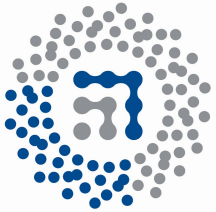

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Use of the structural programs of the Bilbao Crystallographic Server. Group-subgroup relations. The program SUBGROUPS

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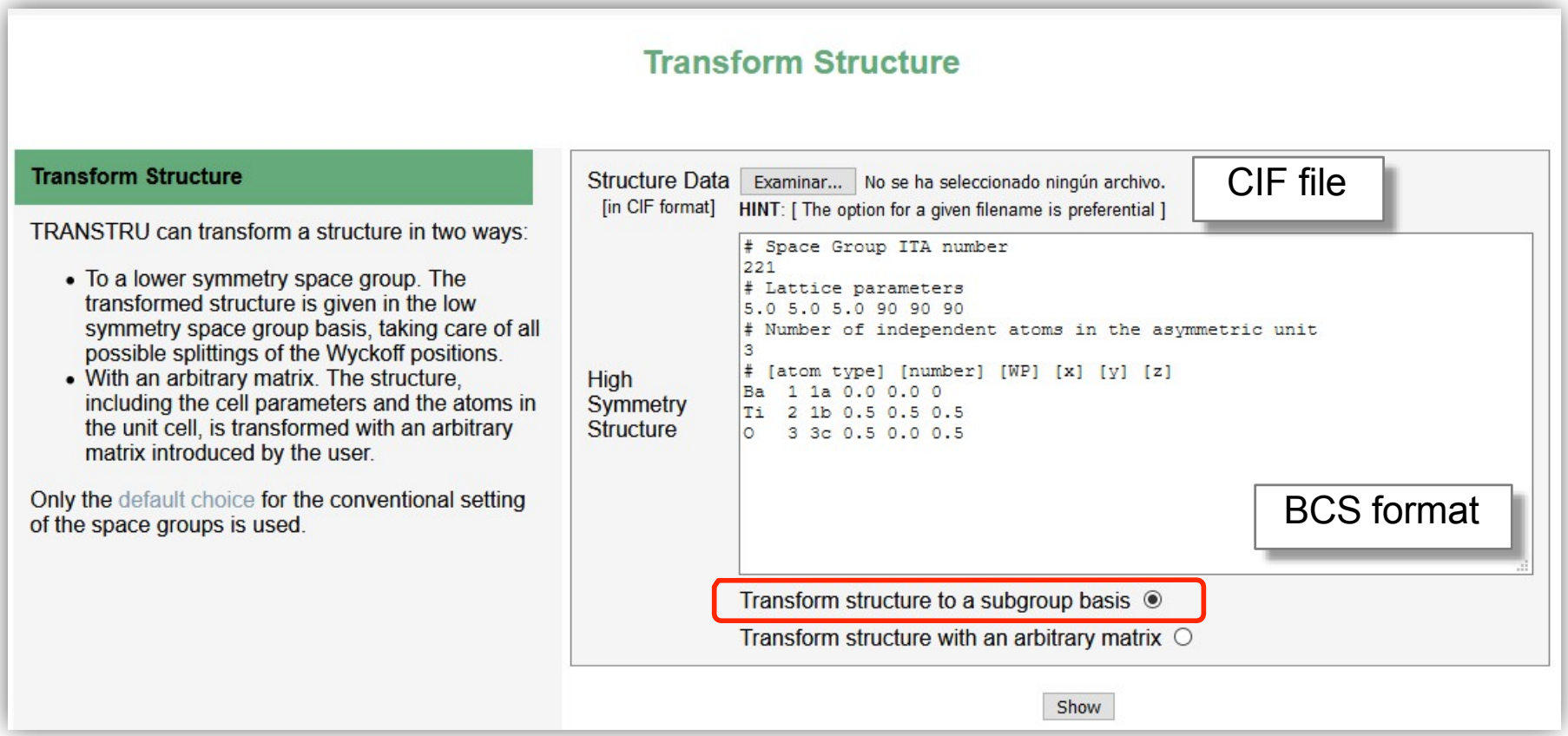
Why we have to derive and work with SUBGROUPS?: DISTORTED STRUCTURES

Symmetry break: G → F (subgroup of G)

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
CIF2STANDARD	Transforms a given CIF (in any setting) to that of standard setting
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

Structure transformation to a lower symmetry

TRANSTRU



To transform a structure described in standard setting to a lower symmetry space group or with an arbitrary matrix

Structure transformation to a lower symmetry

TRANSTRU

Transform Structure

Transform Structure

TRANSTRU transforms the structure to the low symmetry space group basis, taking care of all possible splittings of the Wyckoff positions.

Structure

```
221
3.9064 3.9064 3.9064 90. 90. 90.
3
La      1       1a      0.000000        0.000000        0.000000
Co      1       1b      0.500000        0.500000        0.500000
O       1       3c      0.500000        0.500000        0.000000
```

Low symmetry Space Group *ITA* number: 15

Transformation Matrix:

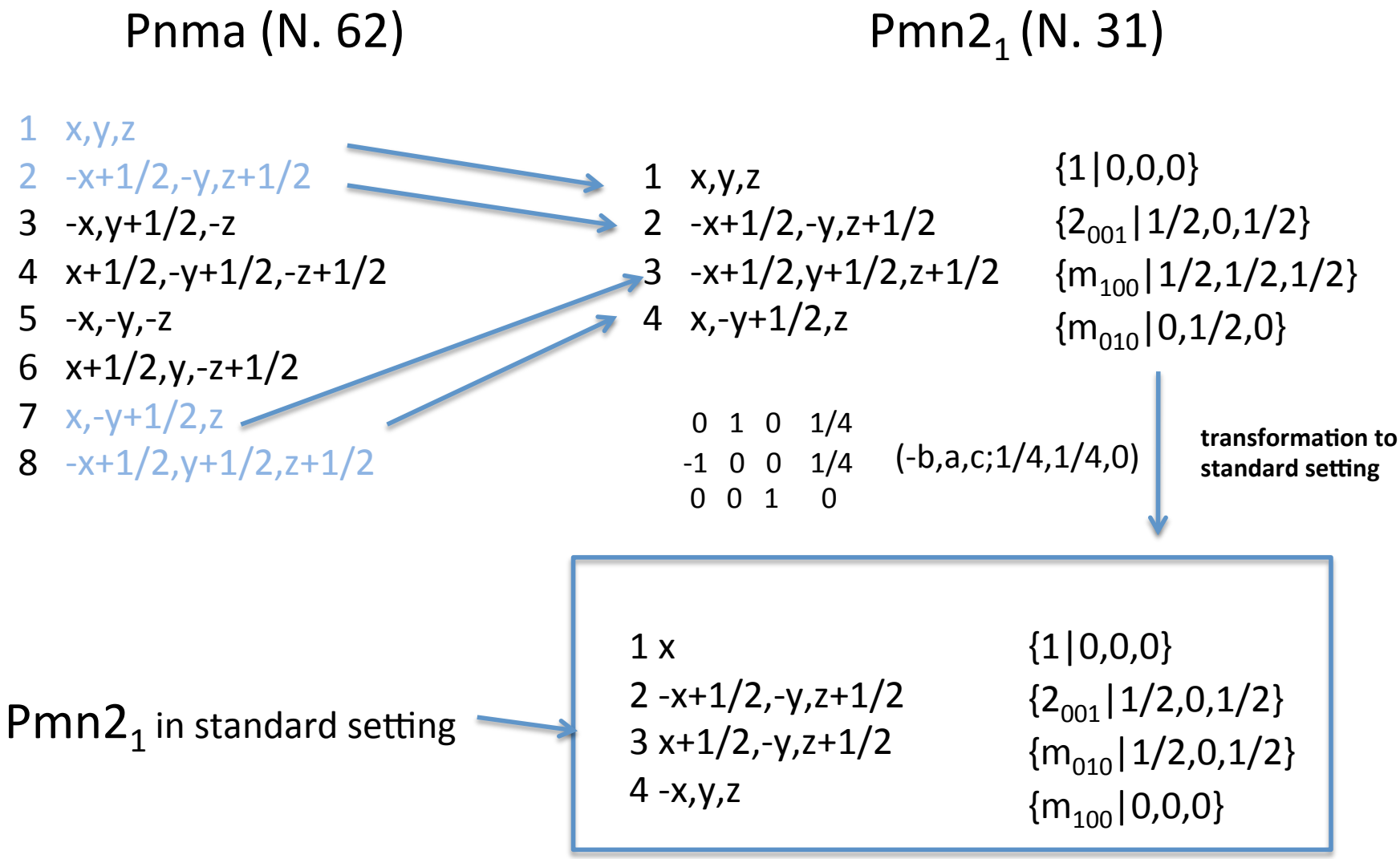
In matrix form:

	Linear part			Origin Shift
	1	-1	-1	0
	2	0	0	1/2
	-1	-1	1	1/2

Show

Transformation of the set of operations forming the subgroup to standard setting of the space group

What is a subgroup of a space group and how we define it:



Structure transformation to a lower symmetry

$SrZrO_3$ Pnma (N. 62)

62
5.8206 8.1949 5.8045 90 90 90
4
Sr 1 4c 0.524000 0.250000 0.004000
Zr 1 4a 0.000000 0.000000 0.000000
O 1 4c -0.013000 0.250000 -0.069000
O 2 8d 0.284000 0.036000 0.215000

7 free parameters

Wyckoff Positions of Group *Pnma* (No. 62)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	d	1	(x,y,z) (-x+1/2,-y,z+1/2) (-x,y+1/2,-z) (x+1/2,-y+1/2,-z+1/2) (-x,-y,-z) (x+1/2,y,-z+1/2) (x,-y+1/2,z) (-x+1/2,y+1/2,z+1/2)
4	c	.m.	(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2)
4	b	-1	(0,0,1/2) (1/2,0,0) (0,1/2,1/2) (1/2,1/2,0)
4	a	-1	(0,0,0) (1/2,0,1/2) (0,1/2,0) (1/2,1/2,1/2)

$SrZrO_3$ $Pmn2_1$ (N. 31)

031
8.194900 5.820600 5.804500 90.000000 90.000000 90.000000
7

Sr	1	2a	0.000000	0.274000	0.004000
Sr	1_2	2a	0.500000	0.226000	0.996000
Zr	1	4b	0.250000	0.750000	0.000000
O	1	2a	0.000000	0.737000	0.931000
O	1_2	2a	0.500000	0.763000	0.069000
O	2	4b	0.214000	0.034000	0.215000
O	2_2	4b	0.714000	0.466000	0.785000

Wyckoff Positions of Group *Pmn*2_1 (No. 31)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
4	b	1	(x,y,z) (-x+1/2,-y,z+1/2) (x+1/2,-y,z+1/2) (-x,y,z)
2	a	m..	(0,y,z) (1/2,-y,z+1/2)

Structure transformation to a lower symmetry

$SrZrO_3$ Pnma (N. 62)

62
5.8206 8.1949 5.8045 90 90 90
4
Sr 1 4c 0.524000 0.250000 0.004000 **2**
Zr 1 4a 0.000000 0.000000 0.000000 **0**
O 1 4c -0.013000 0.250000 -0.069000 **2**
O 2 8d 0.284000 0.036000 0.215000 **6**

7 free parameters

Wyckoff Positions of Group *Pnma* (No. 62)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	d	1	(x,y,z) (-x+1/2,-y,z+1/2) (-x,y+1/2,-z) (x+1/2,-y+1/2,-z+1/2) (-x,-y,-z) (x+1/2,y,-z+1/2) (x,-y+1/2,z) (-x+1/2,y+1/2,z+1/2)
4	c	.m.	(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2)
4	b	-1	(0,0,1/2) (1/2,0,0) (0,1/2,1/2) (1/2,1/2,0)
4	a	-1	(0,0,0) (1/2,0,1/2) (0,1/2,0) (1/2,1/2,1/2)

$SrZrO_3$ $Pmn2_1$ (N. 31)

031
8.194900 5.820600 5.804500 90 90 90
7

Sr	1	2a	0.000000	0.274000	0.004000	**2**
Sr	1_2	2a	0.500000	0.226000	0.996000	**2**
Zr	1	4b	0.250000	0.750000	0.000000	**3**
O	1	2a	0.000000	0.737000	0.931000	**2**
O	1_2	2a	0.500000	0.763000	0.069000	**2**
O	2	4b	0.214000	0.034000	0.215000	**3**
O	2_2	4b	0.714000	0.466000	0.785000	**3**

17 free parameters

Wyckoff Positions of Group *Pmn*2_1 (No. 31)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
4	b	1	(x,y,z) (-x+1/2,-y,z+1/2) (x+1/2,-y,z+1/2) (-x,y,z)
2	a	m..	(0,y,z) (1/2,-y,z+1/2)

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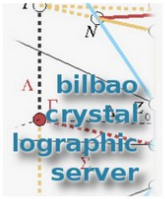

Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
27 June - 1 July 2022, Leioa (Spain)

Forthcoming schools and workshops

News:

- **Space-group symmetry**
  05/2022: The monoclinic and tetragonal ITA-settings database has been completed.
- **New Article**
  04/2022: Regnault *et al.* "Catalogue of flat-band stoichiometric materials". Nature (2022) **603**, 824-828
- **New version of B-IncStrDB**
  02/2022: New version of the data-base of incommensurate structures.
- **New upload option in MAGNDATA**
  10/2021: New feature that permits anyone to submit to this database any published magnetic structure not yet included in the collection.

- Space-group symmetry
- Magnetic Symmetry and Applications
- Group-Subgroup Relations of Space Groups
- Representations and Applications
- Solid State Theory Applications
- Structure Utilities
- Topological Quantum Chemistry
- Subperiodic Groups: Layer, Rod and Frieze Groups
- Structure Databases
- Raman and Hyper-Raman scattering
- Point-group symmetry
- Plane-group symmetry
- Double point and space groups

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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)

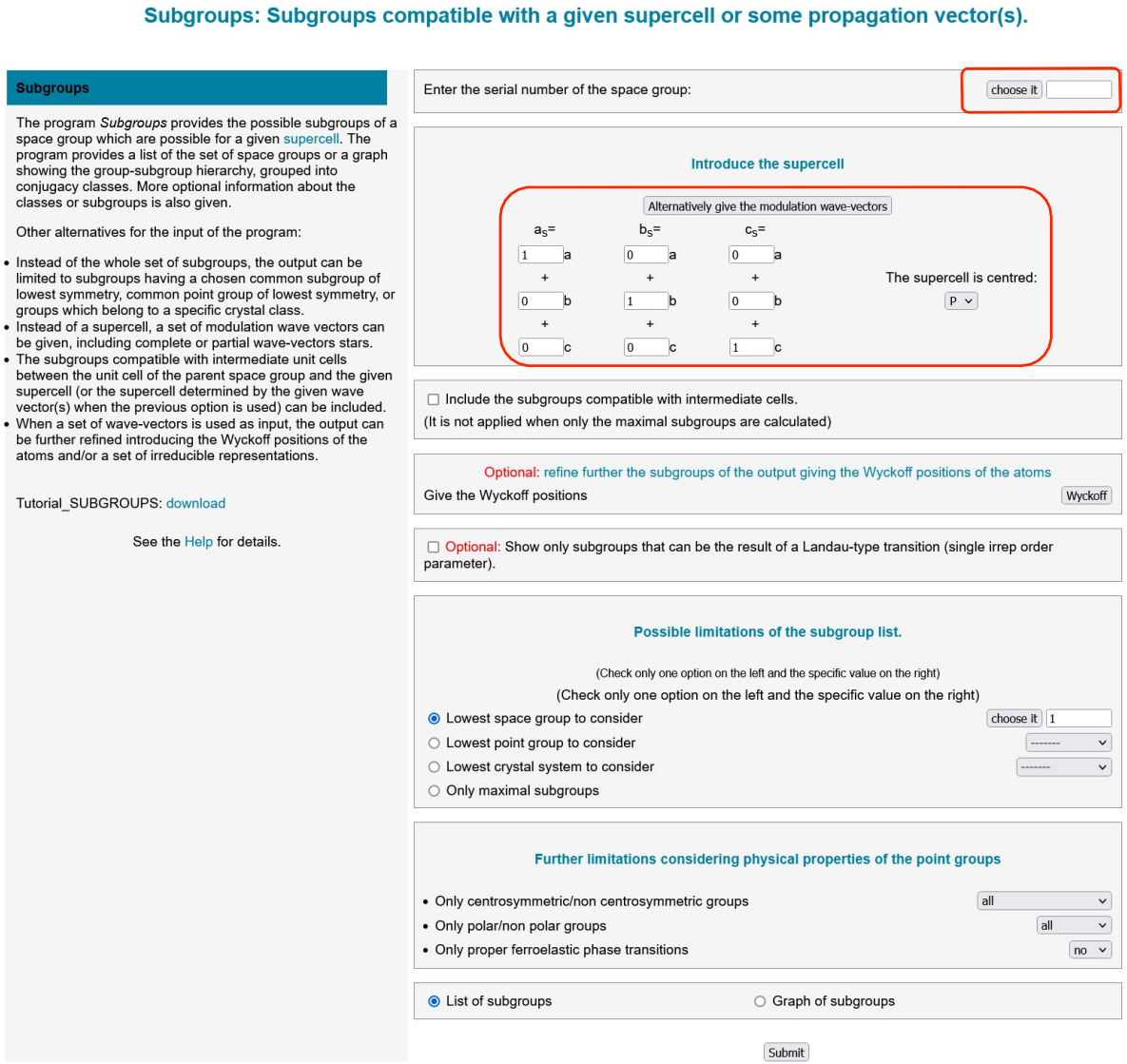
B-incstDB
02/2022: New version of the

Determine and explore online all possible symmetries that can result from the distortion of a parent structure of higher symmetry

database any published magnetic structure not yet included in the collection.

Double point and space groups

SUBGROUPS: https://www.cryst.ehu.es/cgi-bin/cryst/programs/subgrmag1_cell.pl



Parent space group

Supercell or modulation wave-vector

Minimal input

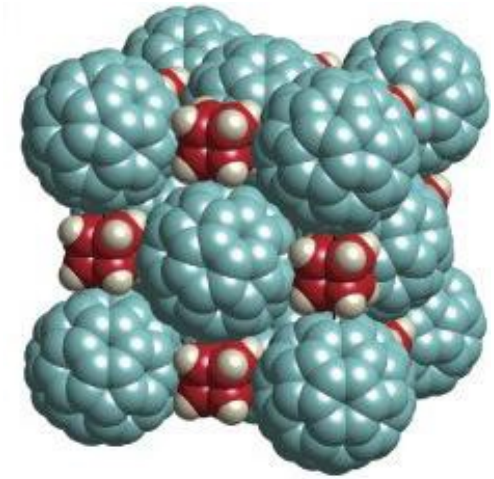
Other alternatives to filtered the results of the program

Example : Fullerene-cubane crystal

High-temperature phase

Low-temperature phase

Fm-3m(No. 225)



Nature Mat. **4**, 764 (2005)

Power diffraction experiments

?

Orthorhombic structure

$$a_o \approx b_o \approx \frac{a_{co}}{\sqrt{2}} \quad ; \; c_o \approx 2a_c$$

phys. stat. sol. (b) 243, 2999 (2006)

J. Phys. Chem. B **113**, 2042 (2009)

Disordered fullerenes molecules 4a (0,0,0)

Disordered cubane molecules 4b (1/2,1/2,1/2)

Possible symmetry (space group) of the detected low symmetry phase?

Example : Fullerene-cubane crystal

Subgroups: Subgroups compatible with a given supercell or some propagation vector(s).

Subgroups

The program *Subgroups* provides the possible subgroups of a space group which are possible for a given supercell. The program provides a list of the set of space groups or a graph showing the group-subgroup hierarchy, grouped into conjugacy classes. More optional information about the classes or subgroups is also given.

Other alternatives for the input of the program:

- Instead of the whole set of subgroups, the output can be limited to subgroups having a chosen common subgroup of lowest symmetry, common point group of lowest symmetry, or groups which belong to a specific crystal class.
- Instead of a supercell, a set of modulation wave vectors can be given, including complete or partial

Enter the serial number of the space group: choose it 225

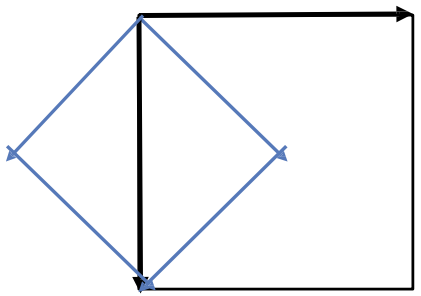
Introduce the supercell

Alternatively give the modulation wave-vectors

a_s=	b_s=	c_s=
1/2 a	1/2 a	0 a
+	+	+
-1/2 b	1/2 b	0 b
+	+	+
0 c	0 c	2 c

The supercell is centred: P

...



◉ List of subgroups ○ Graph of subgroups

Submit

Example : Fullerene-cubane crystal

List of subgroups that fulfill the given conditions

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$P4_2/ncm$ (No. 138)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
2	$P4_2/nmc$ (No. 137)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
3	$P4_2/mcm$ (No. 132)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
4	$P4_2/mmc$ (No. 131)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
5	$P4/ncc$ (No. 130)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
6	$P4/nmm$ (No. 129)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
7	$P4/mcc$ (No. 124)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
8	$P4/mmm$ (No. 123)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
9	$P\bar{4}c2$ (No. 116)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
10	$P\bar{4}c2$ (No. 116)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
11	$P\bar{4}m2$ (No. 115)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

99 subgroups

Input data

Subgroups of the space group :	$Fm\bar{3}m$ (N. 225)
Lowest space group to consider:	$P1$ (N. 1)
Supercell given by:	(1/2,-1/2,0),(1/2,1/2,0),(0,0,2)
Centred supercell:	No

90	Pm (No. 6)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & -2 & 0 & 1/2 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
91	$C2$ (No. 5)	$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
92	$C2$ (No. 5)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
93	$P2_1$ (No. 4)	$\begin{pmatrix} 1/2 & 1/2 & 0 & -1/8 \\ -1/2 & 1/2 & 0 & 1/8 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
94	$P2_1$ (No. 4)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & -2 & 0 & 0 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
95	$P2$ (No. 3)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
96	$P2$ (No. 3)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & -2 & 0 & 0 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
97	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
98	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps
99	$P1$ (No. 1)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	192=4x48	Conjugacy Class	Get irreps

Example: Fullerene-cubane crystal

Go back to the input page

Enter the serial number of the space group: choose it 225

Introduce the supercell

Alternatively give the modulation wave-vectors

a_s=	b_s=	c_s=
1/2 a +	1/2 a +	0 a +
-1/2 b +	1/2 b +	0 b +
0 c	0 c	2 c

The supercell is centred: P

Possible limitations of the subgroup list.

(Check only one option on the left and the specific value on the right)

(Check only one option on the left and the specific value on the right)

- ○ Lowest space group to consider — choose it 1
- ○ Lowest point group to consider — -------
- ◉ Lowest crystal system to consider — Orthorhombic
- ○ Only maximal subgroups

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$P4_2/ncm$ (No. 138)	1/2 1/2 0 1/4; -1/2 1/2 0 0; 0 0 2 -1/4	12=4x3	Conjugacy Class	Get irreps
2	$P4_2/nmc$ (No. 137)	1/2 1/2 0 1/4; -1/2 1/2 0 0; 0 0 2 1/4	12=4x3	Conjugacy Class	Get irreps
3	$P4_2/mcm$ (No. 132)	1/2 1/2 0 0; -1/2 1/2 0 0; 0 0 2 1/2	12=4x3	Conjugacy Class	Get irreps
4	$P4_2/mmc$ (No. 131)	1/2 1/2 0 0; -1/2 1/2 0 0; 0 0 2 0	12=4x3	Conjugacy Class	Get irreps
5	$P4/ncc$ (No. 130)	1/2 1/2 0 1/4; -1/2 1/2 0 0; 0 0 2 1/4	12=4x3	Conjugacy Class	Get irreps
6	$P4/nmm$ (No. 129)	1/2 1/2 0 1/4; -1/2 1/2 0 0; 0 0 2 -1/4	12=4x3	Conjugacy Class	Get irreps

60	$P2_12_12$ (No. 18)	1/2 1/2 0 0; -1/2 1/2 0 0; 0 0 2 -1/4	48=4x12	Conjugacy Class	Get irreps
61	$P222_1$ (No. 17)	1/2 1/2 0 0; -1/2 1/2 0 0; 0 0 2 1/2	48=4x12	Conjugacy Class	Get irreps
62	$P222$ (No. 16)	1/2 1/2 0 0; -1/2 1/2 0 0; 0 0 2 1/2	48=4x12	Conjugacy Class	Get irreps

The list of subgroups is reduced from 99 to 62

Most of them can be discarded symmetry higher than orthorhombic

Orthorhombic point groups: 222, mm2 or mmm

Example: Fullerene-cubane crystal

Go back to the input page

Enter the serial number of the space group: choose it 225

Introduce the supercell

Alternatively give the modulation wave-vectors

a_s=	b_s=	c_s=
1/2 a +	1/2 a +	0 a +
-1/2 b +	1/2 b +	0 b +
0 c	0 c	2 c

The supercell is centred: P

Possible limitations of the subgroup list.

(Check only one option on the left and the specific value on the right)

(Check only one option on the left and the specific value on the right)

- ○ Lowest space group to consider — choose it 1
- ◉ Lowest point group to consider — 8: mmm
- ○ Lowest crystal system to consider — -------
- ○ Only maximal subgroups

List of subgroups that fulfill the given conditions

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$P4_2/ncm$ (No. 138)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
2	$P4_2/nmc$ (No. 137)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
3	$P4_2/mcm$ (No. 132)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
4	$P4_2/mmc$ (No. 131)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
5	$P4/ncc$ (No. 130)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
6	$P4/nmm$ (No. 129)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
7	$P4/mcc$ (No. 124)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
8	$P4/mmm$ (No. 123)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
9	$Ccce$ (No. 68)	$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
10	$Cmme$ (No. 67)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
11	$Cccm$ (No. 66)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
12	$Cmmm$ (No. 65)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
13	$Cmce$ (No. 64)	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
14	$Cmcm$ (No. 63)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
15	$Pnma$ (No. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
16	$Pmmn$ (No. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
17	$Pccn$ (No. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
18	$Pmma$ (No. 51)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
19	$Pccm$ (No. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
20	$Pmmm$ (No. 47)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

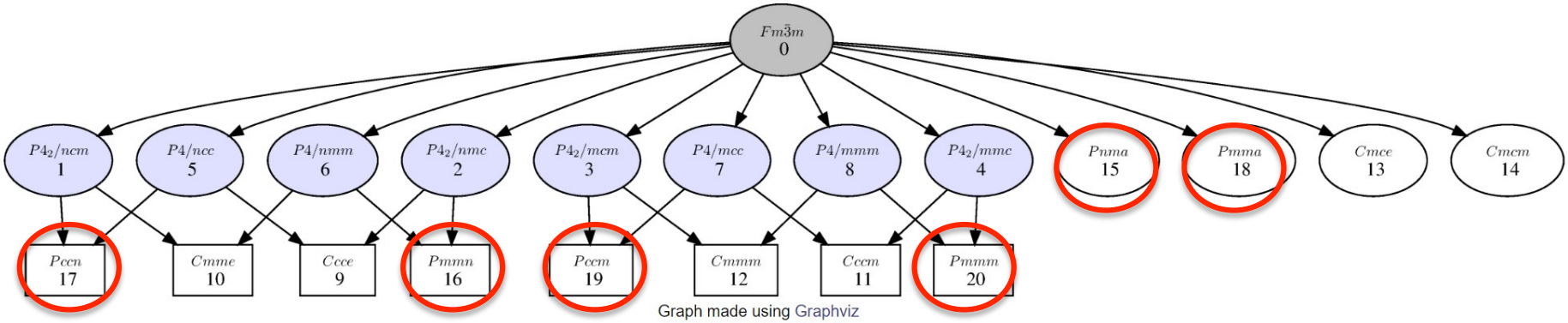
Example: Fullerene-cubane crystal

Input data

Subgroups of the space group :	$Fm\bar{3}m$ (N. 225)
Lowest point group to consider:	*mmm* (N. 8)
Supercell given by:	(1/2,-1/2,0),(1/2,1/2,0),(0,0,2)
Centred supercell:	No

Graph of subgroups that fulfill the given conditions

Get the full list of subgroups



Graph made using Graphviz
Download a postscript file

Remove labels

Get information about the groups of the conjugacy class with label [ ] Get information

Get the subgraph between the group (or conjugacy class) with label [ ] and the group (or conjugacy class) with label [ ] according to these rules Get graph

Graph showing the group-subgroup hierarchy of these 20 subgroups

Example : Fullerene-cubane crystal

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$P4_2/ncm$ (No. 138)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
2	$P4_2/nmc$ (No. 137)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
3	$P4_2/mcm$ (No. 132)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
4	$P4_2/mmc$ (No. 131)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
5	$P4/ncc$ (No. 130)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
6	$P4/nmm$ (No. 129)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
7	$P4/mcc$ (No. 124)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
8	$P4/mmm$ (No. 123)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps
9	$Ccce$ (No. 68)	$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
10	$Cmme$ (No. 67)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
11	$Cccm$ (No. 66)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
12	$Cmmm$ (No. 65)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
13	$Cmce$ (No. 64)	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
14	$Cmcm$ (No. 63)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
15	$Pnma$ (No. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
16	$Pmmn$ (No. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
17	$Pccn$ (No. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
18	$Pmma$ (No. 51)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
19	$Pccm$ (No. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
20	$Pmmm$ (No. 47)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

Tetragonal subgroups

C centered orthorhombic

The unit cell of the LS-phase is known to be primitive orthorhombic

6 possible symmetries

Example : Fullerene-cubane crystal

15	*Pnma* (No. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
16	*Pmmn* (No. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
17	*Pccn* (No. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
18	*Pmma* (No. 51)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
19	*Pccm* (No. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
20	*Pmmm* (No. 47)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

The irreducible representations of the parent structure that are compatible with this specific symmetry for the distorted structure

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Input data

Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→*Pnma* (N. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	$Fm\bar{3}m$ (No. 225) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,0)	*I*4/*mmm* (No. 139) a/2-b/2,a/2+b/2,c;0,0,0	
	GM_5^+: (a,0,0)	*Immm* (No. 71) a/2+b/2,-1/2a+b/2,c;0,0,0	
DT: (0,1/2,0)(1/2,0,0)**(0,0,1/2)**	DT_5: (0,0,0,0,0,0,0,0,a,0,0,a)	*Pnma* (No. 62) -2c,a/2+b/2,a/2-b/2;0,1/4,-1/4	matrices of the irreps
X: (0,1,0)(1,0,0)**(0,0,1)**	X_2^-: (0,0,a)	$P4_2/nmc$ (No. 137) a/2-b/2,a/2+b/2,c;0,1/4,1/4	matrices of the irreps
	X_3^-: (0,0,a)	*P*4/*nmm* (No. 129) a/2-b/2,a/2+b/2,c;1/4,0,1/4	

The symmetry break
$\mathrm{Fm\text{-}3m} \longrightarrow Pnma$
can be realized through a
Landau type phase transition

Example : Fullerene-cubane crystal

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

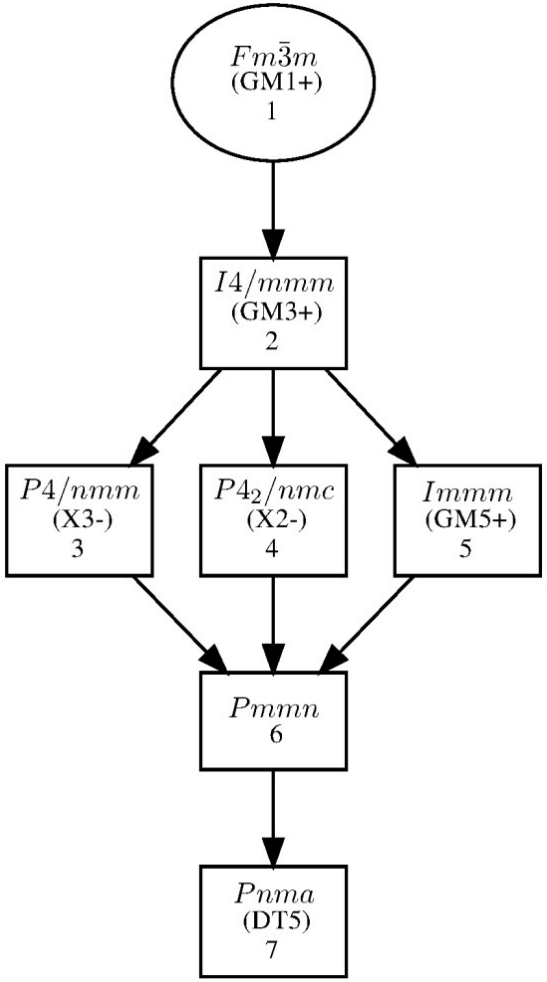
Input data

Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→*Pnma* (N. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	$Fm\bar{3}m$ (No. 225) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,0)	*I*4/*mmm* (No. 139) a/2-b/2,a/2+b/2,c;0,0,0	
	GM_5^+: (a,0,0)	*Immm* (No. 71) a/2+b/2,-1/2a+b/2,c;0,0,0	
DT: (0,1/2,0)(1/2,0,0)**(0,0,1/2)**	DT_5: (0,0,0,0,0,0,0,0,a,0,0,a)	*Pnma* (No. 62) -2c,a/2+b/2,a/2-b/2;0,1/4,-1/4	matrices of the irreps
X: (0,1,0)(1,0,0)**(0,0,1)**	X_2^-: (0,0,a)	$P4_2/nmc$ (No. 137) a/2-b/2,a/2+b/2,c;0,1/4,1/4	matrices of the irreps
	X_3^-: (0,0,a)	*P*4/*nmm* (No. 129) a/2-b/2,a/2+b/2,c;1/4,0,1/4	



Example : Fullerene-cubane crystal

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

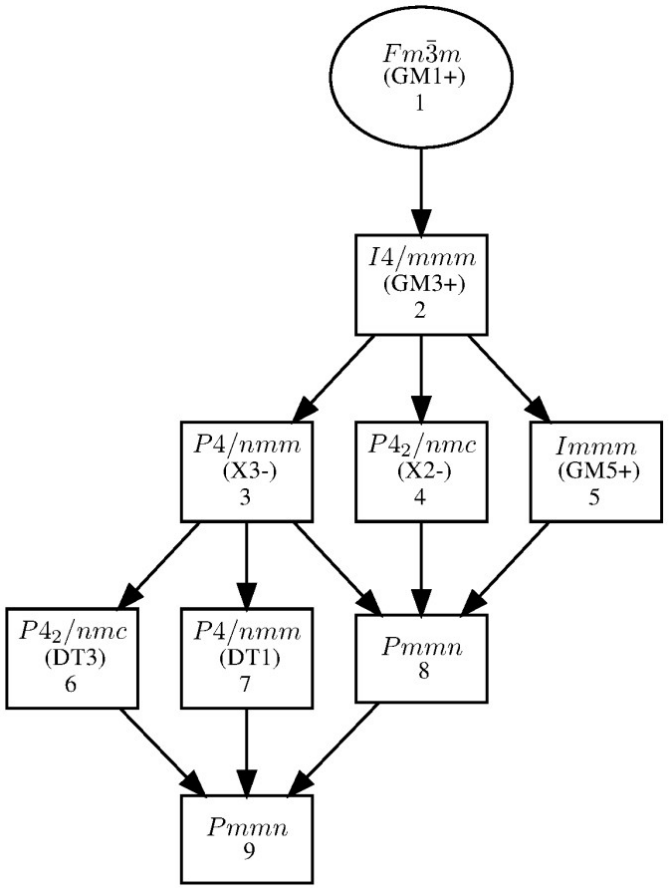
Input data

Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→$Pmmn$ (N. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	$Fm\bar{3}m$ (No. 225) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,0)	$I4/mmm$ (No. 139) a/2-b/2,a/2+b/2,c;0,0,0	
	GM_5^+: (a,0,0)	$Immm$ (No. 71) a/2+b/2,-1/2a+b/2,c;0,0,0	
DT: (0,1/2,0)(1/2,0,0)**(0,0,1/2)**	DT_1: (0,0,0,0,a,a)	$P4/nmm$ (No. 129) a/2-b/2,a/2+b/2,2c;1/4,0,-1/4	matrices of the irreps
	DT_3: (0,0,0,0,a,-a)	$P4_2/nmc$ (No. 137) a/2-b/2,a/2+b/2,2c;1/4,0,-1/4	
X: (0,1,0)(1,0,0)**(0,0,1)**	X_2^-: (0,0,a)	$P4_2/nmc$ (No. 137) a/2-b/2,a/2+b/2,c;0,1/4,1/4	matrices of the irreps
	X_3^-: (0,0,a)	$P4/nmm$ (No. 129) a/2-b/2,a/2+b/2,c;1/4,0,1/4	



Example: Fullerene-cubane crystal

Use the option *Get irreps* for the other possible symmetries

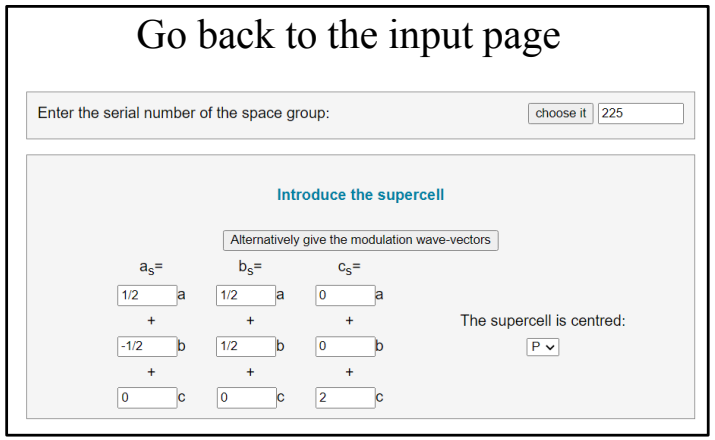
15	*Pnma* (No. 62)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
16	*Pmmn* (No. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
17	*Pccn* (No. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
18	*Pmma* (No. 51)	$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
19	*Pccm* (No. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
20	*Pmmm* (No. 47)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

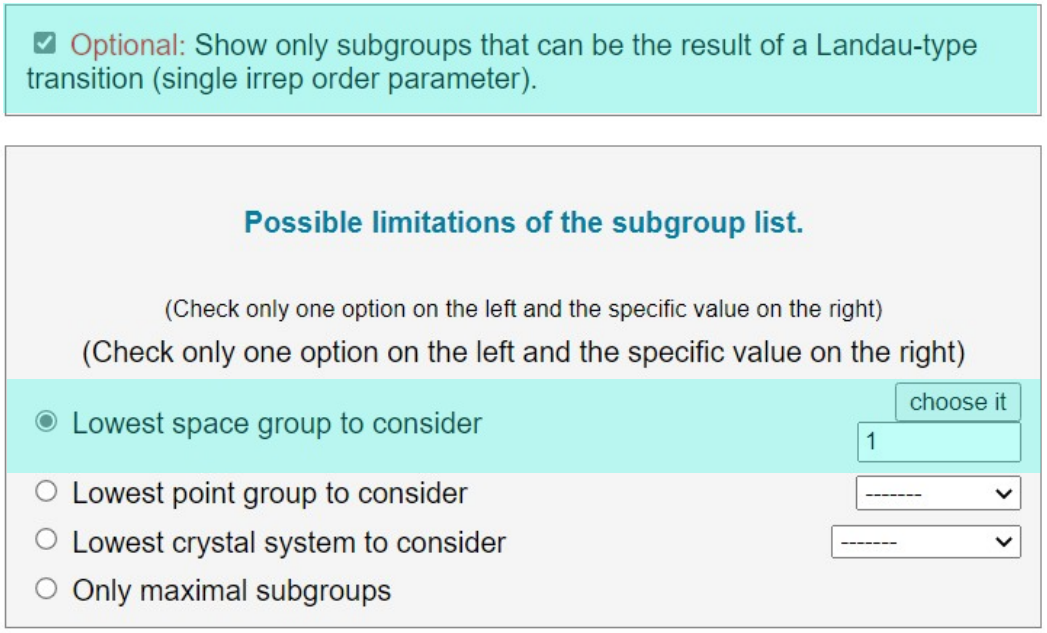
Only two of the symmetries can be result of a single irrep order parameter (fulfill the Landau condition)

$$\mathrm{Fm\text{-}3m} \xrightarrow{\mathbf{DT5}} \mathrm{Pnma}\ (-2c, -1/2a + 1/2b, 1/2a - 1/2b; 0, 1/4, -1/4)$$

$$\mathrm{Fm\text{-}3m} \xrightarrow{\mathbf{DT5}} \mathrm{Pmma}\ (-2c, 1/2a + 1/2b, 1/2a - 1/2b; 0, 0, 1/2)$$

Example: Fullerene-cubane crystal

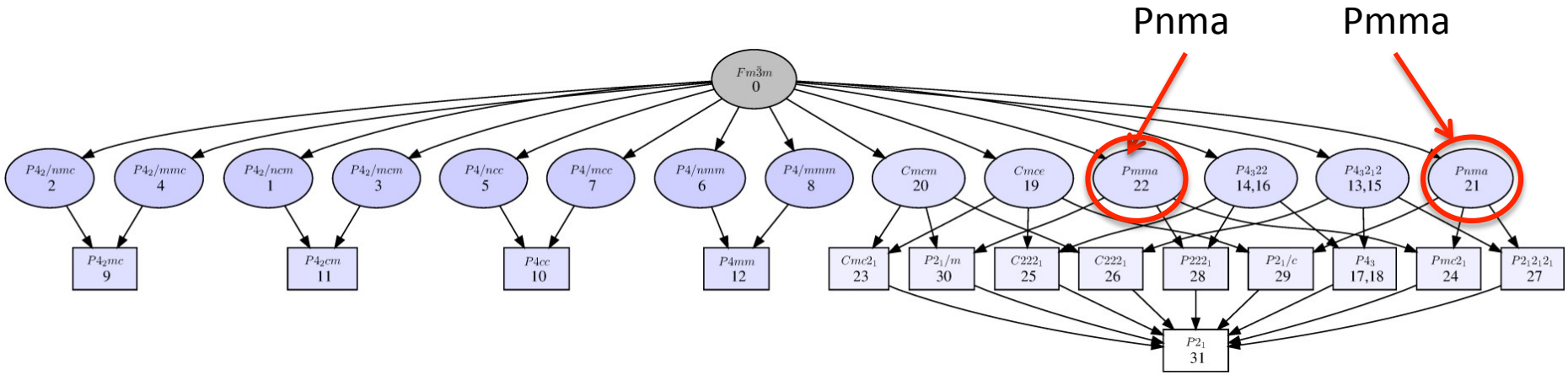




This option allows to discard all possible symmetries that cannot be reached by the action of a **single *irrep* distortion (a single order parameter)**

Example: Fullerene-cubane crystal

Landau-type possible symmetry breaks (one order parameter according to an irrep)



This condition reduces the number of possible distinct symmetries from 99 to 31

From the six-non-centered subgroups with point group mmm, only the subroups of type Pnma and Pmma appear

Structure transformation to a lower symmetry

TRANSTRU

Transform Structure

Transform Structure

TRANSTRU transforms the structure to the low symmetry space group basis, taking care of all possible splittings of the Wyckoff positions.

Structure

```
221
3.9064 3.9064 3.9064 90. 90. 90.
3
La      1       1a      0.000000        0.000000        0.000000
Co      1       1b      0.500000        0.500000        0.500000
O       1       3c      0.500000        0.500000        0.000000
```

Low symmetry Space Group *ITA* number: 15

Transformation Matrix:

In matrix form:

	Linear part			Origin Shift
	1	-1	-1	0
	2	0	0	1/2
	-1	-1	1	1/2

Show

Transformation of the set of operations forming the subgroup to standard setting of the space group

TRANSTRU is now linked directly with SUBGROUPS!

Input data

Subgroups of the space group : $Fm\bar{3}m$ (N. 225)
Lowest space group to consider: $P1$ (N. 1)
Supercell given by: (1/2,-1/2,0),(1/2,1/2,0),(0,0,2)
Centred supercell: No
Only subgroups compatible with a Landau-type transition

List of subgroups that can be the result of a Landau-type transition

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	TRANSTRU
1	$P4_2/ncm$ (No. 138)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	
2	$P4_2/nmc$ (No. 137)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	
3	$P4_2/mcm$ (No. 132)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	
4	$P4_2/mmc$ (No. 131)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	
5	$P4/ncc$ (No. 130)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	
6	$P4/nmm$ (No. 129)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \end{pmatrix}$	12=4x3	Conjugacy Class	Get irreps	

Pnma

Pmma

21	$Pnma$ (No. 62)	$\begin{pmatrix} 0 & -1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps	☑
22	$Pmma$ (No. 51)	$\begin{pmatrix} 0 & -1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps	☑
23	$Cmc2_1$ (No. 36)	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
24	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
25	$C222_1$ (No. 20)	$\begin{pmatrix} 1 & 0 & 0 & 1/4 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
26	$C222_1$ (No. 20)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
27	$P2_12_12_1$ (No. 19)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 1/8 \\ -1/2 & 1/2 & 0 & -1/8 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
28	$P222_1$ (No. 17)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
29	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1/2 & 0 & -1 & 0 \\ -1/2 & 0 & 0 & 1/4 \\ 0 & 2 & 0 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
30	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & -2 & 0 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps	
31	$P2_1$ (No. 4)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & -2 & 0 & 0 \end{pmatrix}$	96=4x24	Conjugacy Class	Get irreps	

* Clases with the same i superscript are conjugated through an improper symmetry operation.

Submit selected subgroups to TRANSTRU Submit

This example was already in one of our tutorials from 2010:

Tutorial_SPT_abr2010.pdf (can be downloaded from the BCS but obsolete)

2011

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Low Temperature Structure and Supramolecular Interactions of the C_{60}−Cubane Cocrystal

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ABSTRACT: The rotor−stator phase of the fullerene−cubane cocrystal, $C_{60}\cdot C_8H_8$, has an orientational ordering phase transition at around 140 K. On the basis of a simulated annealing analysis of the powder X-ray diffraction data, we determined the previously unknown crystal structure of the orthorhombic oriented phase: the space group is *Pnma*, the positions and the orientations of the constituent molecules significantly changed relative to the rock salt structure of the ambient temperature phase. The experimental structure is confirmed by cohesive energy calculations based on a pair potential method. Related structures, allowed by symmetry considerations, can be excluded by both the experiments and the calculations. The stability of the oriented phase is predominantly controlled by the nearest neighbor fullerene−fullerene and fullerene−cubane interactions.

This example was already in one of our tutorials from 2010:

Tutorial_SPT_abr2010.pdf (can be downloaded from the BCS but obsolete)

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Low Temperature Structure and Supramolecular Interactions of the C_{60}−Cubane Cocrystal

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More Examples:

More examples in the tutorial of SUBGROUPS that can be downloaded from the webpage of the program ...