Mathematics and Computer Science for Materials Innovation: Crystal-lattice Classifications

Satellite of 33rd European Crystallographic Meeting

UNIVERSITY OF LIVERPOOL

5-9 September 2022

ONLINE CRYSTALLOGRAPHY BY THE BILBAO CRYSTALLOGRAPHIC SERVER

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20-21 August 2018

ews:

- 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
  - New program: DGENPOS
    04/2017: General positions of Double Space Groups
  - New program: REPRESENTATIONS DPG
    04/2017: Irreducible representations of

- 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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Working Environment

Crystallographic databases

Symmetry relations between crystallographic groups

Structure utilities

Representations of crystallographic groups

Solid-state applications

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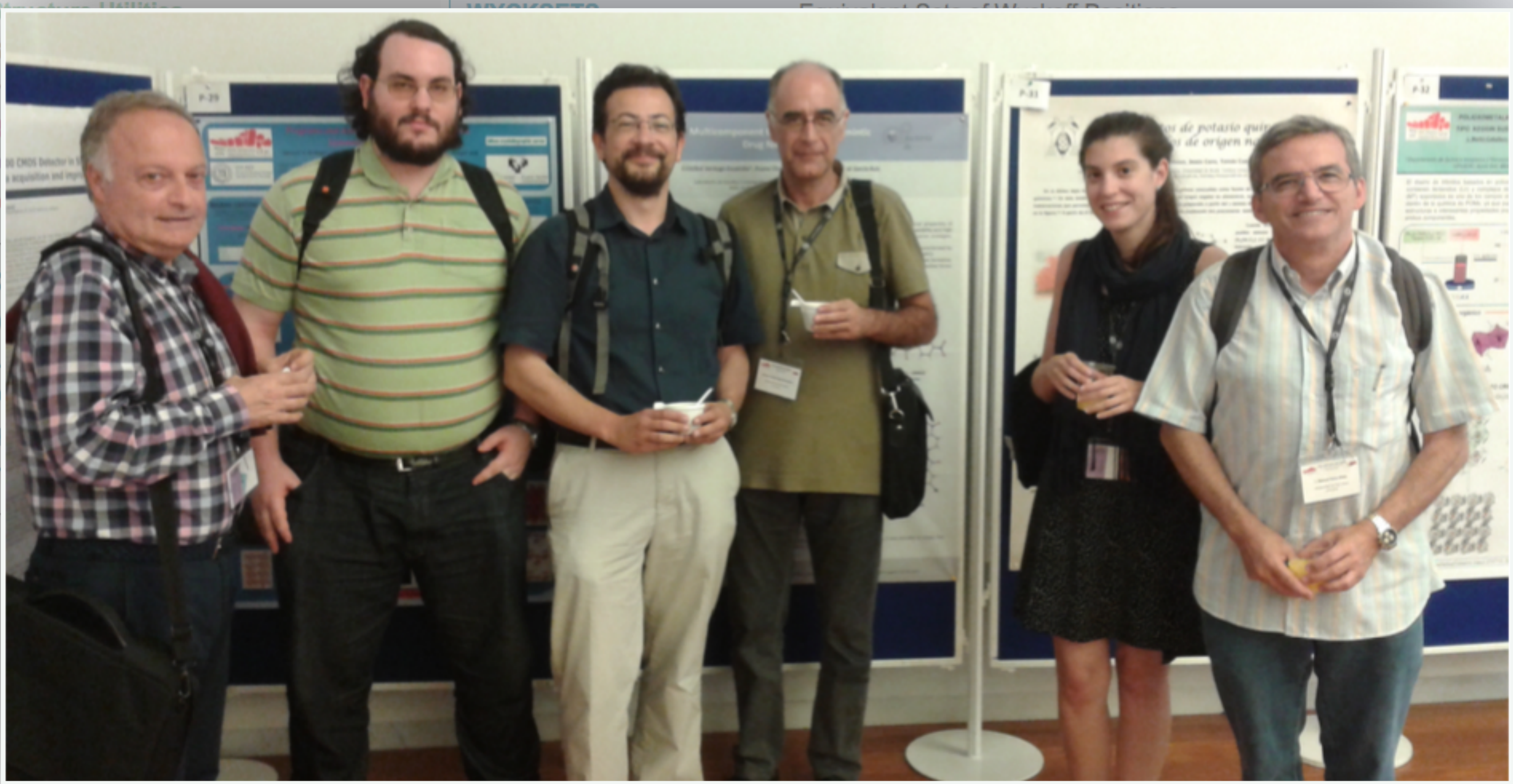
present team

Gemma de la Flor | Gotzon Madariaga
Emre Tasci | J. Manuel Perez-Mato
Luis Elcoro | Mois. I. Aroyo



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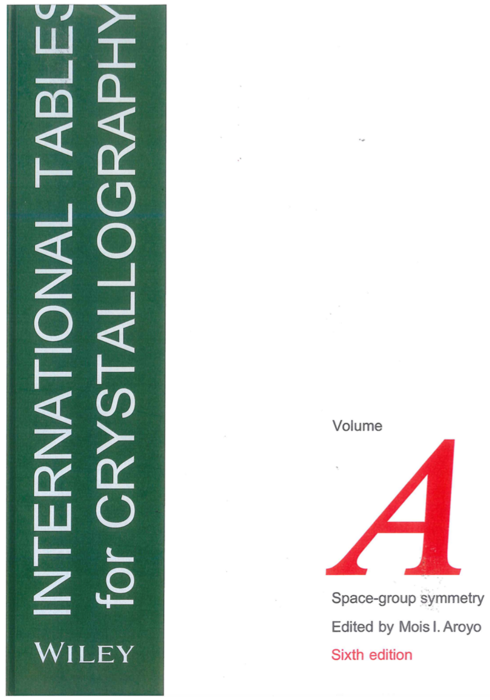

SPACE-GROUP SYMMETRY

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News:

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- **New program: BANDREP**
  04/2017: Band representations and Elementary

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

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Problem: Matrix-column presentation
Geometrical interpretation

GENPOS

Generators and General Positions

space group

How to select the group

The space groups are specified by their sequential 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**] or [**ITA Settings**] for checking the non

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

choose it 14

Show:

Generators only

All General Positions

Standard/Default Setting

Non Conventional Setting

ITA Settings

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

Space-group symmetry operations

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

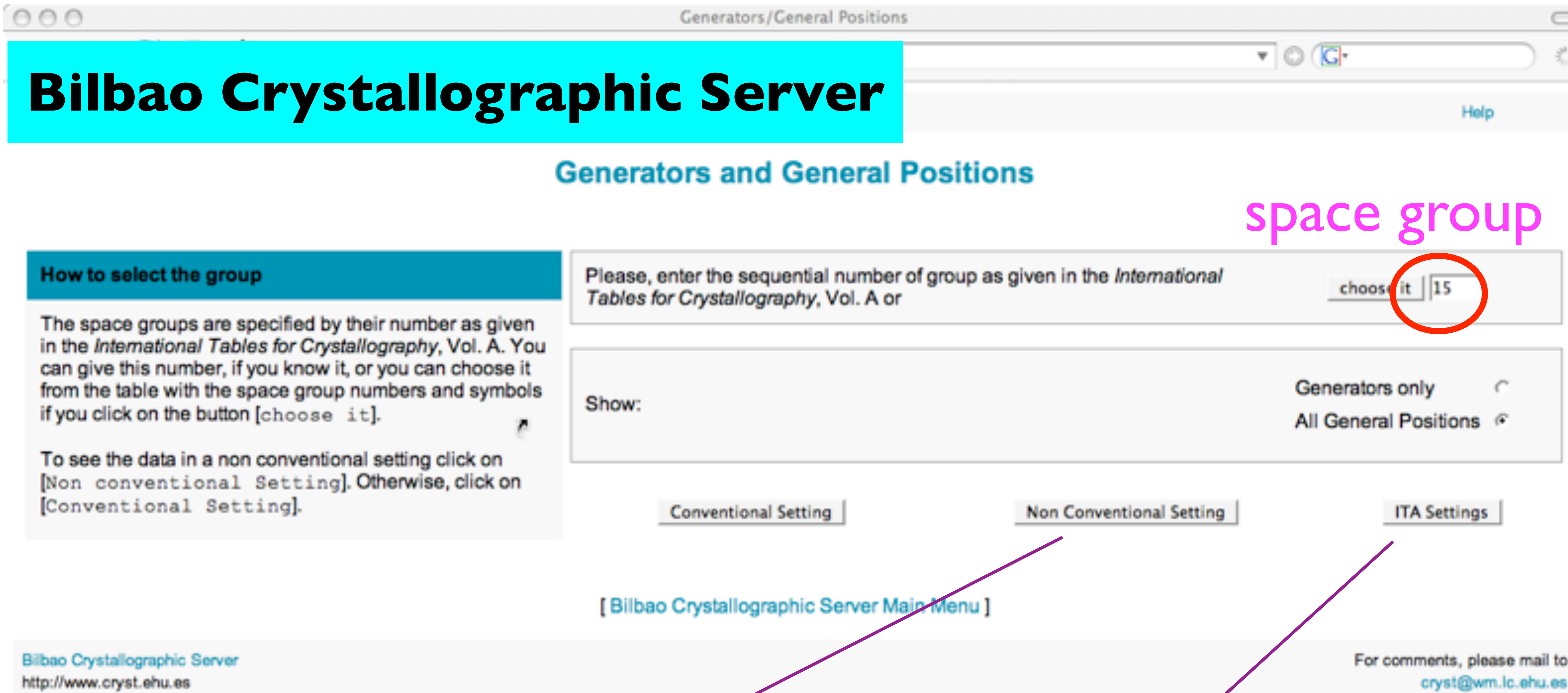
Symmetry operations

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

Problem: Co-ordinate transformations in crystallography

Generators
General positions

GENPOS



space group

Transformation of the basis

ITA-settings symmetry data

Example **GENPOS**:

default setting C12/c1

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

final setting A112/a

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.

$$(a, b, c)_n = (a, b, c)_s P$$

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

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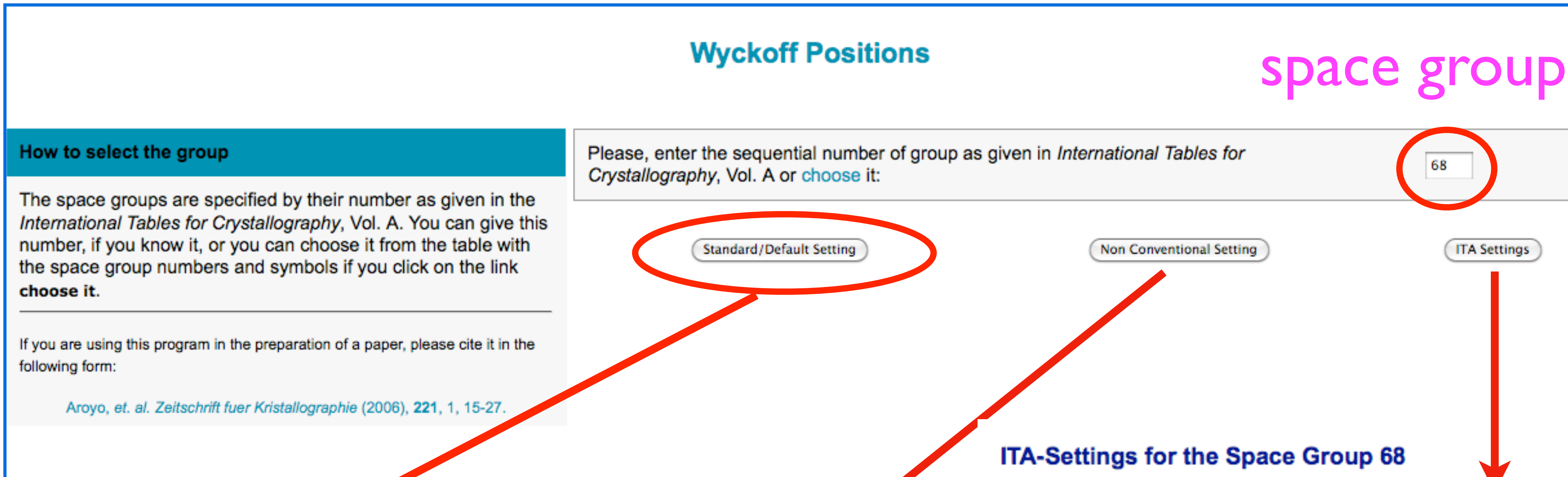
Problem: Wyckoff positions / Site-symmetry groups — WYCKPOS



Conventional/ standard basis

Transformation of the basis

ITA ettings

ITA-Settings for the Space Group 68

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

$(a, b, c)_n = (a, b, c)_s P$

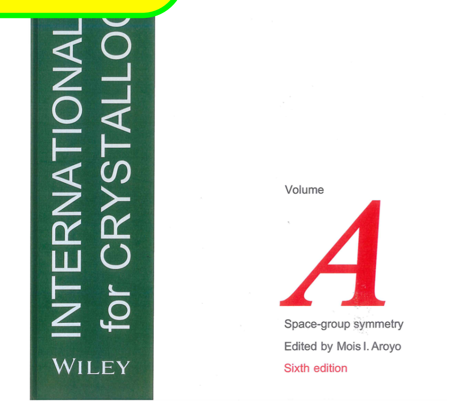
ITA number	Setting	P	P^{-1}
68	*C c c e* [origin 1]	**a,b,c**	**a,b,c**
68	*A e a a* [origin 1]	**c,a,b**	**b,c,a**
68	*B b e b* [origin 1]	**b,c,a**	**c,a,b**
68	*C c c e* [origin 2]	**a,b,c**	**a,b,c**
68	*A e a a* [origin 2]	**c,a,b**	**b,c,a**

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

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	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+$
8	*g*	..2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+$
8	*f*	.2.	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$
8	*e*	2..	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},$
8	*d*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$
8	*c*	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$
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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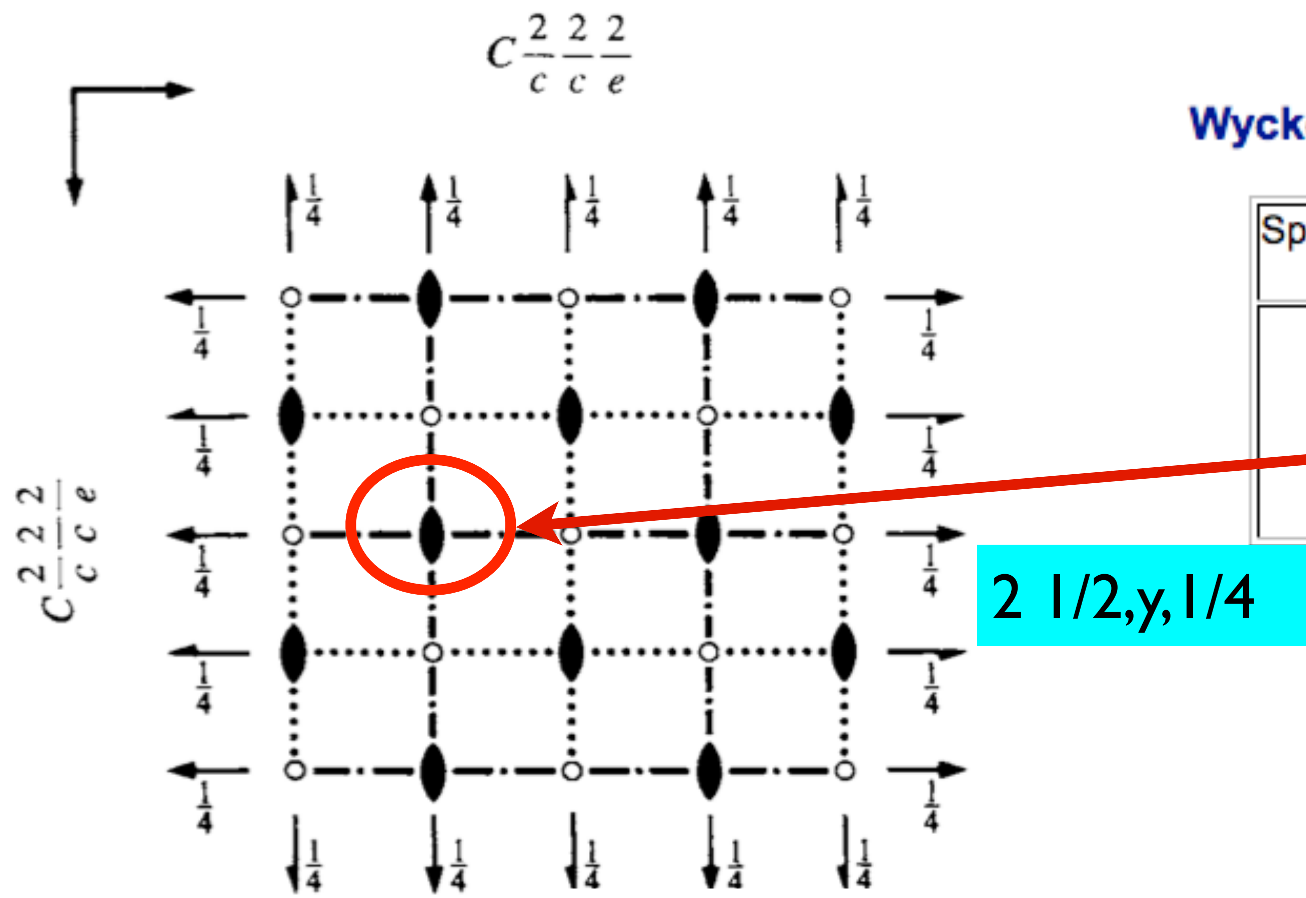
Example **WYCKPOS**: Wyckoff Positions Ccce (68)



2 x,1/4,1/4

Wyckoff position and site symmetry group of a specific point

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

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

Show

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

Site Symmetry Group 222

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

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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.

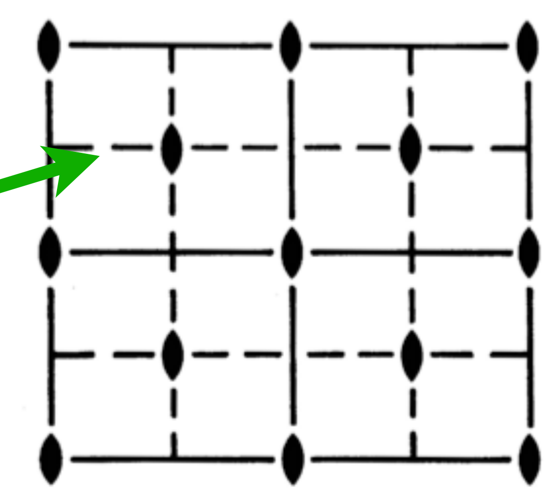
Introduce the crystal system	
Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A	choose it 35
Matrix column representation of symmetry operation	-x+1/2,y+1/2,z

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 (*Cmm*2)

-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



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
```

SYMMETRY RELATIONS BETWEEN SPACE GROUPS

Group-Subgroup Relations of Space Groups	
SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS	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)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

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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.

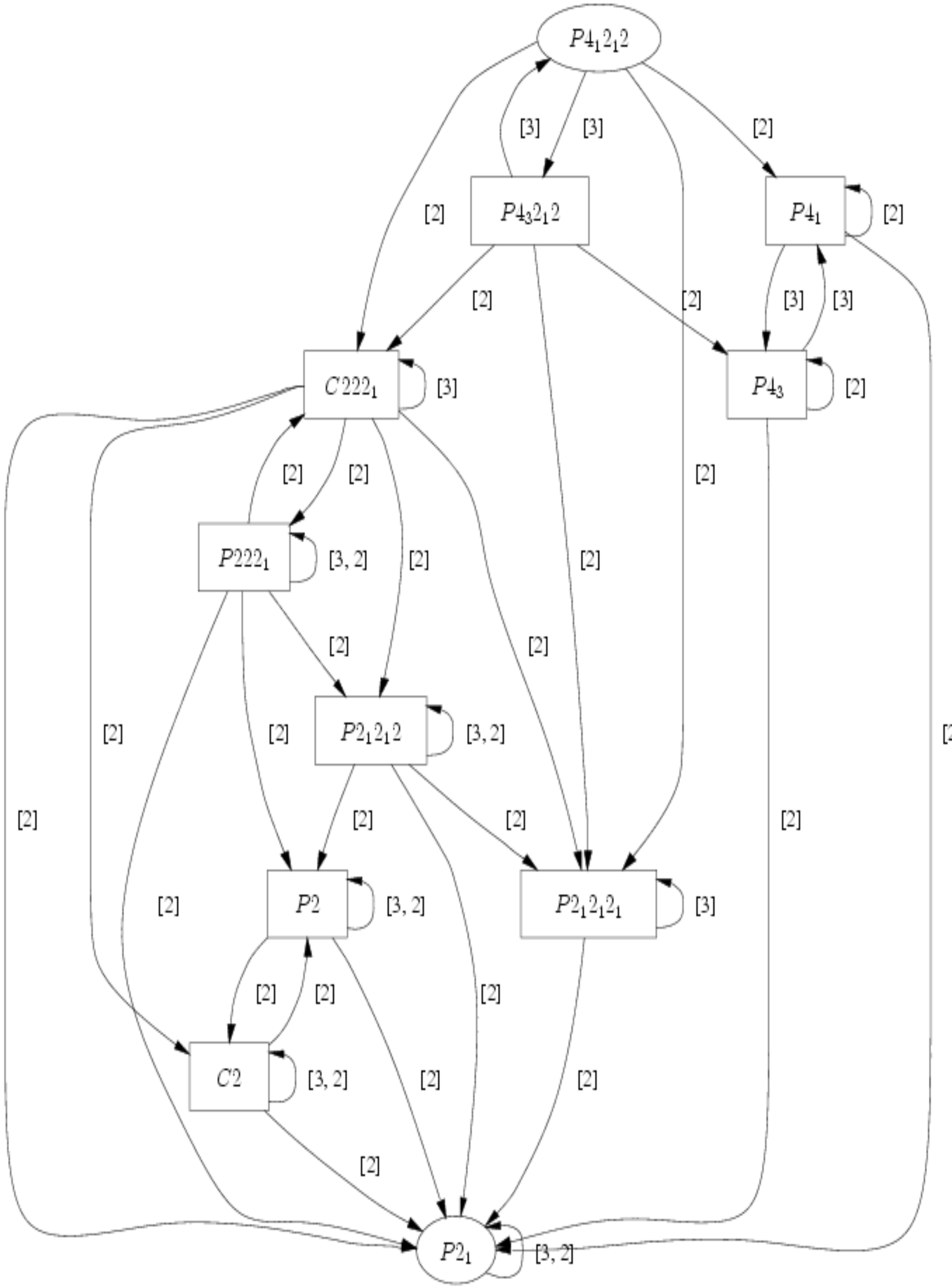
Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:	
Enter supergroup number (G) or choose it:	99
Enter subgroup number (H) or choose it:	4
Enter the index [G:H] (optional):	

Construct the lattice

subgroup index

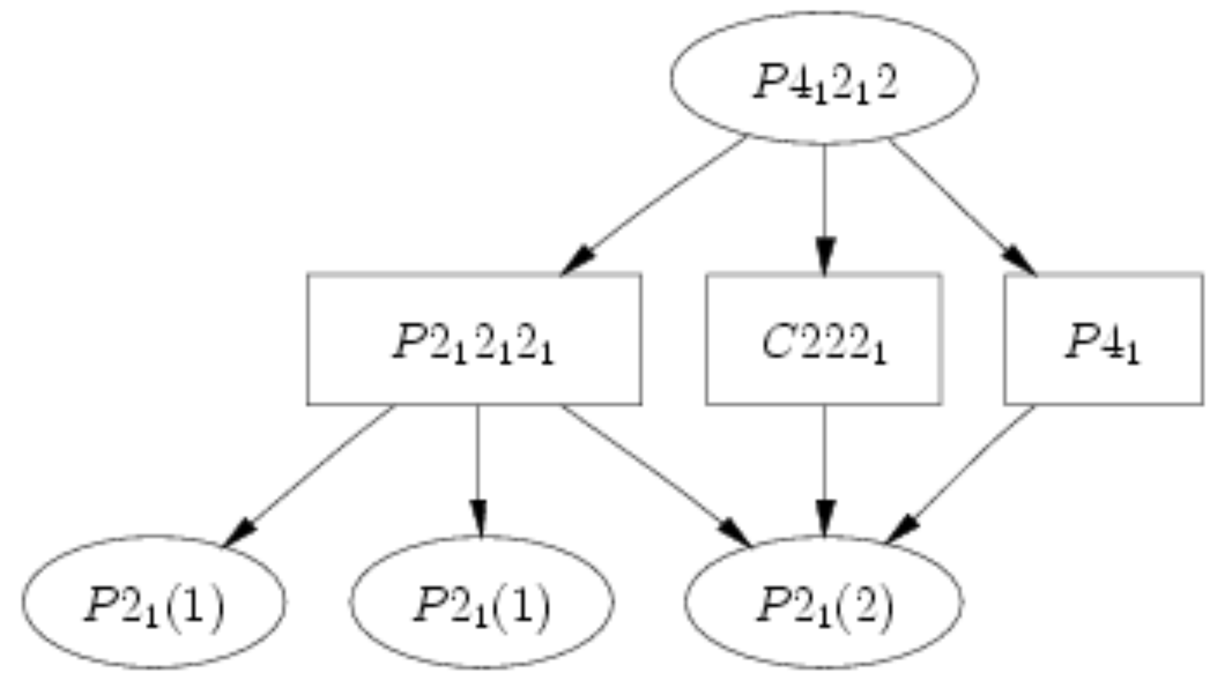
$[i]=[i_P].[i_L]$

SUBGROUPGRAPH
$P4_12_12 > P2_1$



General graph for $P4_12_12 > P2_1$

maximal subgroup graph



three $P2_1$ subgroups in two conjugacy classes

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

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

twins: $i_P=P_G/P_H$

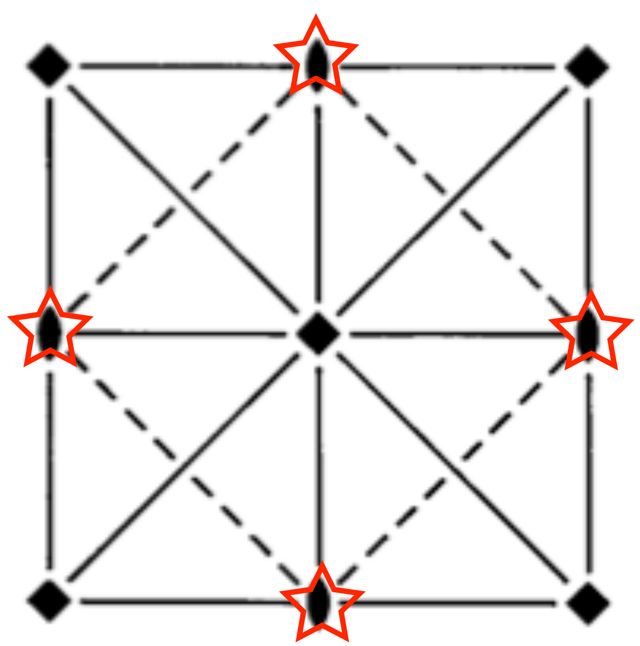
antiphase: $i_L=Z_{H,p}/Z_{G,p}=V_{H,p}/V_{G,p}$

Problem: SPLITTING OF WYCKOFF POSITIONS **WYCKSPLIT**

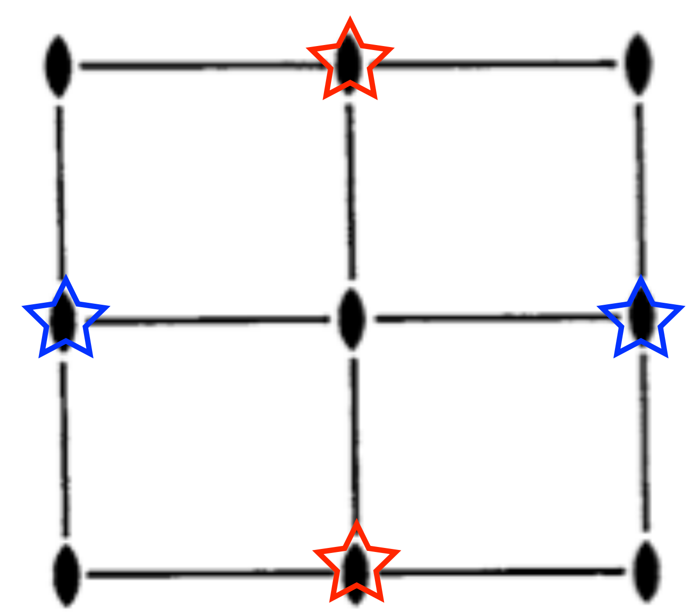
Group-subgroup pair *P4mm*>*Pmm2*, [i]=2

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**,	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$	$2a$	$2b$	$4c$	$8d$	$8d$	$2\times4c$	$2\times8d$

Example

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)

SUPERGROUPS OF SPACE GROUPS

Definition:

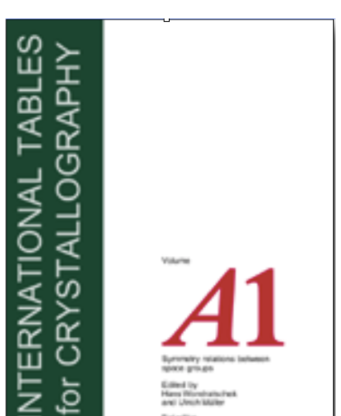
The group G is a supergroup of H if
H is a subgroup of G, $G \geq H$

If H is a maximal subgroup of G, $H<G$,
then G is a minimal supergroup of H, $G>H$

Types of minimal supergroups:

translationengleiche (***t***-type)
klassengleiche (***k***-type)

non-isomorphic   isomorphic

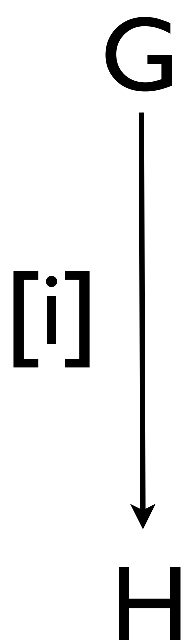


minimal non-isomorphic *k*-
and ***t*- supergroups types**

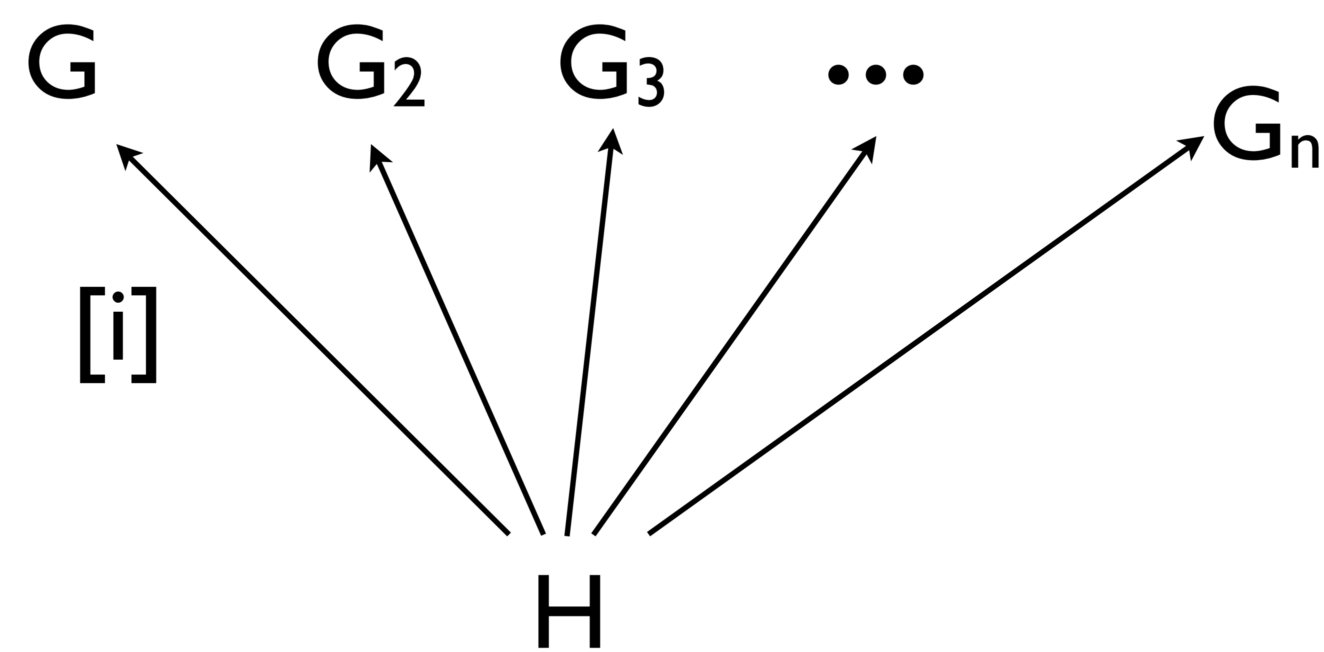
Problem: SUPERGROUPS OF SPACE GROUPS

SUPERGROUPS

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



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



all $G_k>H$ contain H as subgroup

$$G_k = H + Hg_2 + \ldots + Hg_{ik}$$

Normalizer procedure

different $G_k>H$: $N(H) \cap N(G)$

all $G_k>H$: decomposition of $[N(H): N(H) \cap N(G)]$

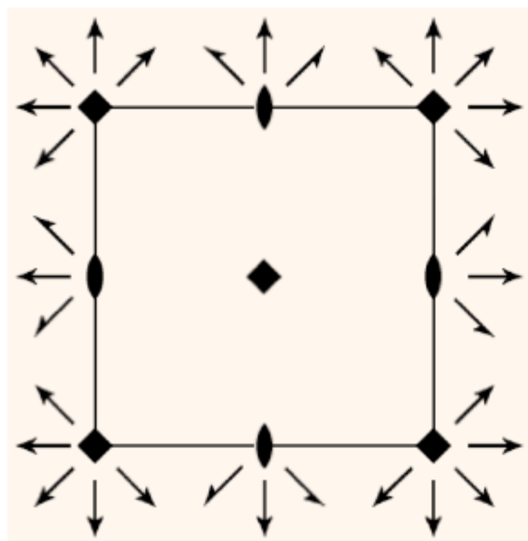
Example: Supergroups P422 of P222

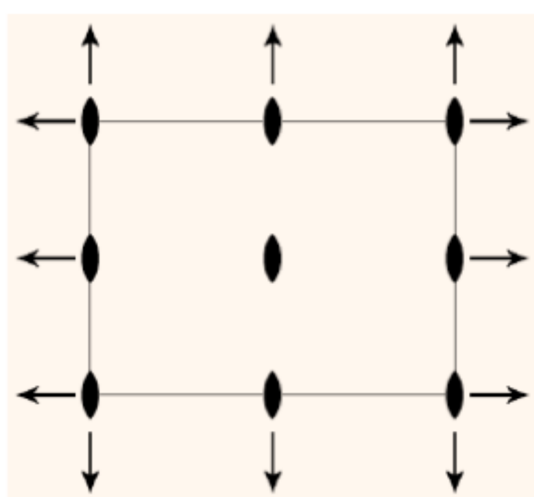
Group-subgroup pair P422>P222

P422

[2]

P222





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

Supergroups P422 of the group P222

$P4_z22$ $P4_x22$ $P4_y22$

[2]

P222

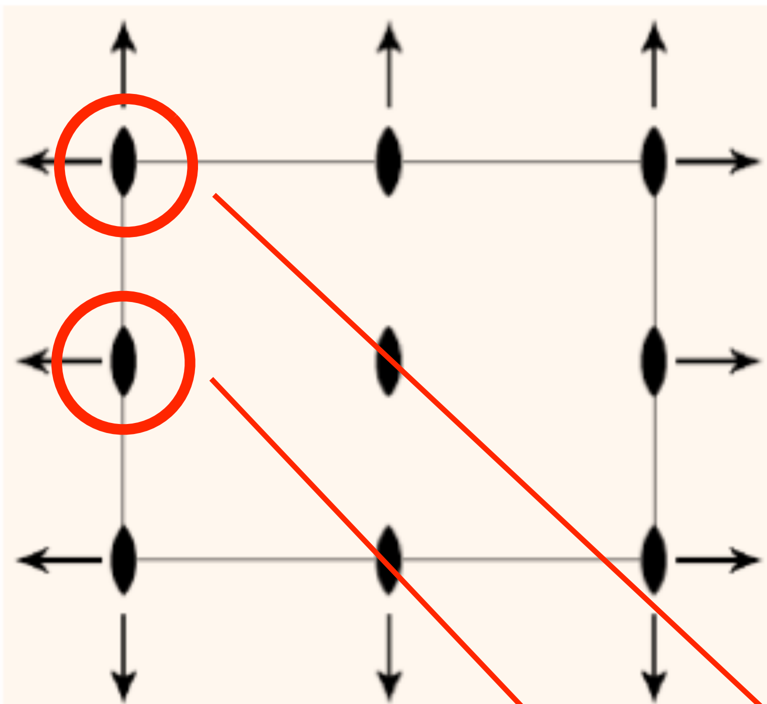
$$P4_z22 = P222 + (P222)(4_z,0)$$

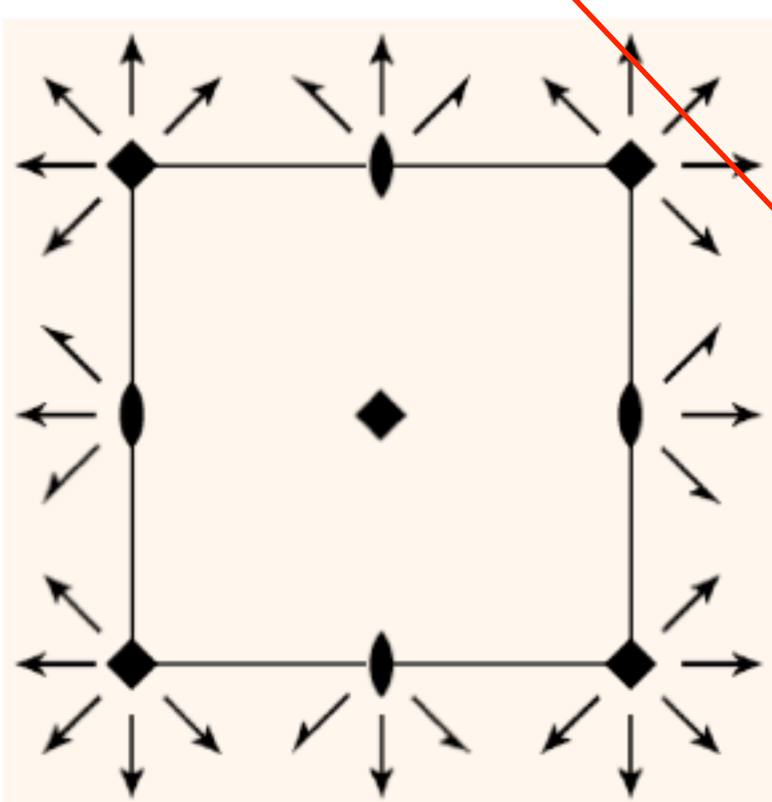
$$P4_x22 = P222 + (P222)(4_x,0)$$

$$P4_y22 = P222 + (P222)(4_y,0)$$

Are there more supergroups P422 of P222?

Example: Supergroups P422 of P222



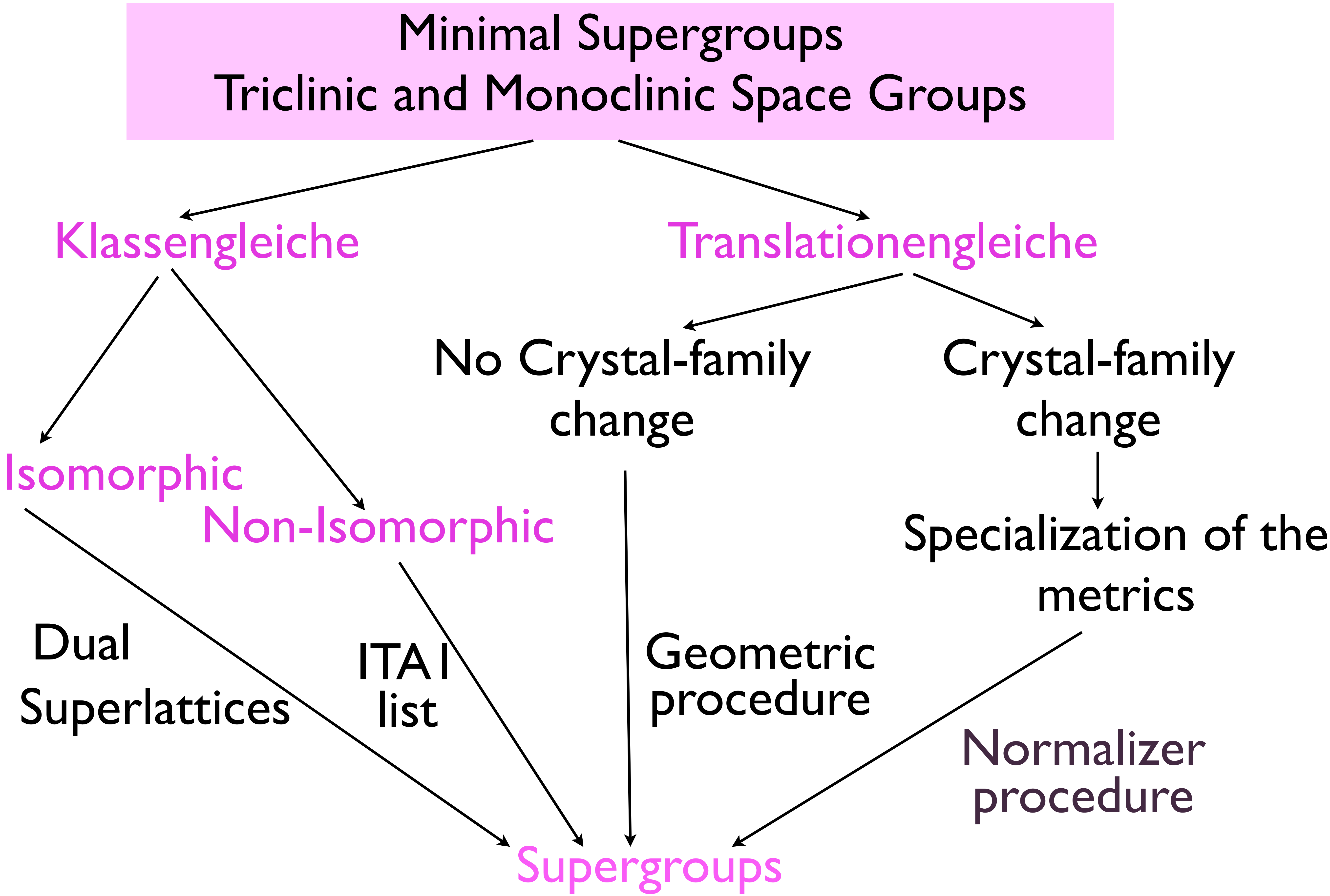


$\mathcal{H} = \mathrm{P}\mathbf{222}$

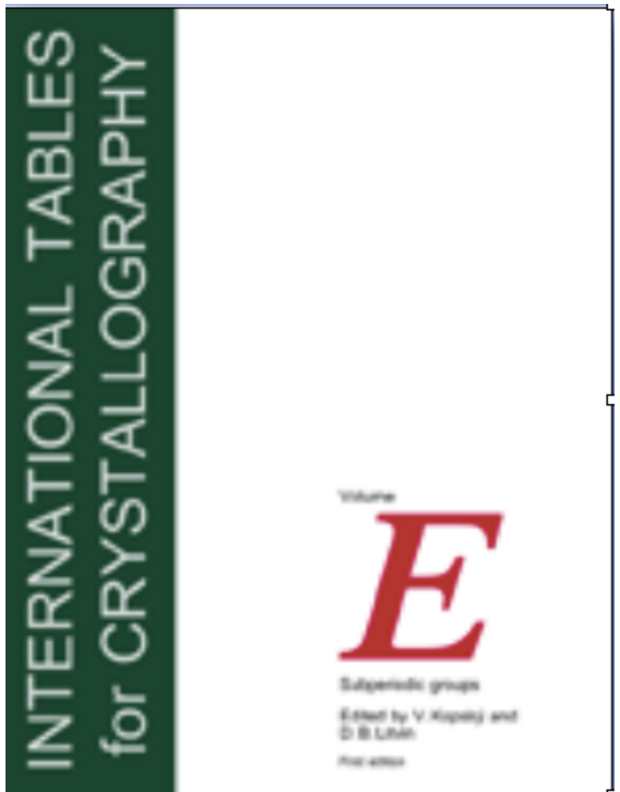
$\mathcal{G} = \mathrm{P}\mathbf{422}$

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

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


Minimal Supergroups
Triclinic and Monoclinic Space Groups
Klassengleiche
Translationengleiche
No Crystal-family change
Crystal-family change
Isomorphic
Non-Isomorphic
Specialization of the metrics
Dual Superlattices
ITA1 list
Geometric procedure
Normalizer procedure
Supergroups

SUBPERIODIC 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

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

Point-group symmetry

ECM31-Oviedo Satellite

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

- 04/2017: General positions of Double Space Groups
- New program: REPRESENTATIONS DPG

MAGNETIC SYMMETRY

FCT/ZTF

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  - **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 induced 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

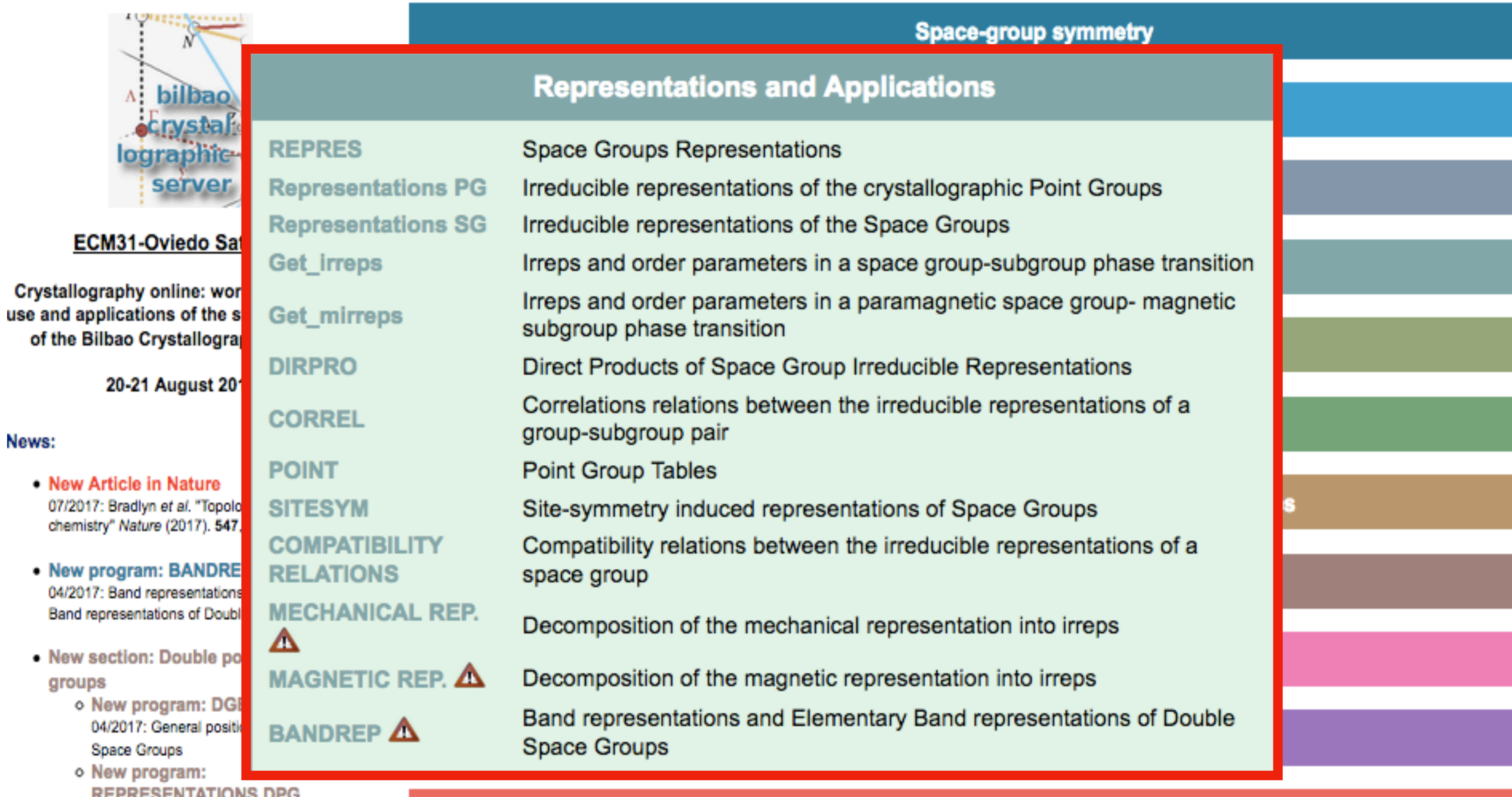
Point group symmetry

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/D...html

Captura de pantalla

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS



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 point and space groups

POINT

character tables
multiplication tables
symmetrized products
subgroup relations
subduced reps

k-VEC

wave-vector data
Brillouin zones
representation domains
parameter ranges
irrep tables

Retrieval tools

Database on Representations of Point Groups

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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

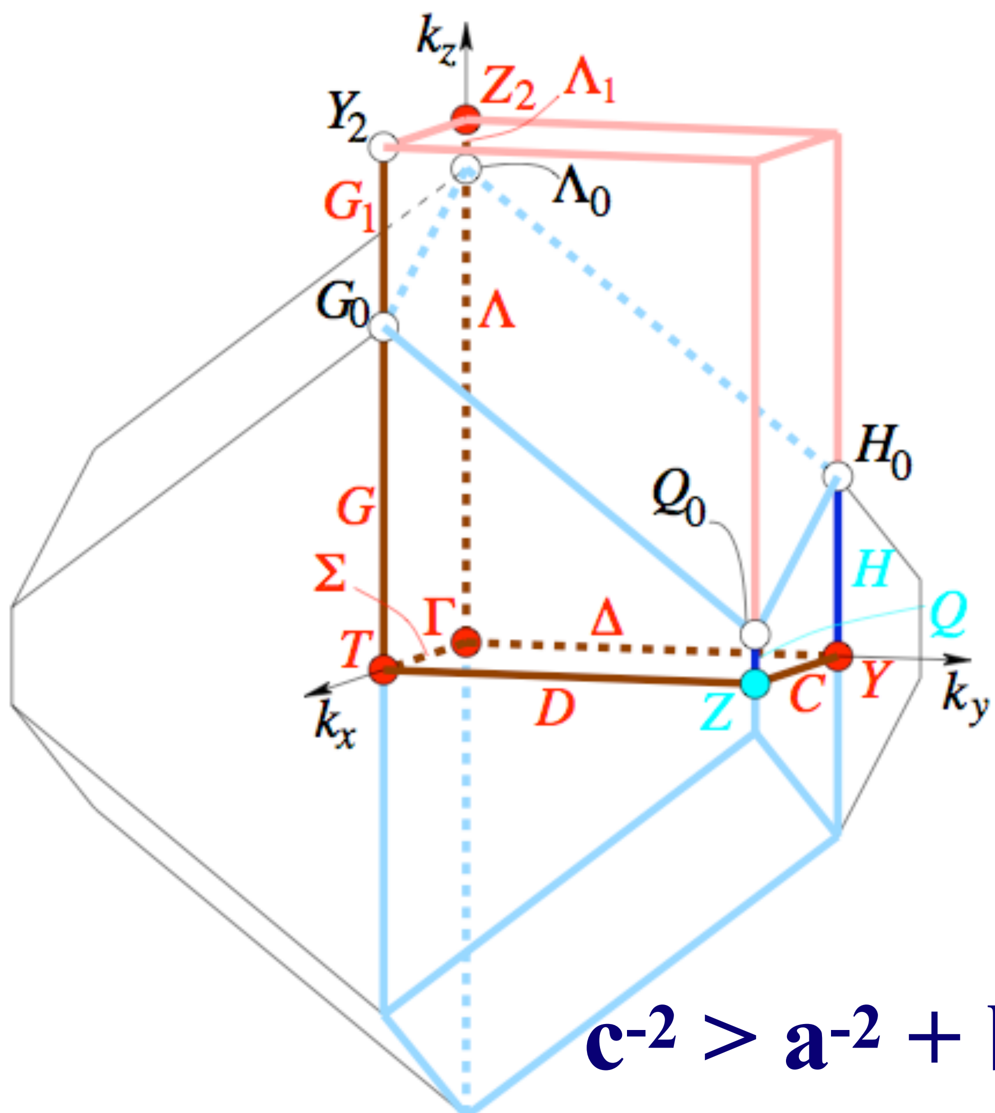
↔

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~T$_2$			b	2	222	1/2,0,0
Z	1/2,1/2,0	0,0,1	c	2	222	0,0,1/2
Y	1/2,0,1/2	0,1,0	d	2	222	0,1/2,0
Y~Y$_2$			d	2	222	1/2,0,1/2
SM	0,u,u ex	2u,0,0	e	4	2..	x,0,0 : 0 < x <= sm$_0$
U	1,1/2+u,1/2+u ex	2u,1,1	e	4	2..	x,1/2,1/2 : 0 < x < u$_0$
U~SM$_1$=[SM$_0$ T$_2$]			e	4	2..	x,0,0 : 1/2-u$_0$=sm$_0$ < x < 1/2
SM+SM$_1$=[GM T$_2$]			e	4	2..	x,0,0 : 0 < x < 1/2
A	1/2,1/2+u,u ex	2u,0,1	f	4	2..	x,0,1/2 : 0 < x <= a$_0$
C	1/2,u,1/2+u ex	2u,1,0	f	4	2..	x,1/2,0 : 0 < x < c$_0$

DOUBLE CRYSTALLOGRAPHIC GROUPS

FCT/ZTF

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Space-group symmetry

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Representations and Applications

Double point and space groups

DGENPOS ⚠	General positions of Double Space groups
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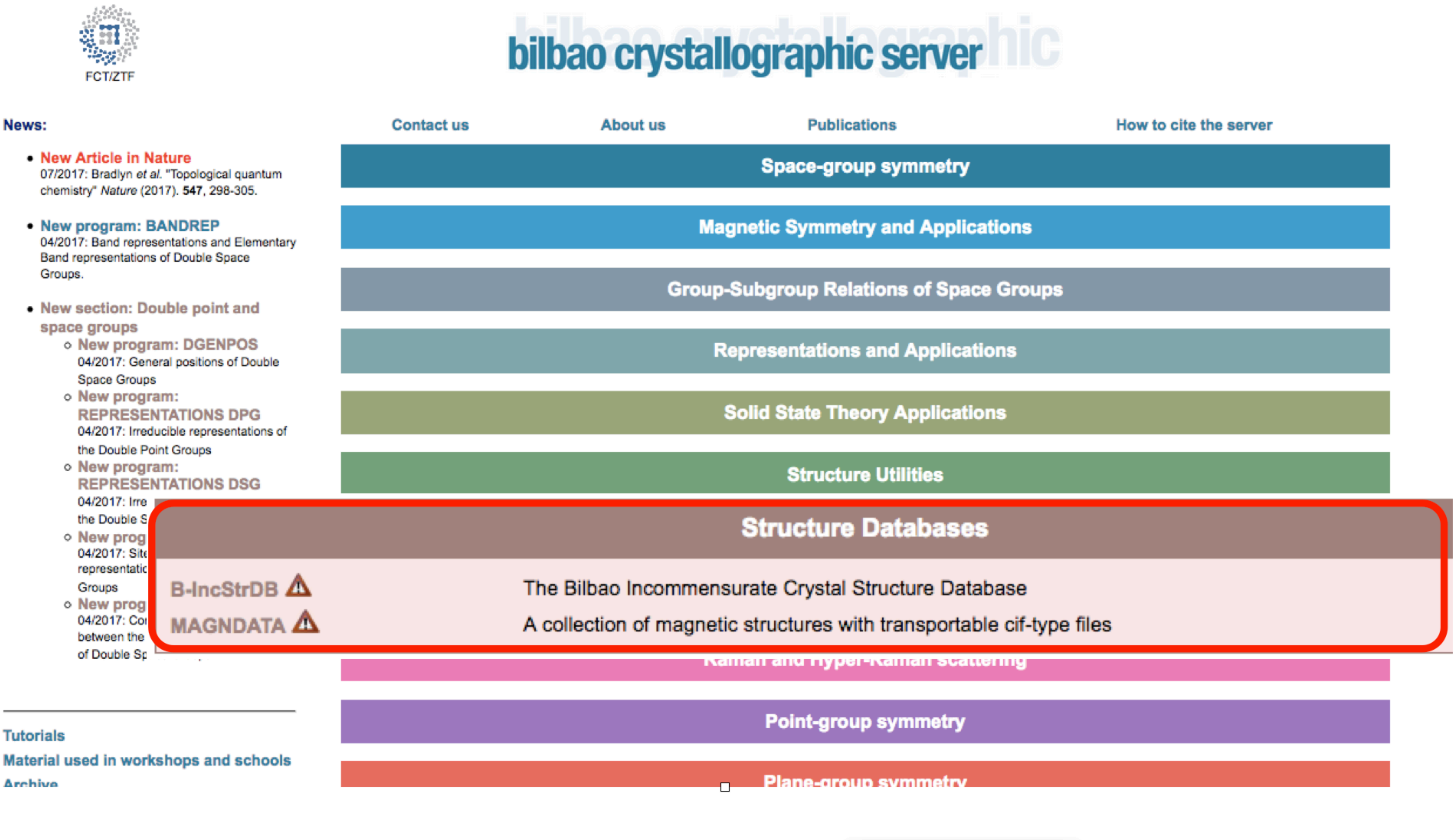
BANDREP ⚠	Band representations and Elementary Band representations of Double Space Groups

STRUCTURE DATABASES



STRUCTURE UTILITIES

Gemma DE LA FLOR MARTIN ...

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Space-group symmetry

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Structure Utilities

CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
VISUALIZE	Visualize structures using Jmol
COMPSTRU	Comparison of Similar Structures with the same Symmetry
STRUCTURE RELATIONS	Finds the transformation matrix that relates the two given group-subgroup related structures within a tolerance.

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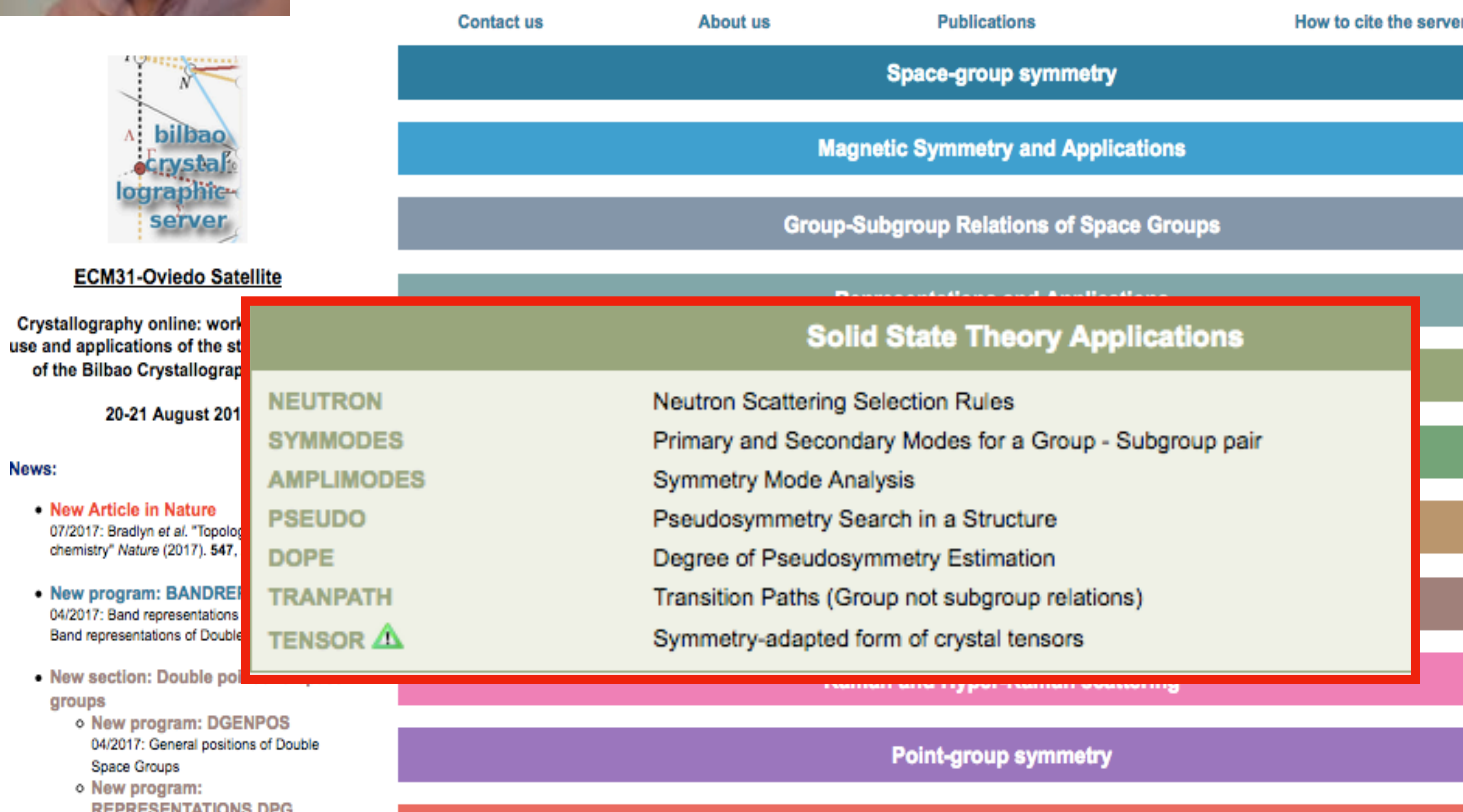
Plane-group symmetry

Double point and space groups

STRUCTURAL RELATIONSHIPS



THANK YOU
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YOUR ATTENTION!