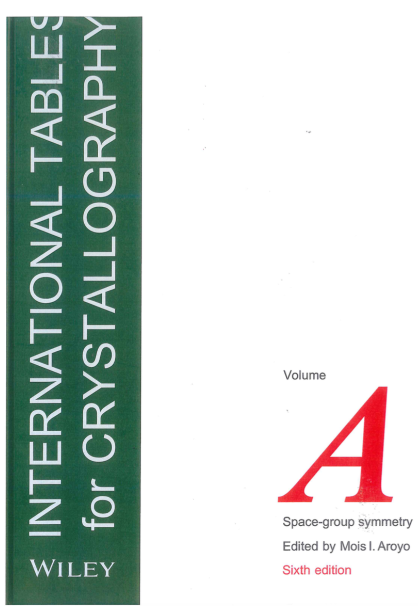
Extensive tabulations and illustrations of the 17 plane groups and of the 230 space groups

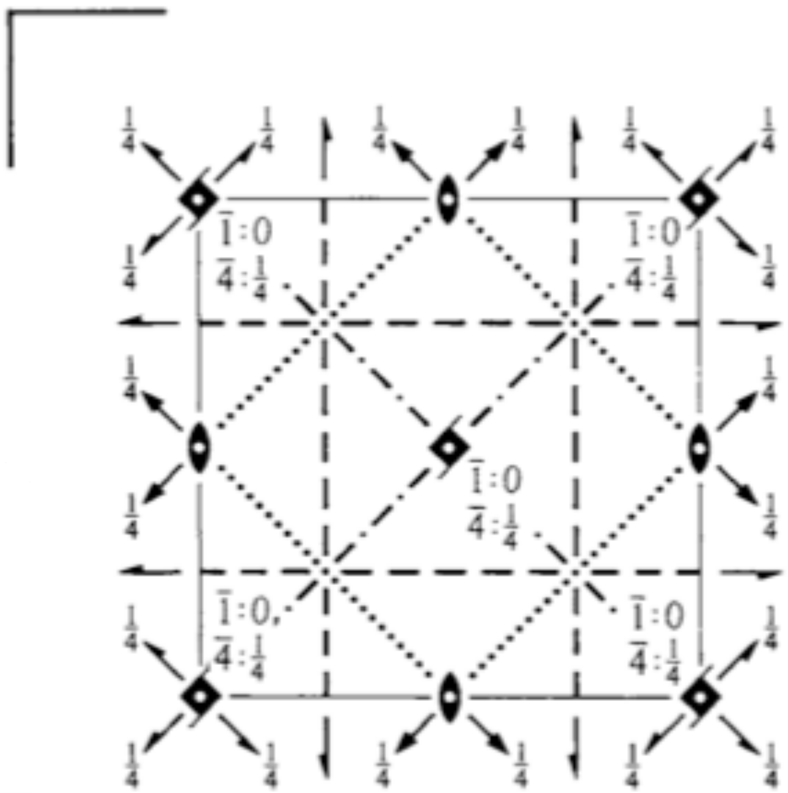
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection conditions;
- symmetries of special projections;

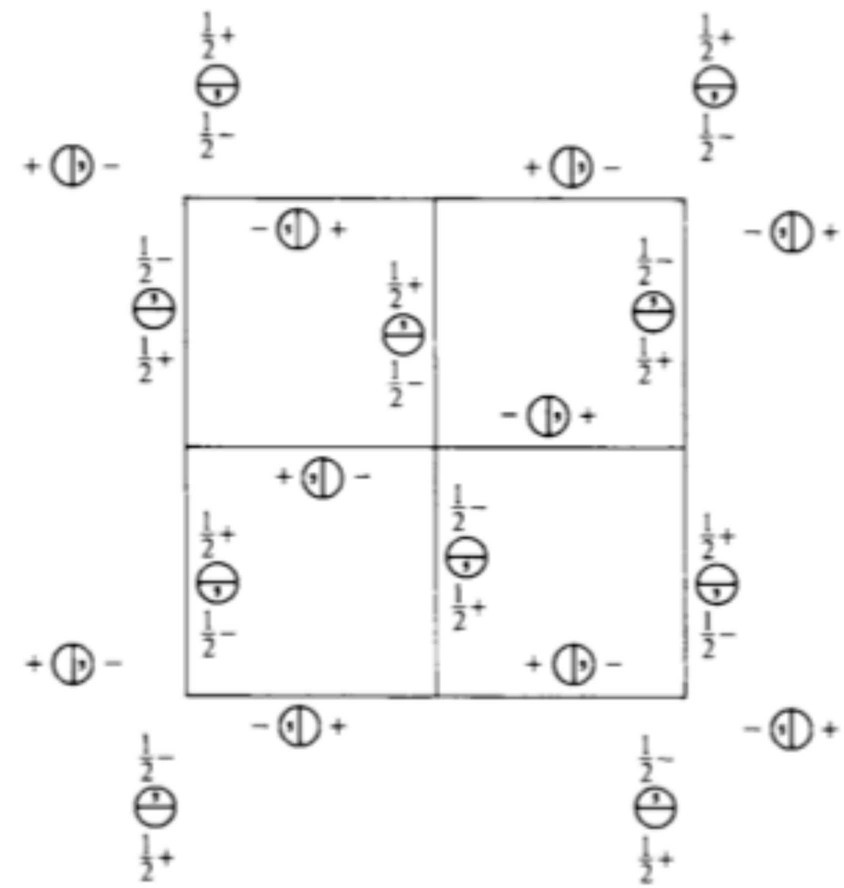
International Tables for Crystallography (2006). Vol. A, Space group 135, pp. 466–467.

$P4_2/mbc$ $\quad D_{4h}^{13}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 135 $\quad P\ 4_2/m\ 2_1/b\ 2/c$ $\quad$ Patterson symmetry $P4/mmm$







Origin at centre ($2/m$) at $4_2/m\,1\,n$

Asymmetric unit $\quad 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,0,z$	(4) $4^-(0,0,\frac{1}{2})\quad 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\quad 0,0,z;\quad 0,0,\frac{1}{4}$	(12) $\bar{4}^-\quad 0,0,z;\quad 0,0,\frac{1}{4}$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection condi
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl : $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	h	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	g	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	hkl : $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	
8	f	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	
8	e	$2..$	$0,0,z$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	
4	d	2.22	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl : $h+k,l=2n$
4	c	$2/m..$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$
4	b	$\bar{4}..$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	hkl : $h+k,l=2n$
4	a	$2/m..$	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$

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    04/2017: Irreducible representations of

Space-group symmetry

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 symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

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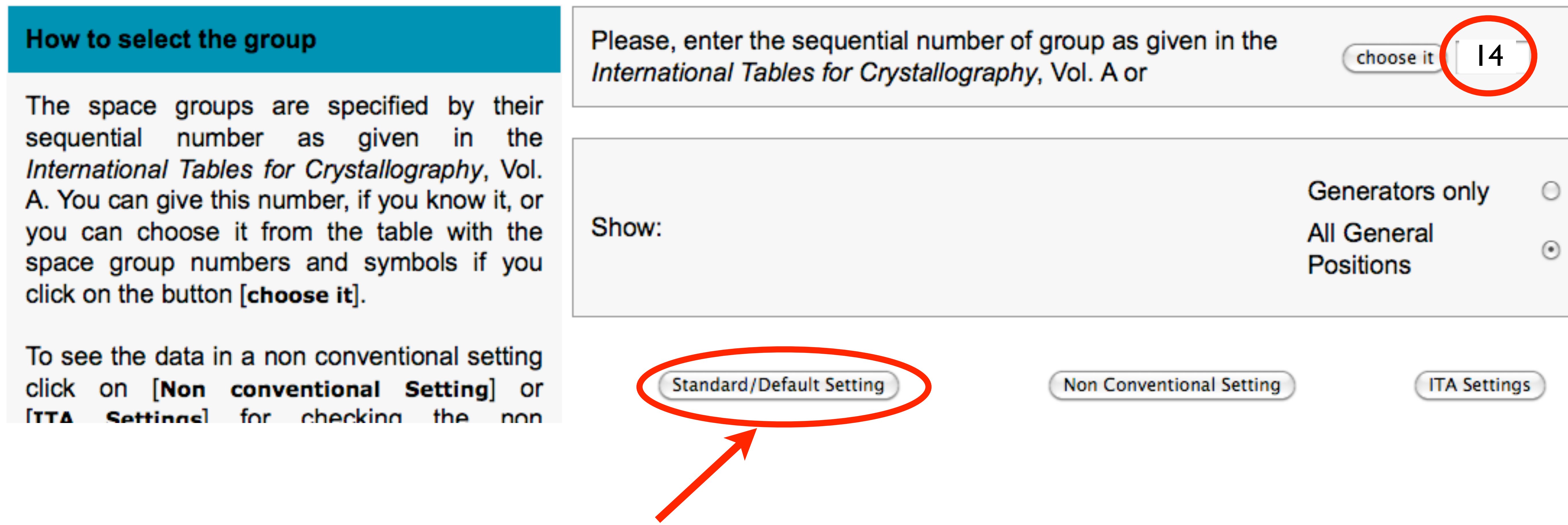
Problem: Matrix-column presentation
Geometrical interpretation

GENPOS

Generators and General Positions

space group



Example GENPOS: Space group $P2_1/c$ (14)

Space-group symmetryoperations

short-hand notation

matrix-column presentation $\begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$

Geometric interpretation

Seitz symbols

General Positions of the Group 14 ($P2_1/c$) [unique axis b]

Click here to get the general positions in text format

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x,y+1/2,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 0,y,1/4	{ 2_{010} | 0 1/2 1/2 }
3	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	{ -1 | 0 }
4	x,-y+1/2,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,1/4,z	{ m_{010} | 0 1/2 1/2 }

ITA data

General positions

4 e 1 (1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

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Problem: Wyckoff positions
Site-symmetry groups

WYCKPOS

Wyckoff Positions

space group

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it.**

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

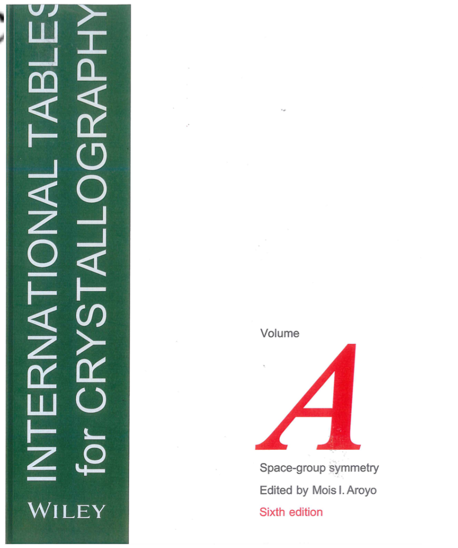
Aroyo, *et. al. Zeitschrift fuer Kristallographie* (2006), **221**, 1, 15-27.

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

Standard/Default Setting | Non Conventional Setting | ITA Settings

$Ccce$ D_{2h}^{22} mmm Orthorhombic

No. 68 $C\ 2/c\ 2/c\ 2/e$ Patterson symmetry $Cmmm$



16	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$
8	h	$..2$	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$
8	g	$..2$	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$
8	f	$.2.$	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	
8	e	$2..$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	
8	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	
8	c	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	
4	b	222	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$		
4	a	222	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$		

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

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

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

Site Symmetry Group 222

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

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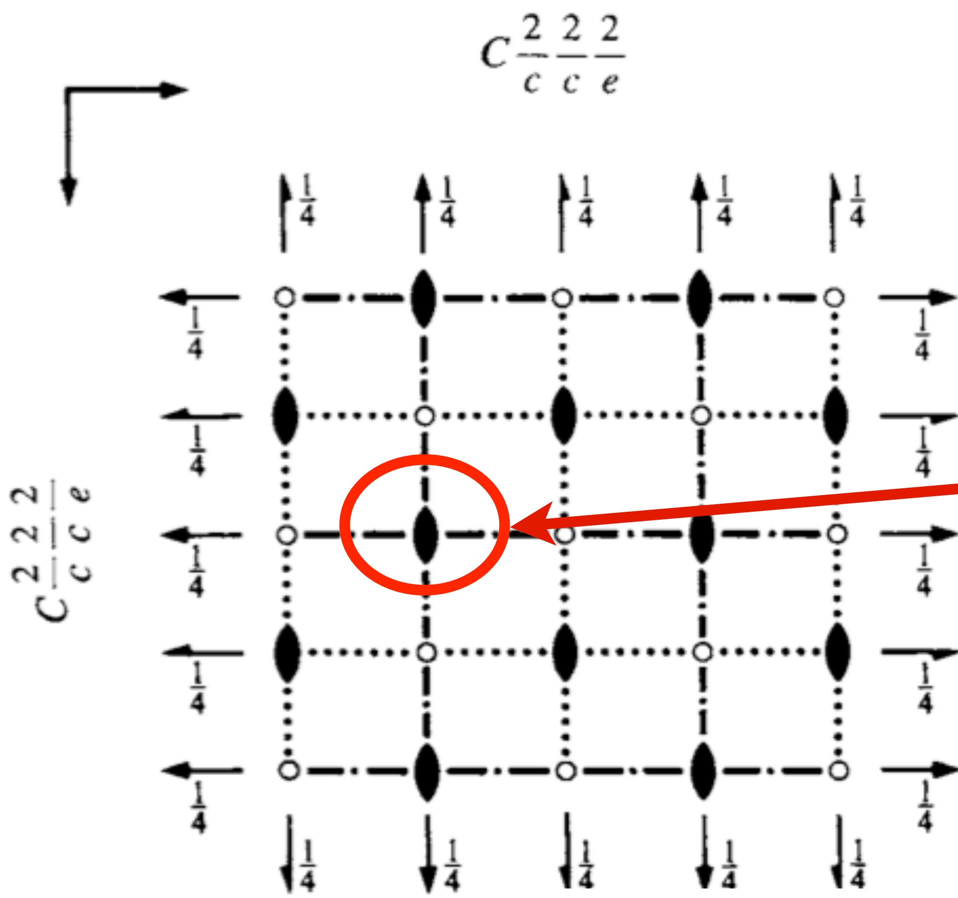
Example **WYCKPOS**: Wyckoff Positions Ccce (68)



Wyckoff position and site symmetry group of a specific point

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

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

Show

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

Site Symmetry Group 222

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

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Problem: Geometric Interpretation of (W,w) SYMMETRY OPERATION

Geometric Interpretation of Matrix Column Representation of Symmetry Operation

Symmetry Operation

This program calculates the geometric interpretation of matrix column representation of symmetry operation for a given crystal system or space group.

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

If you want to work on a non conventional setting click on **Non conventional setting**, this will show you a form where you have to introduce the transformation matrix relating the conventional setting of the group you have chosen with the non conventional one you are interested in.

Output:

We obtain the geometric interpretation of the symmetry operation.

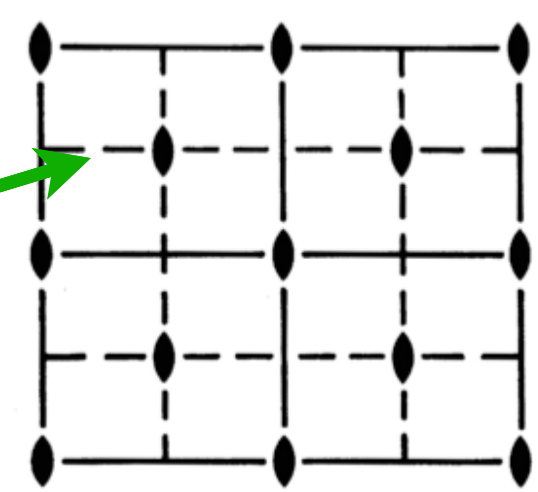
Introduce the crystal system	
Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A	choose it 35
Matrix column representation of symmetry operation	-x+1/2,y+1/2,z

In matrix form	Rotational part			Translation
	1	0	0	0
	0	1	0	0
	0	0	1	0

Standard/Default Setting Non Conventional Setting ITA Settings

Symmetry operation of the space group 35 (*Cmm2*)

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



EXERCISES

Problem 1.1

1. Characterize geometrically the matrix-column pairs listed under *General position* of the space group *P4mm* in ITA.

2. Consider the diagram of the symmetry elements of *P4mm*. Try to determine the matrix-column pairs of the symmetry operations whose symmetry elements are indicated on the unit-cell diagram.

3. Compare your results with the results of the program SYMMETRY OPERATIONS

EXERCISES

Problem 1.2

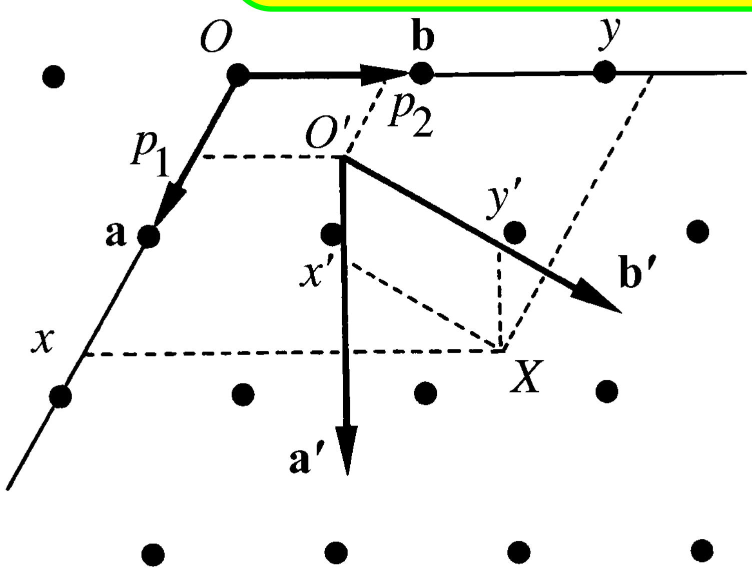
Consider the special Wyckoff positions of the the space group *P4mm*.

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

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

Compare your results with the results of the program WYCKPOS.

Co-ordinate transformations in crystallography



3-dimensional space

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

$$\Big\downarrow (P,p)$$

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

Transformation matrix-column pair (*P*,*p*)

(i) linear part: change of orientation or length:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$$

$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}).$$

(ii) origin shift by a shift vector *p*(p_1,p_2,p_3):

$$O' = O + p$$

the origin *O’* has coordinates (p_1,p_2,p_3) in the old coordinate system

Co-ordinate transformations in crystallography

Transformation of space-group operations (W,w) by $(\boldsymbol{P},\boldsymbol{p})$:

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

Structure-description transformation by $(\boldsymbol{P},\boldsymbol{p})$

unit cell parameters:

metric tensor $\boldsymbol{G}$: $\boxed{\boldsymbol{G}'=\boldsymbol{P}^t\,\boldsymbol{G}\,\boldsymbol{P}}$

atomic coordinates X(x,y,z):

$$\boxed{(X')=(P,p)^{-1}(X)}$$

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

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left(\begin{array}{ccc|c} P11 & P12 & P13 & p1 \\ P21 & P22 & P23 & p2 \\ P31 & P32 & P33 & p3 \end{array}\right)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Problem: **ITA SETTINGS**

530 ITA settings of **orthorhombic** and **monoclinic** groups

Monoclinic descriptions

	Transf.	**abc**	**c$\bar{\mathbf{b}}$a**	**abc**	**ba$\bar{\mathbf{c}}$**	**abc**	**$\bar{\mathbf{a}}$cb**	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

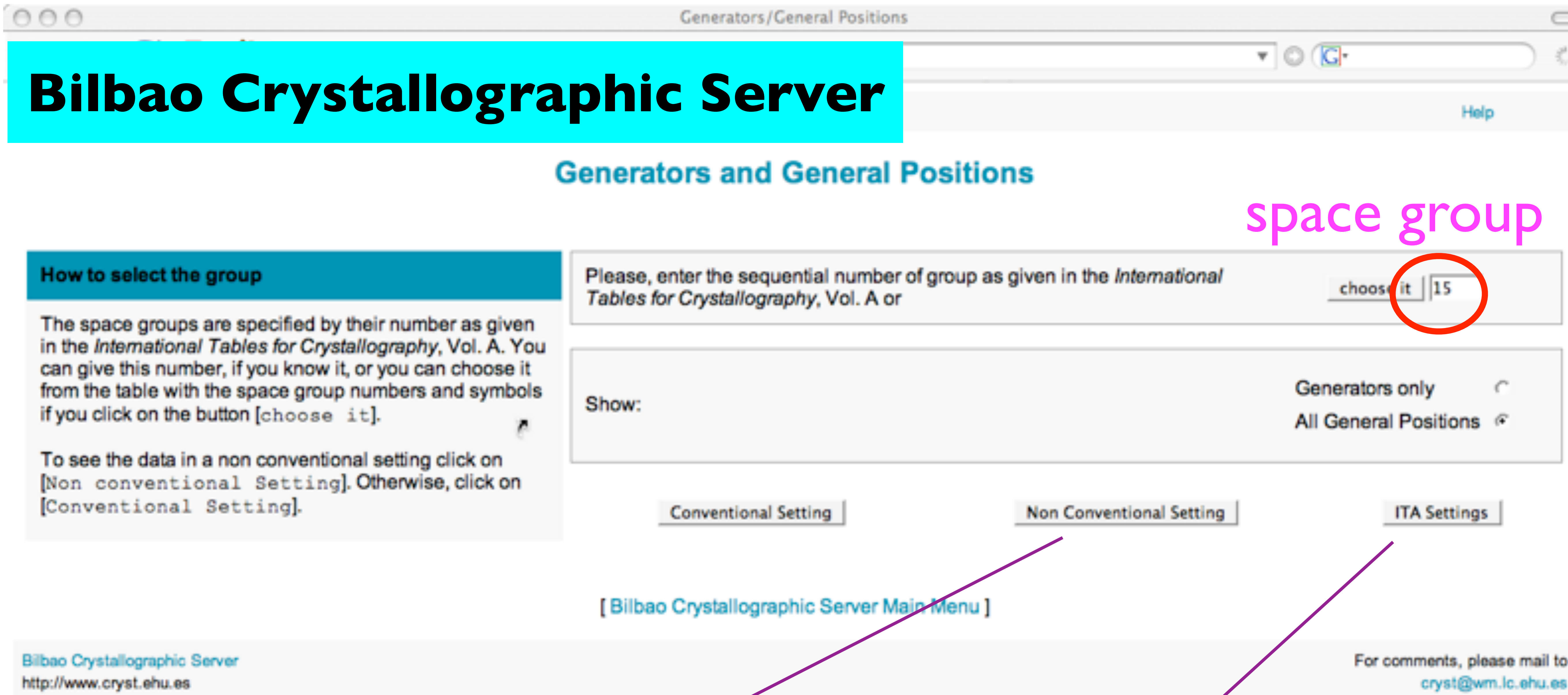
Orthorhombic descriptions

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

Problem: Co-ordinate transformations in crystallography

Generators
General positions **GENPOS**

Bilbao Crystallographic Server



space group

Transformation of the basis

ITA-settings symmetry data

ITA-Settings for the Space Group 15

Note: The transformation matrices must be read by columns. **P** is the transformation from standard to the ITA-setting.

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

Example **GENPOS**:

default setting C12/c1

$(W,w)_{A112/a}=$
$(P,p)^{-1}(W,w)_{C12/c1}(P,p)$

final setting A112/a

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,-b,-a-c	a,-b,a-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

Example **GENPOS**: ITA settings of C2/c(15)

The general positions of the group 15 (*A* 1 1 2/*a*)

N	Standard/Default Setting *C2/c*			ITA-Setting *A* 1 1 2/*a*		
	(x,y,z) form	matrix form	symmetry operation	(x,y,z) form	matrix form	symmetry operation
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
2	-x, y, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4	-x+1/2, -y, z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/4,0,z
3	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0
4	x, -y, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,0,z	x+1/2, y, -z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	a x,y,0
5	x+1/2, y+1/2, z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	t (1/2,1/2,0)	x, y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (0,1/2,1/2)
6	-x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 1/4,y,1/4	-x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,1/4,z
7	-x+1/2, -y+1/2, -z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 1/4,1/4,0	-x, -y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 0,1/4,1/4
8	x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (1/2,0,1/2) x,1/4,z	x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	n (1/2,1/2,0) x,y,1/4

default setting **A112/*a* setting**

Bilbao Crystallographic Server

Problem: Coordinate transformations Wyckoff positions **WYCKPOS**

Wyckoff Positions

space group

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

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

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

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

Standard/Default Setting | Non Conventional Setting | ITA Settings

Transformation of the basis

ITA settings

ITA-Settings for the Space Group 68

:es must be read by columns. **P** is the transformation f

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

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

Bilbao Crystallographic Server

Problem: Space-group identification by a set of generators in arbitrary basis

IDENTIFY GROUP

IDENTIFY GROUP: Identifies a Space Group given a set of generators

IDENTIFY GROUP identifies a Space Group given a set of generators and shows the transformation matrix to a standard or reference (default) description of the Space Group.

Enter the generators of the Space Group in the box below, given in any basis

x+1/2,y+1/2,z

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

Assumed lattice translations:

x + 1 , y , z

x , y + 1 , z

x , y , z + 1

```
x,y,z
```

EXERCISES

Problem 1.3

Consider the space group $P2_1/c$ (No. 14). Show that the relation between the *General* and *Special* position data of $P112_1/a$ (setting *unique axis c*) can be obtained from the data $P12_1/c1$ (setting *unique axis b*) applying the transformation $(\mathbf{a'},\mathbf{b'},\mathbf{c'})_{\mathbf{c}} = (\mathbf{a},\mathbf{b},\mathbf{c})_{\mathbf{b}}\boldsymbol{P}$, with $\boldsymbol{P}= \boldsymbol{c},\boldsymbol{a},\boldsymbol{b}$.

Use the retrieval tools GENPOS (generators and general positions) and WYCKPOS (Wyckoff positions) for accessing the space-group 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 *ITA*.

EXERCISES

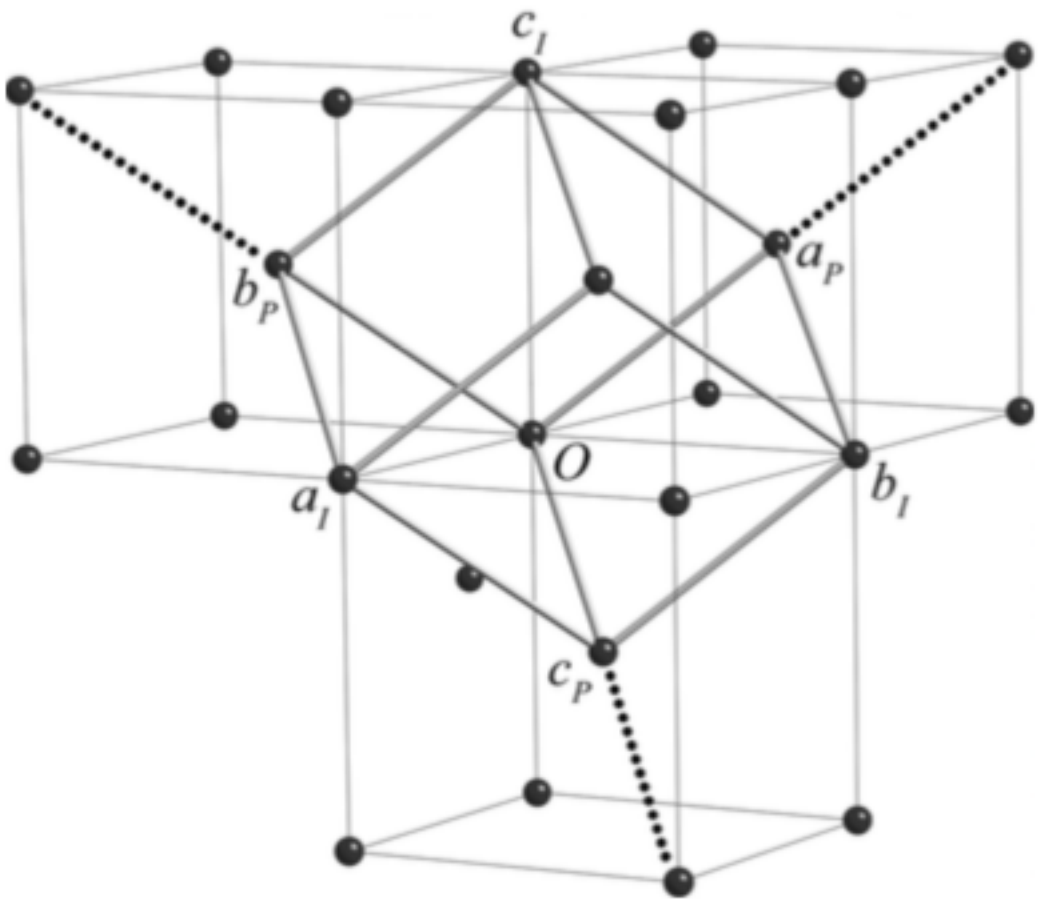
Problem 1.4

Use the retrieval tools GENPOS or *Generators* and *General positions*, WYCKPOS (or *Wyckoff positions*) for accessing the space-group data on the *Bilbao Crystallographic Server* or *Symmetry Database* server. 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 ITA.

Consider the General position data of the space group *Im-3m* (No. 229). Using the option *Non-conventional setting* obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation (**a**',**b**',**c**') = 1/2(-**a**+**b**+**c**,**a**-**b**+**c**,**a**+**b**-**c**)

EXERCISES

Problem 1.5



A body-centred cubic lattice (*cI*) has as its conventional basis the conventional basis (**$\mathbf{a_P}$**,**$\mathbf{b_P}$**,**$\mathbf{c_P}$**) of a primitive cubic lattice, but the lattice also contains the centring vector $1/2\mathbf{a_P}+1/2\mathbf{b_P}+1/2\mathbf{c_P}$ which points to the centre of the conventional cell.

Calculate the coefficients of the metric tensor for the body-centred cubic lattice:

(i) for the conventional basis ($\mathbf{a_P}$,$\mathbf{b_P}$,$\mathbf{c_P}$);

(ii) for the primitive basis:

$\mathbf{a_I}=1/2(-\mathbf{a_P}+\mathbf{b_P}+\mathbf{c_P})$, $\mathbf{b_I}=1/2(\mathbf{a_P}-\mathbf{b_P}+\mathbf{c_P})$, $\mathbf{c_I}=1/2(\mathbf{a_P}+\mathbf{b_P}-\mathbf{c_P})$

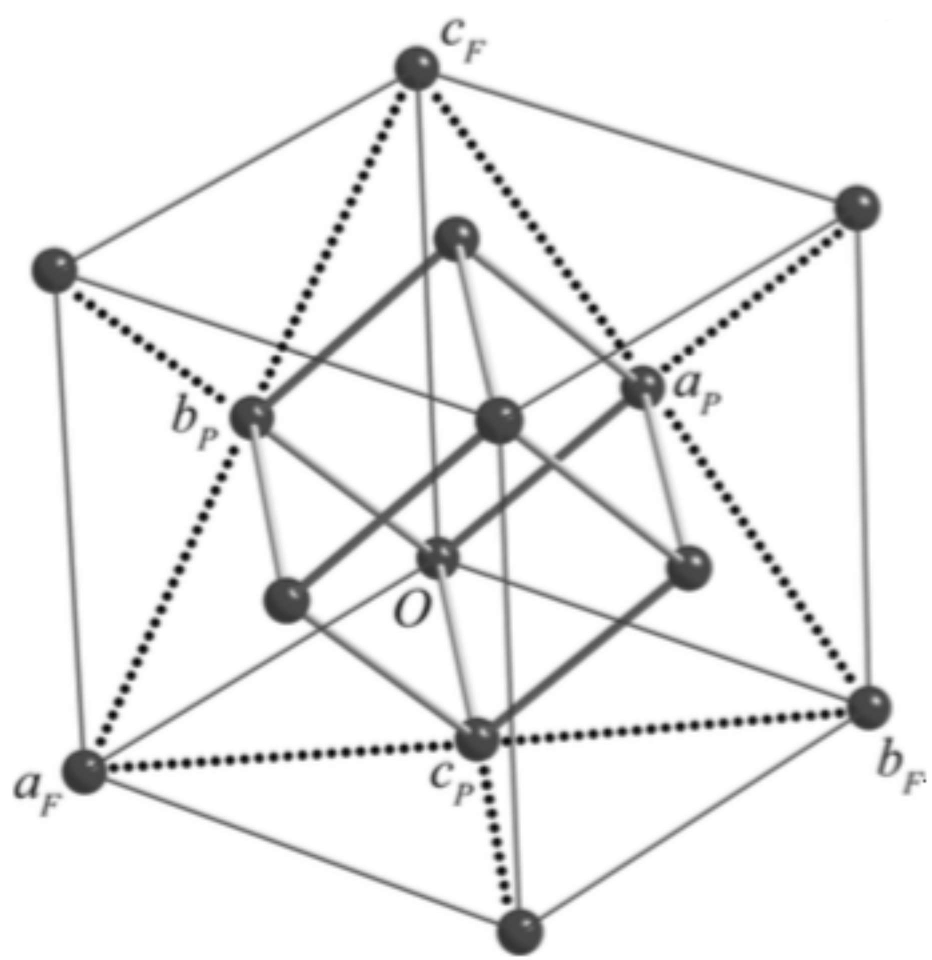
(iii) determine the lattice parameters of the primitive cell if a_P=4 Å

Hint

metric tensor transformation $\boldsymbol{G'=P^t\,G\,P}$

EXERCISES

Problem 1.6



A face-centred cubic lattice (*cF*) has as its conventional basis the conventional basis ($\mathbf{a_P}$,$\mathbf{b_P}$,$\mathbf{c_P}$) of a primitive cubic lattice, but the lattice also contains the centring vectors $1/2\mathbf{b_P}+1/2\mathbf{c_P}$, $1/2\mathbf{a_P}+1/2\mathbf{c_P}$, $1/2\mathbf{a_P}+1/2\mathbf{b_P}$, which point to the centres of the faces of the conventional cell.

Calculate the coefficients of the metric tensor for the face-centred cubic lattice:

(i) for the conventional basis ($\mathbf{a_P}$,$\mathbf{b_P}$,$\mathbf{c_P}$);

(ii) for the primitive basis:

$\mathbf{a_F}=1/2(\mathbf{b_P}+\mathbf{c_P})$, $\mathbf{b_F}=1/2(\mathbf{a_P}+\mathbf{c_P})$, $\mathbf{c_F}=1/2(\mathbf{a_P}+\mathbf{b_P})$

(iii) determine the lattice parameters of the primitive cell if a_P=4 Å

GROUP-SUBGROUP RELATIONS OF SPACE GROUPS

bilbao crystallographic server

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Space-group symmetry

Magnetic Symmetry and Applications

ECM31-Oviedo S

Crystallography online: w
use and applications of the
of the Bilbao Crystallogr

20-21 August 2

News:

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

Group-Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS ⚠	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

International Tables for Crystallography, Vol. A1

eds. H. Wondratschek, U. Mueller

Maximal subgroups of space groups

$P4mm$ No. 99 $P4mm$

I Maximal *translationengleiche* subgroups

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

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

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

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

- **Series of maximal isomorphic subgroups**

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

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

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

$P4mm$ (99)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p > 2;\ 0 \leq u < p;\ 0 \leq v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

Bilbao Crystallographic Server

Problem: SUBGROUPS OF SPACE GROUPS

SUBGROUPGRAPH

Bilbao Crystallographic Server → SUBGROUPGRAPH | Help

Group-Subgroup Lattice and Chains of Maximal Subgroups

Lattice and chains ...

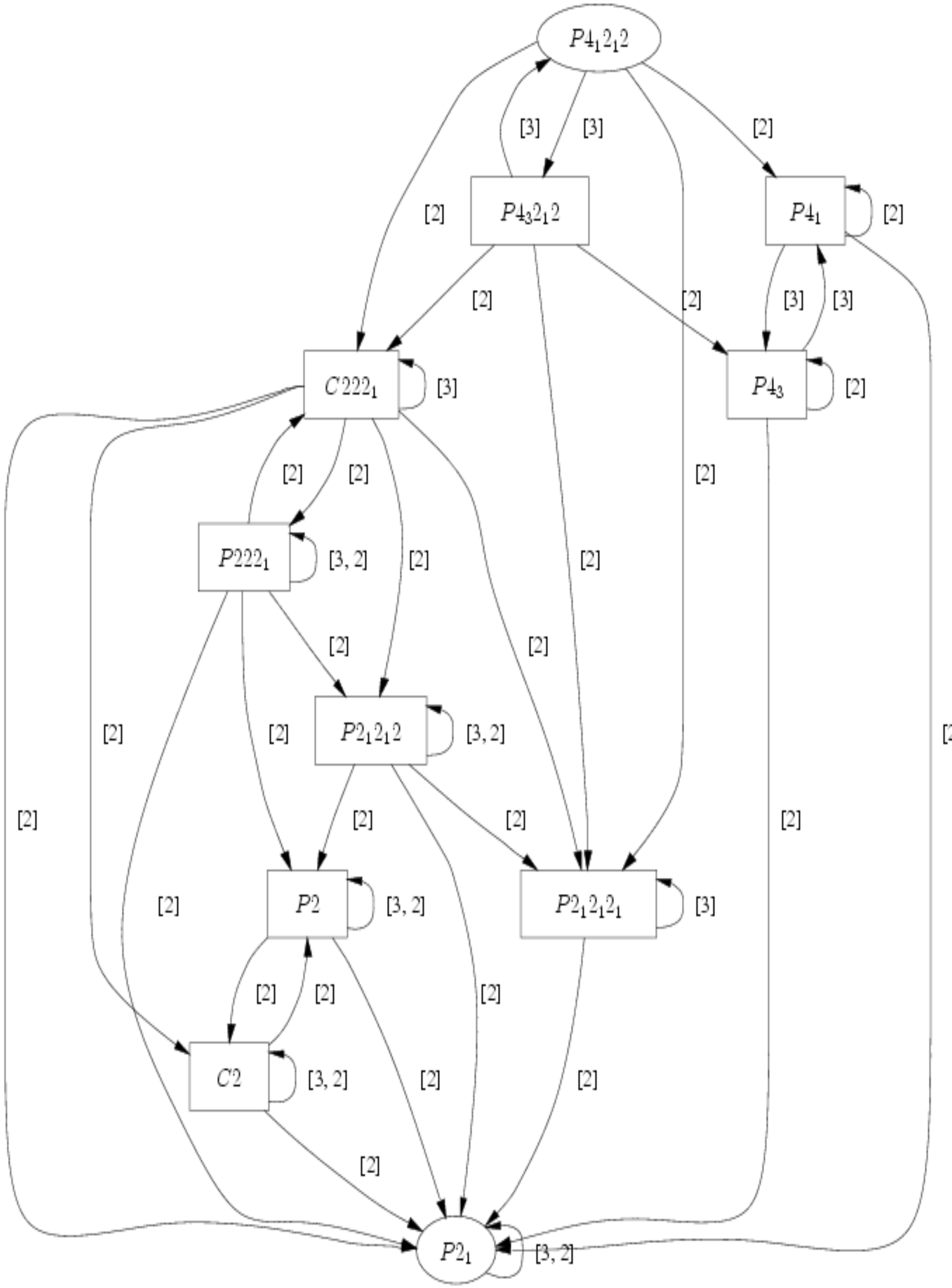
For a given group and supergroup the program SUBGROUPGRAPH will give the lattice of maximal subgroups that relates these two groups and, in the case that the index is specified, all of the possible chains of maximal subgroup that relate the two groups. In the latter case, also there is a possibility to obtain all of the different subgroups of the same type.

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup number (G) or choose it:	99
Enter subgroup number (H) or choose it:	4
Enter the index [G:H] (optional):	

Construct the lattice

subgroup index

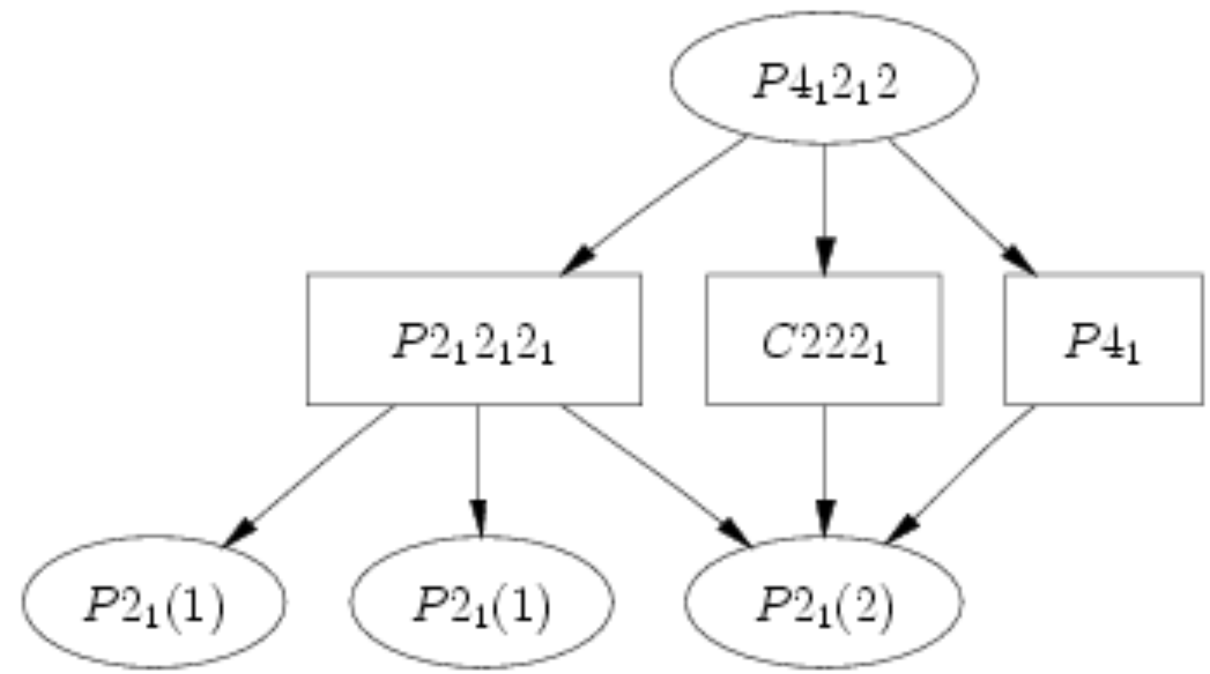
$[i]=[i_P]\cdot[i_L]$



SUBGROUPGRAPH

$P4_12_12 > P2_1$

maximal subgroup graph



three $P2_1$ subgroups in two conjugacy classes

General graph for $P4_12_12 > P2_1$

Graph for $P4_12_12 > P2_1$ index [i]=4

PROBLEM: Domain-structure analysis

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

Hermann, 1929:

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

number of domain states

twins and antiphase domains

twinning operation

symmetry groups of the domain states; multiplicity and degeneracy

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

twins $i_P=P_G/P_H$

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

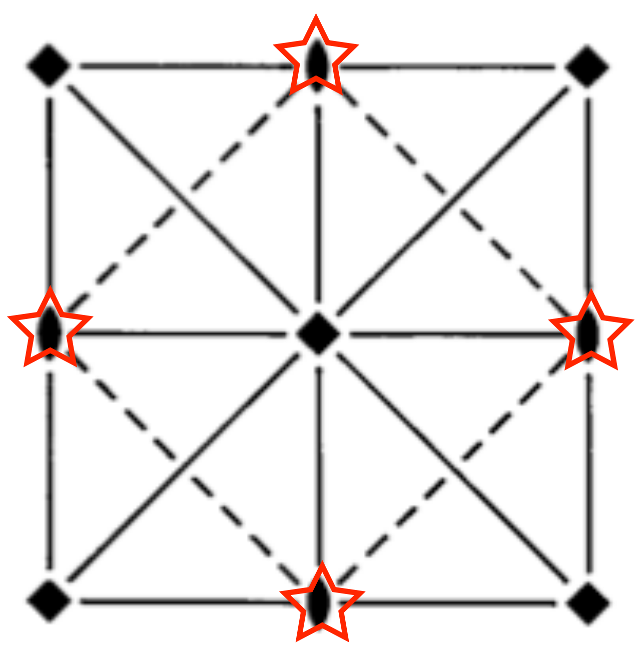
Bilbao Crystallographic Server

Problem: SPLITTING OF WYCKOFF POSITIONS **WYCKSPLIT**

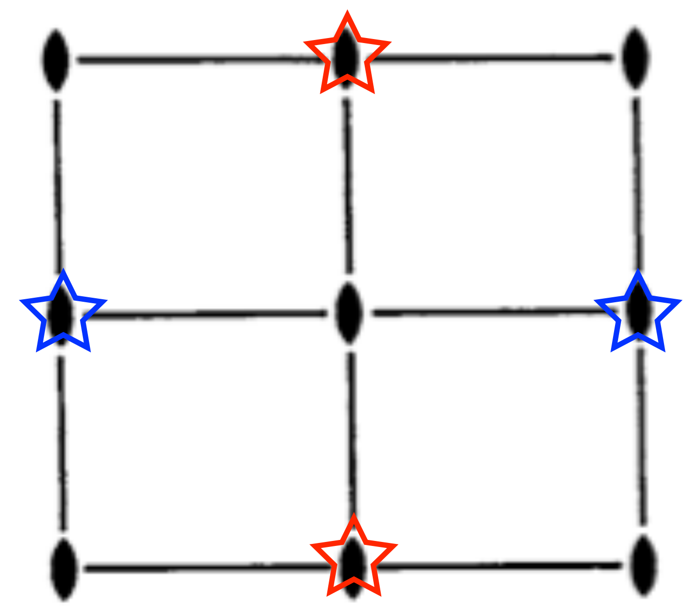
Group-subgroup pair *P4mm*>*Pmm2*, [i]=2

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

P4mm



Pmm2



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

→ 1/2 0 z 1c mm2

→ 0 1/2 z' 1b mm2

Data on Relations between Wyckoff Positions in *International Tables for Crystallography*, Vol. A1

No. 99 $P4mm$

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$2c$	$4d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups									
[2] $P4$ (75)			$1a$	$1b$	$2c$	$4d$	$4d$	$4d$	$2\times4d$
[2] $Pmm2$ (25)			$1a$	$1d$	$1b;1c$	$4i$	$2e;2g$	$2f;2h$	$2\times4i$
[2] $Cmm2$ (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a$	$2b$	$4c$	$4d;4e$	$8f$	$8f$	$2\times8f$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $I4cm$ (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4a$	$4b$	$8c$	$16d$	$16d$	$2\times8c$	$2\times16d$
[2] $I4cm$ (108)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$4a$	$8c$	$16d$	$2\times8c$	$16d$	$2\times16d$
[2] $I4mm$ (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times2a$	$4b$	$8c$	$2\times8d$	$2\times8c$	$16e$	$2\times16e$
[2] $I4mm$ (107)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$2\times2a$	$8c$	$2\times8d$	$16e$	$2\times8c$	$2\times16e$
[2] $P4_2mc$ (105)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$2\times2c$	$8f$	$2\times4d$	$2\times4e$	$2\times8f$
[2] $P4cc$ (103)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$8d$	$8d$	$8d$	$2\times8d$
[2] $P4_2cm$ (101)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$2\times4d$	$8e$	$8e$	$2\times8e$
[2] $P4bm$ (100)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2a$	$2b$	$4c$	$8d$	$8d$	$2\times4c$	$2\times8d$

Example

Bilbao Crystallographic Server

WYCKSPLIT

Wyckoff Positions Splitting

Conventional Settings

Non conventional Settings

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup or choose it	136 group
Enter subgroup or choose it	subgroup 65
Please, define the transformation relating the group and the subgroup bases. (NOTE: If you don't know the transformation click here for possible workarounds)	
rotational matrix: Transformation matrix (P,p)	1 1 0 -1 1 0 0 0 1
origin shift:	0 0 0

Show group-subgroup data.

Two-level input:

Choice of the Wyckoff positions

Wyckoff Positions Splitting

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

Group Data	Subgroup Data
	16r (x, y, z)
	8q (x, y, 1/2)
	8p (x, y, 0)
All positions	8o (x, 0, z)
16k (x, y, z)	8n (0, y, z)
8j (x, x, z)	8m (1/4 , 1/4 , z)
8i (x, y, 0)	4l (0, 1/2 , z)
8h (0, 1/2 , z)	4k (0, 0, z)
4g (x, - x, 0)	4j (0, y, 1/2)
4f (x, x, 0)	4i (0, y, 0)
4e (0, 0, z)	4h (x, 0, 1/2)
4d (0, 1/2 , 1/4)	4g (x, 0, 0)

Wyckoff Positions Splitting

Bilbao Crystallographic Server

WYCKSPLIT

99 (*P4mm*) > 8 (*Cm*) [unique axis b]

Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	8g	4b 4b 4b 4b	Relations
2	4f	4b 4b	Relations
3	4e	4b 4b	Relations
4	4d	4b 2a 2a	Relations
5	2c	4b	Relations
6	1b	2a	Relations
7	1a	2a	Relations

Two-level output:

Relations between coordinate triplets

Splitting of Wyckoff position 4d

Representative			Subgroup Wyckoff position	
No	group basis	subgroup basis	name[n]	representative
1	(x, x, z)	(0, x, z)	$4b_1$	(x_1, y_1, z_1)
2	(-x, -x, z)	(0, -x, z)		(x_1, -y_1, z_1)
3	(x+1, x, z)	(1/2, x+1/2, z)		(x_1+1/2, y_1+1/2, z_1)
4	(-x+1, -x, z)	(1/2, -x+1/2, z)		(x_1+1/2, -y_1+1/2, z_1)
5	(-x, x, z)	(-x, 0, z)	$2a_1$	(x_2, 0, z_2)
6	(-x+1, x, z)	(-x+1/2, 1/2, z)		(x_2+1/2, 1/2, z_2)
7	(x, -x, z)	(x, 0, z)	$2a_2$	(x_3, 0, z_3)
8	(x+1, -x, z)	(x+1/2, 1/2, z)		(x_3+1/2, 1/2, z_3)

MAGNETIC SYMMETRY AND APPLICATIONS

FCT/ZTF

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News:

- New Article in Nature
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305.
- New program: BANDREP
  04/2017: Band representations and Elementary Band representations of Double Space Groups.
- New section: Double point ar… space groups
  - New program: DGENPO…
    04/2017: General positions of D… Space Groups
  - New program: REPRESENTATIONS DP…
    04/2017: Irreducible representa… the Double Point Groups
  - New program: REPRESENTATIONS DS…
    04/2017: Irreducible representa… the Double Space Groups
  - New program: DSITESY…
    04/2017: Site-symmetry induce… representations of Double Spac… Groups
  - New program: DCOMPR…
    04/2017: Compatibility relations between the irreducible represe… of Double Space Groups

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Space-group symmetry

Magnetic Symmetry and Applications

Magnetic Symmetry and Applications

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MNORMALIZER	Normalizers of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MPOINT ⚠	Magnetic Point Group Tables
MAGNEXT	Systematic Absences of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files
MVISUALIZE ⚠	3D Visualization of magnetic structures with Jmol
MTENSOR ⚠	Symmetry-adapted form of crystal tensors in magnetic phases

Point-group symmetry

Tutorials
Material used in workshops and schools
Archive

H. Stokes, B.J. Campbell ***Magnetic Space-group Data***
http://stokes.byu.edu/magneticspacegroups.html

D.B. Litvin ***Magnetic Space Groups v. V3.02***
http://www.bk.psu.edu/faculty/litvin/Download.html

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

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Space-group symmetry

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20-21 August 20

News:

- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topolo chemistry" *Nature* (2017). 547
- **New program: BANDRE**
  04/2017: Band representations Band representations of Doubl
- **New section: Double po groups**
  - **New program: DGI**
    04/2017: General positi Space Groups
  - **New program: REPRESENTATIONS DPG**

Representations and Applications

REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group
MECHANICAL REP. ⚠	Decomposition of the mechanical representation into irreps
MAGNETIC REP. ⚠	Decomposition of the magnetic representation into irreps
BANDREP ⚠	Band representations and Elementary Band representations of Double Space Groups

Databases of Representations

Representations of space and point groups

wave-vector data

Brillouin zones
representation domains
parameter ranges

POINT

character tables
multiplication tables
symmetrized products

Retrieval tools

Database on Representations of Point Groups

Bilbao Crystallographic Server

Point Group Tables of C_{6v}(6mm)

Character Table

C_{6v}(6mm)	#	1	2	3	6	m_d	m_v	functions
Mult.	-	1	1	2	2	3	3	.
A_1	Γ_1	1	1	1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	1	1	-1	-1	J_z
B_1	Γ_3	1	-1	1	-1	1	-1	.
B_2	Γ_4	1	-1	1	-1	-1	1	.
E_2	Γ_6	2	2	-1	-1	0	0	(x^2-y^2,xy)
E_1	Γ_5	2	-2	-1	1	0	0	$(x,y),(xz,yz),(J_x,J_y)$

[List of irreducible representations in matrix form]

character tables
matrix representations
basis functions

group-subgroup relations

The Rotation Group D(L)

L	2L+1	A_1	A_2	B_1	B_2	E_2	E_1
0	1	1	.	.	.	.	.
1	3	1	.	.	.	.	1
2	5	1	.	.	.	1	1
3	7	1	.	1	1	1	1
4	9	1	.	1	1	2	1
5	11	1	.	1	1	2	2
6	13	2	1	1	1	2	2
7	15	2	1	1	1	2	3
8	17	2	1	1	1	3	3
9	19	2	1	2	2	3	3
10	21	2	1	2	2	4	3

Point Subgroups

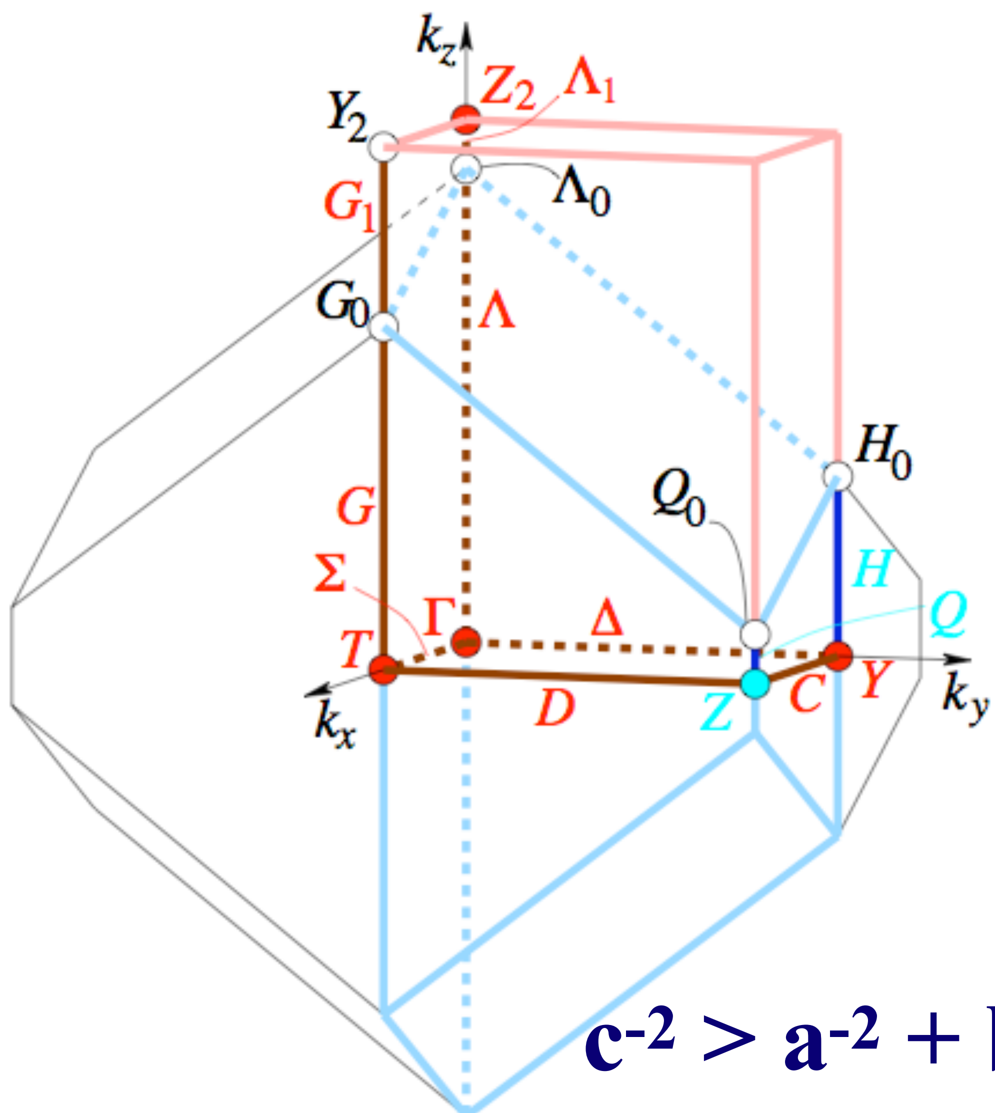
Subgroup	Order	Index
6mm	12	1
6	6	2
3m	6	2
3	3	4
mm2	4	3
2	2	6
m	2	6
1	1	12

Brillouin Zone Database
Crystallographic Approach

Reciprocal space groups
Brillouin zones
Representation domain
Wave-vector symmetry

↔

Symmorphic space groups
IT unit cells
Asymmetric unit
Wyckoff positions



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

The k-vector Types of Group 22 [*F222*]

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
$T \sim T_2$			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
$Y \sim Y_2$			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
$U \sim SM_1 = [SM_0\ T_2]$			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

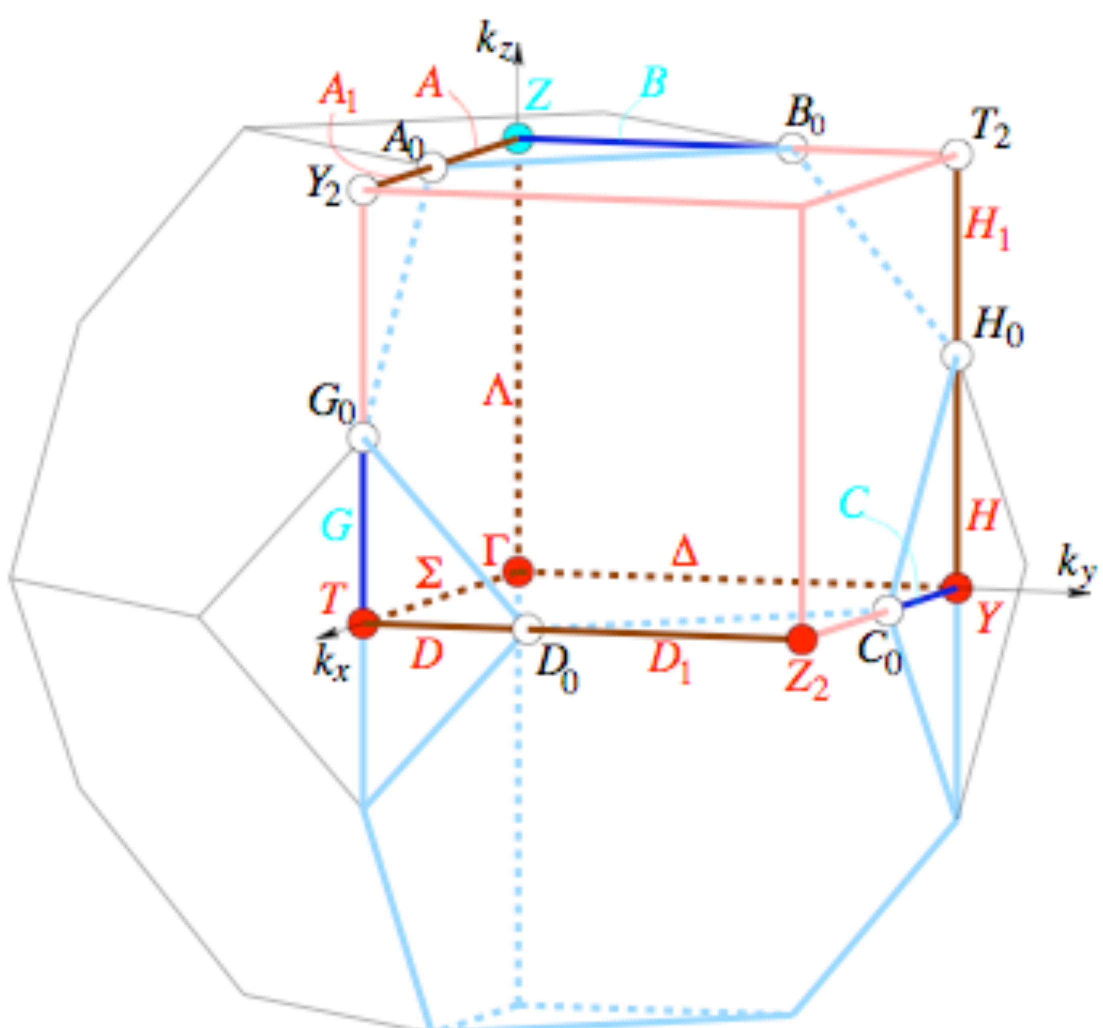
Brillouin zone Database

Bilbao Crystallographic Server

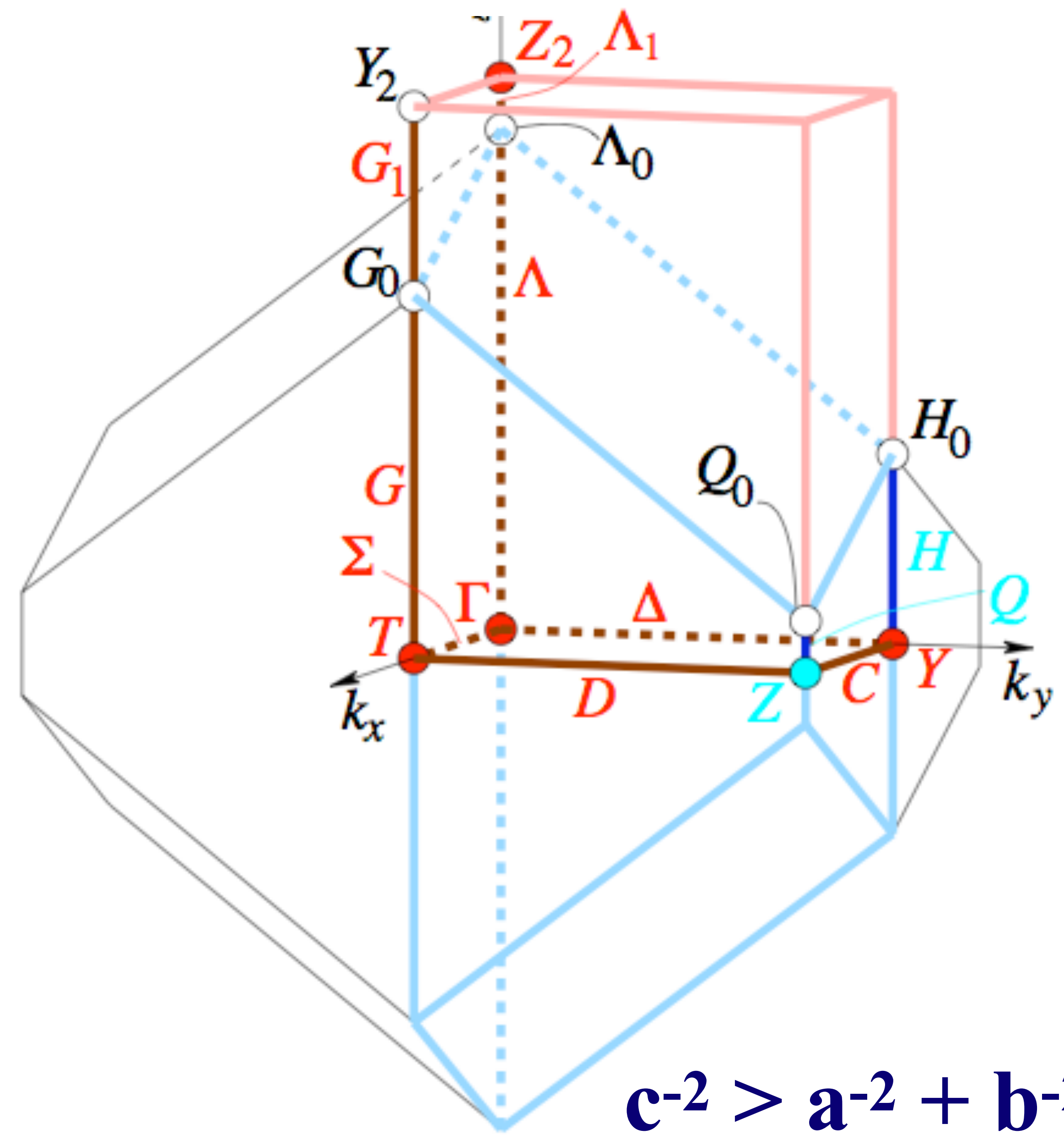
The k-vector Types of Group 22 [*F*222]

Brillouin zone

(Diagram for arithmetic crystal class 222F)

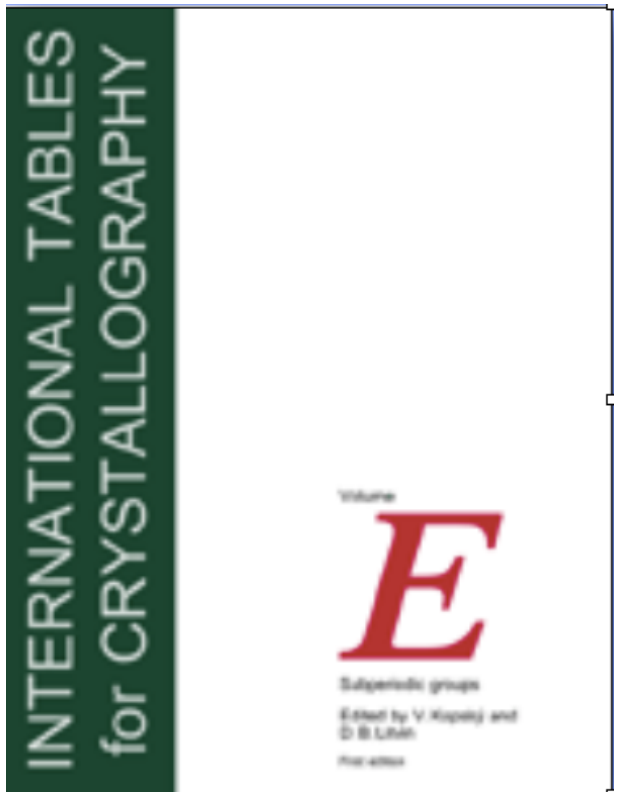


$c^{-2} < a^{-2} + b^{-2}$



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

SUBPERIODIC GROUPS: LAYER, ROD AND FRIEZE GROUPS



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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

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Subperiodic Groups: Layer, Rod and Frieze Groups

GENPOS	Generators and General Positions of Subperiodic Groups
WPOS	Wyckoff Positions of Subperiodic Groups
MAXSUB	Maximal Subgroups of Subperiodic Groups
KVEC ⚠	The k-vector types and Brillouin zones of Layers Groups
SECTIONS ⚠	Identification of Layer Symmetry of Periodic Sections

04/2017: General positions of Double Space Groups

- New program: REPRESENTATIONS DPG

Point-group symmetry