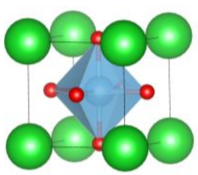
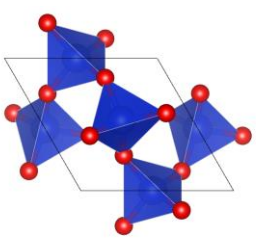
Crystal-Structure Tools

Crystallography Online: Workshop on the use and applications of the structural and magnetic tools of the Bilbao Crystallographic Server





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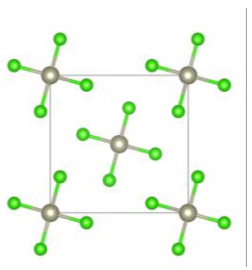

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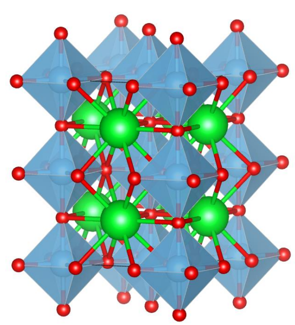
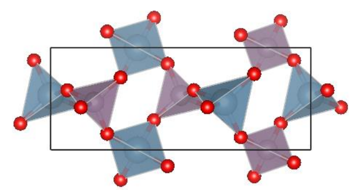
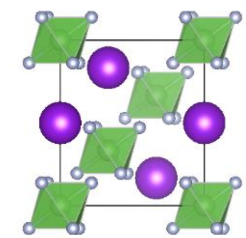


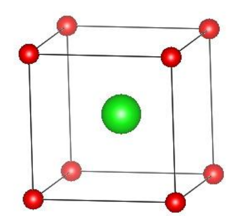
SUBGROUPS

TRANSTRU



EQUIVSTRU





POSSIBLE SYMMETRIES OF DISTORTED STRUCTURES

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

FCT/ZTF

bilbao crystallographic server

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-IncStrDB

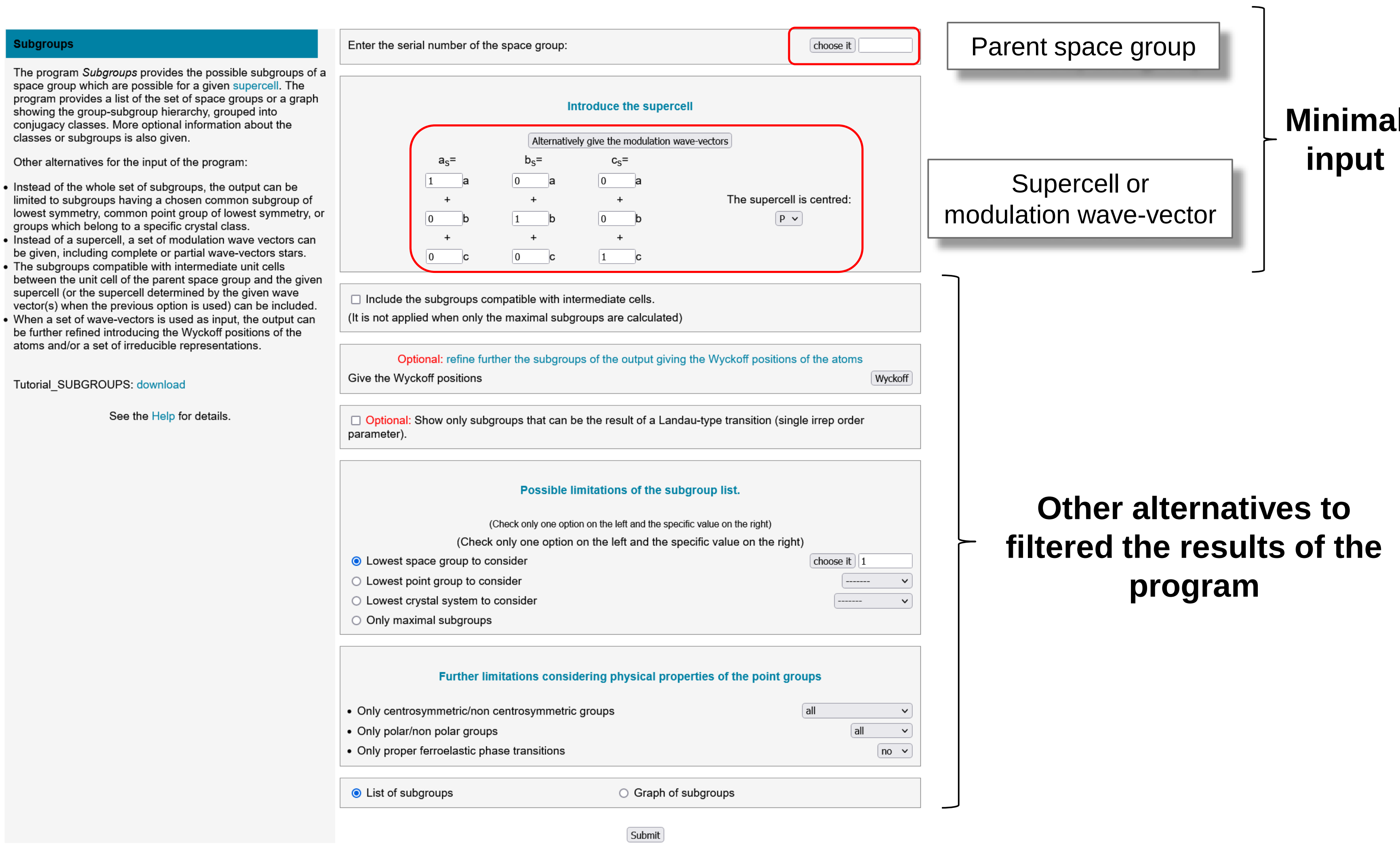
02/2022: New version of the

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


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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be included.
- When a set of wave-vectors is used as input, the output can be further refined introducing the Wyckoff positions of the atoms and/or a set of irreducible representations.

Tutorial_SUBGROUPS: download

See the Help for details.

Enter the serial number of the space group: choose it

Introduce the supercell

Alternatively give the modulation wave-vectors

a_s=	b_s=	c_s=
1 a	0 a	0 a
+	+	+
0 b	1 b	0 b
+	+	+
0 c	0 c	1 c

The supercell is centred: P

☐ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms
Give the Wyckoff positions — Wyckoff

☐ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

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 — -------
- ○ Only maximal subgroups

Further limitations considering physical properties of the point groups

- Only centrosymmetric/non centrosymmetric groups — all
- Only polar/non polar groups — all
- Only proper ferroelastic phase transitions — no

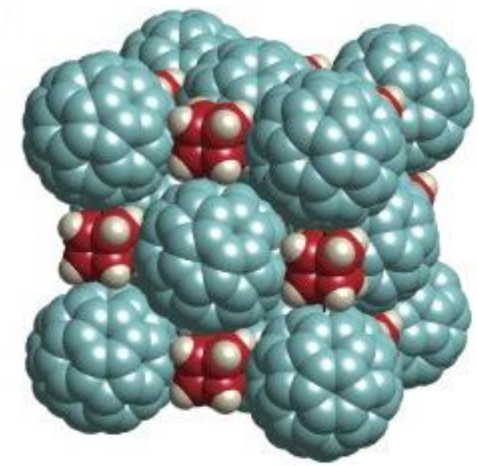
◉ List of subgroups ○ Graph of subgroups

Submit

Example 1: Fullerene-cubane crystal

High-temperature phase

$Fm\bar{3}m$ (No. 225)



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

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

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

Power diffraction experiments

Low-temperature phase

?

Orthorhombic structure

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

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

Restrict the symmetry of the low-symmetry phase to a minimal set of most probable space groups

Example 1: Fullerene-cubane crystal (a)

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

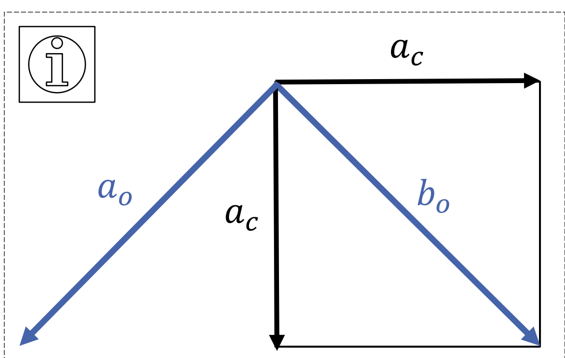
Enter the serial number of the space group: choose it 225

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 1: Fullerene-cubane crystal (a)

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

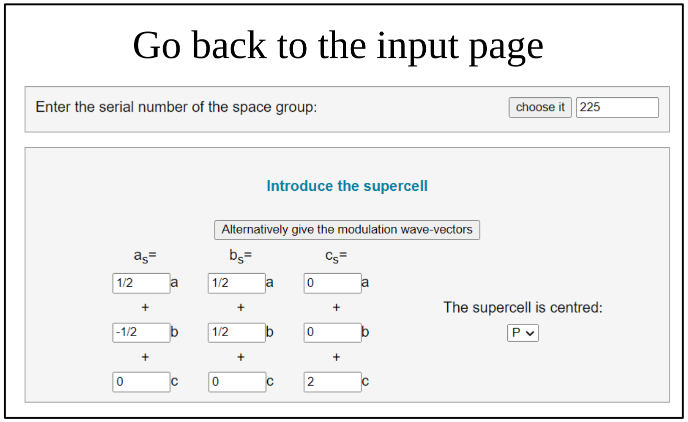
Input data

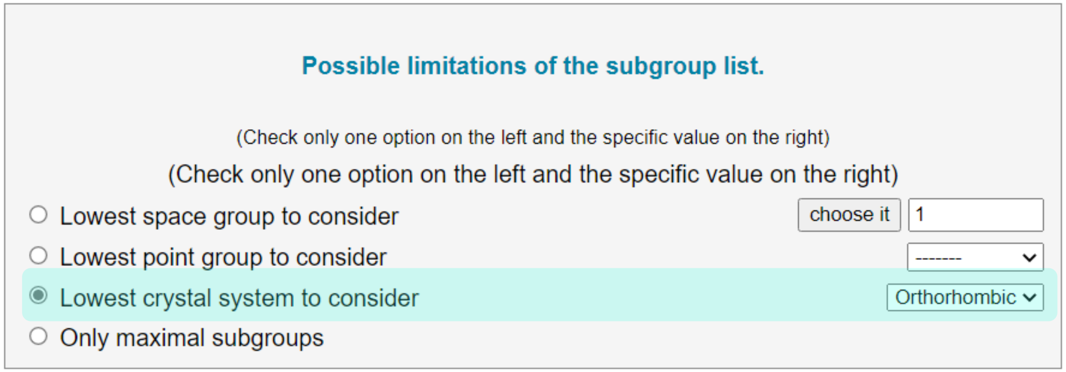
Subgroups of the space group :	$Fm\bar{3}m$ (N. 225)
Lowest space group to consider:	$P1$ (N. 1)
Supercell given by:	(1/2,-1/2,0),(1/2,1/2,0),(0,0,2)
Centred supercell:	No

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

99 subgroups

Example 1: Fullerene-cubane crystal (a)





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
60	$P2_12_12$ (No. 18)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
61	$P222_1$ (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
62	$P222$ (No. 16)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps

The list of maximal 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 1: Fullerene-cubane crystal (b)

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= 1/2 a + -1/2 b + 0 c

b_s= 1/2 a + 1/2 b + 0 c

c_s= 0 a + 0 b + 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

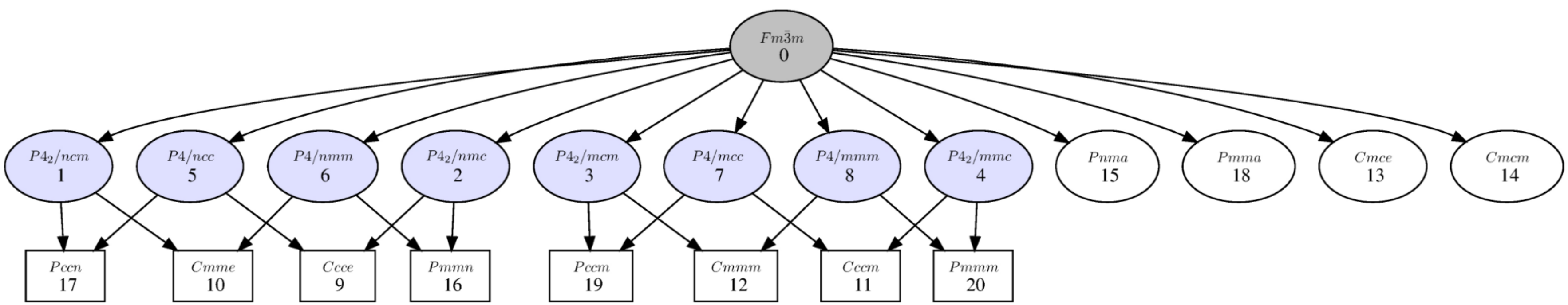
Example 1: Fullerene-cubane crystal (b)

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 1: Fullerene-cubane crystal (b)

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 (rows 1–8)

C centered orthorhombic (rows 9–14)

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

6 possible symmetries

Example 1: Fullerene-cubane crystal (c)

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)	*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_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)	*P4/nmm* (No. 129) a/2-b/2,a/2+b/2,c;1/4,0,1/4	

The symmetry break

$$Fm\bar{3}m \longrightarrow Pnma$$

can be realized through a Landau type phase transition

Example 1: Fullerene-cubane crystal (d)

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

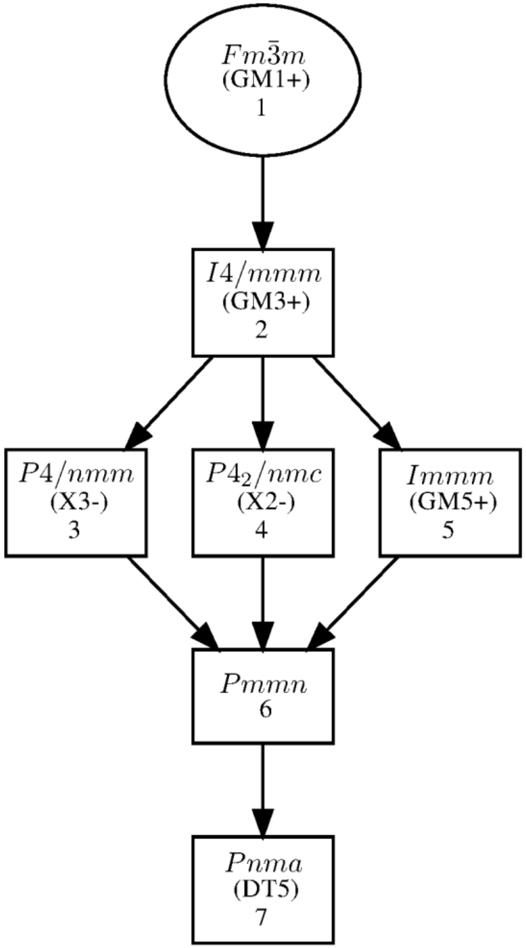
Input data

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)	*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_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)	*P4/nmm* (No. 129) a/2-b/2,a/2+b/2,c;1/4,0,1/4	



Example 1: Fullerene-cubane crystal (e)

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)

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

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

Example 1: Fullerene-cubane crystal (f)

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

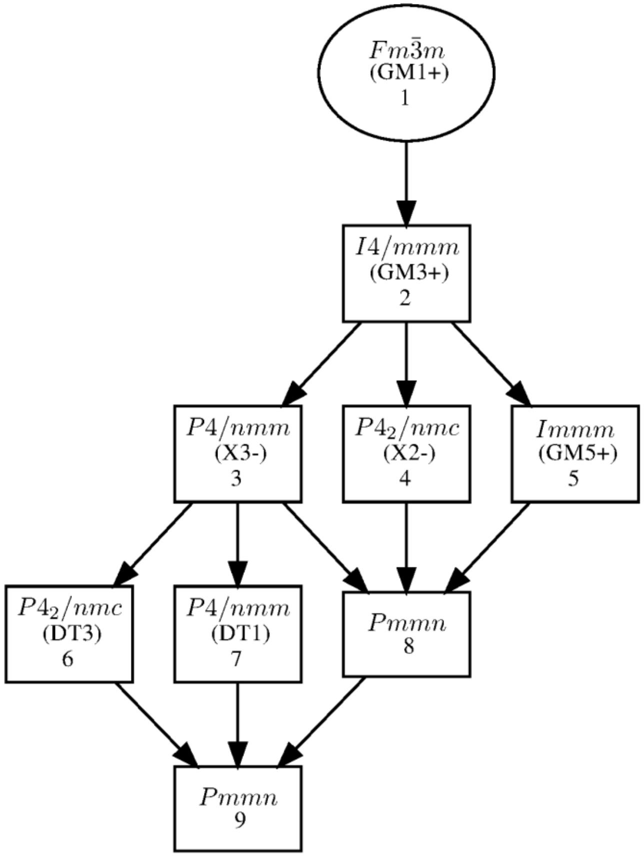
Input data

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)	*P*4_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)	*P*4_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	



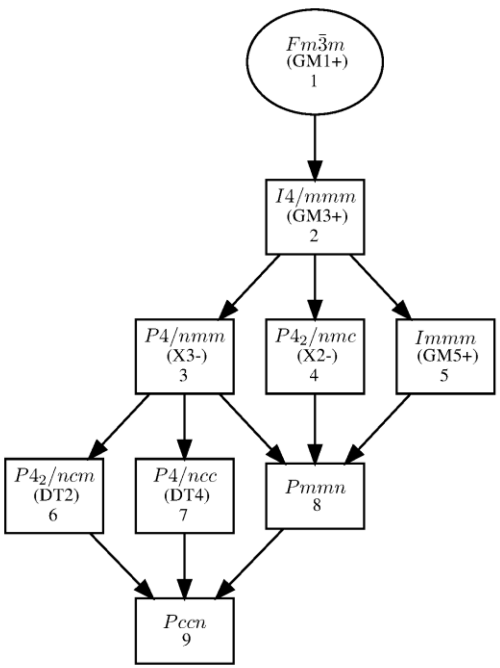
Example 1: Fullerene-cubane crystal (g)

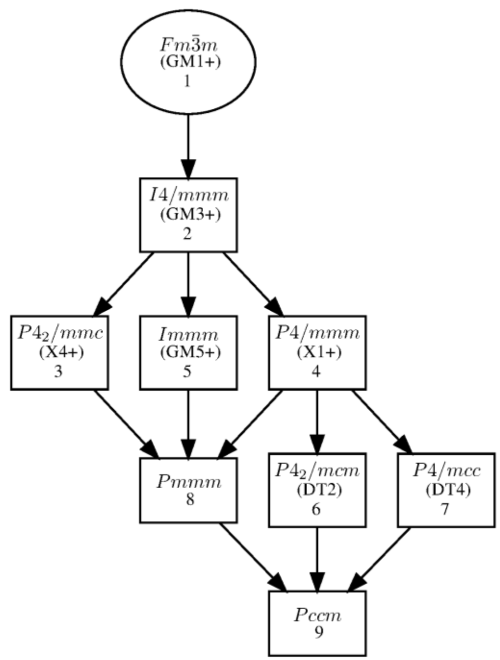
Do the same process as in the previous step for the other 3 possible symmetries

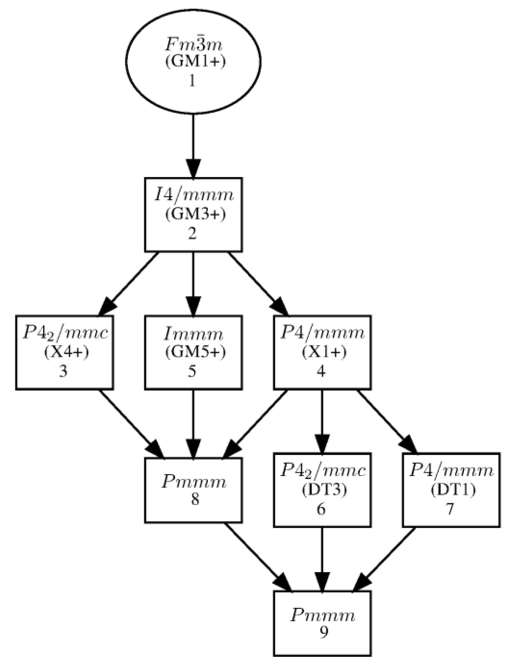
Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→$Pccn$ (N. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$

Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→$Pccm$ (N. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$

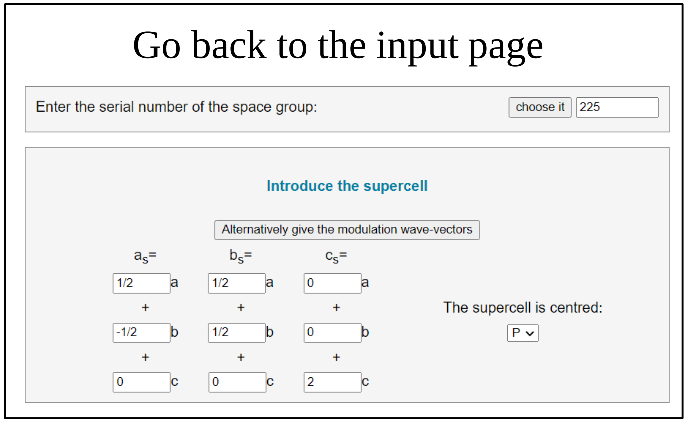
Group→subgroup	Transformation matrix
$Fm\bar{3}m$ (N. 225)→$Pmmm$ (N. 47)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$

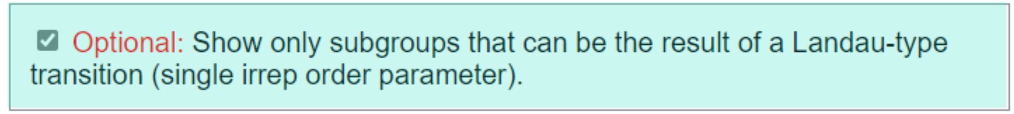


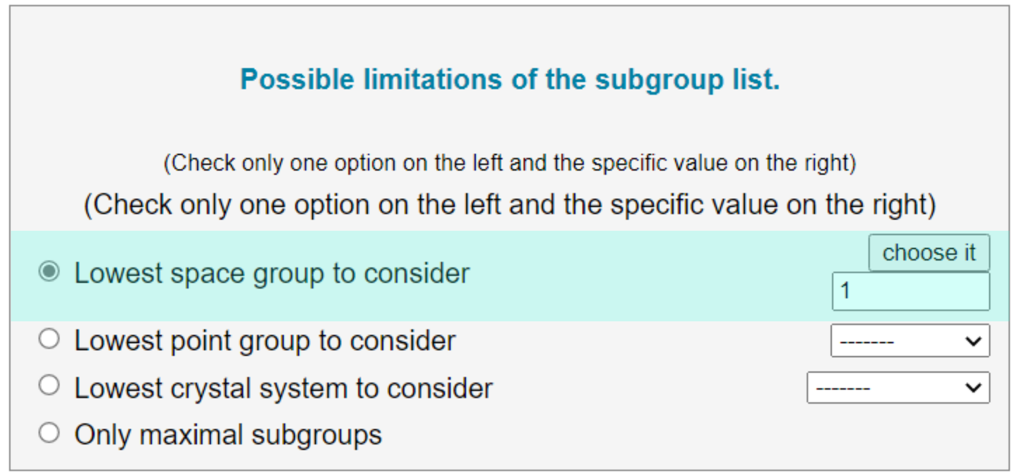




Example 1: Fullerene-cubane crystal (h)

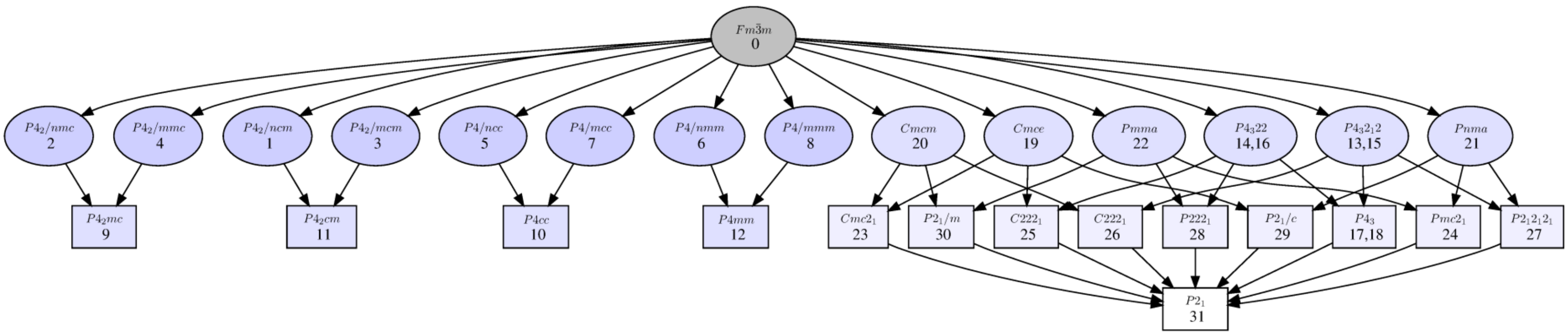






This option allows to discard all possible symmetries that cannot be reached by the action of a **single *irrep* distortion**

Example 1: Fullerene-cubane crystal (h)



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 here

Example 2: Parent space group $\boldsymbol{Pnma}$

Let us suppose that we observe a structure with symmetry $Pnma$, which exhibits when lowering the temperature a phase transition. Diffraction experiments in the low symmetry phase give evidence of superstructure reflections, which can be indexes as $(h, k, l + 1/2)$.

This additional diffraction peaks indicates a **distortion** $\Longrightarrow$ duplication of the c parameter

Modulation wave vector (0, 0, 1/2)

We wish to know the possible space group symmetries that this low temperature phase can have, in order to construct structural models that could fit the diffraction data

Example 2: Parent space group $Pnma$ (a)

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.

Enter the serial number of the space group: choose it 62

Introduce the supercell

Alternatively give the modulation wave-vectors

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

The supercell is centred: P

. . .

◉ List of subgroups ○ Graph of subgroups

Submit

Example 2: Parent space group *Pnma* (a)

Input data

Subgroups of the space group :	*Pnma* (N. 62)
Lowest space group to consider:	*P*1 (N. 1)
Supercell given by:	(1,0,0),(0,1,0),(0,0,2)
Centred supercell:	No

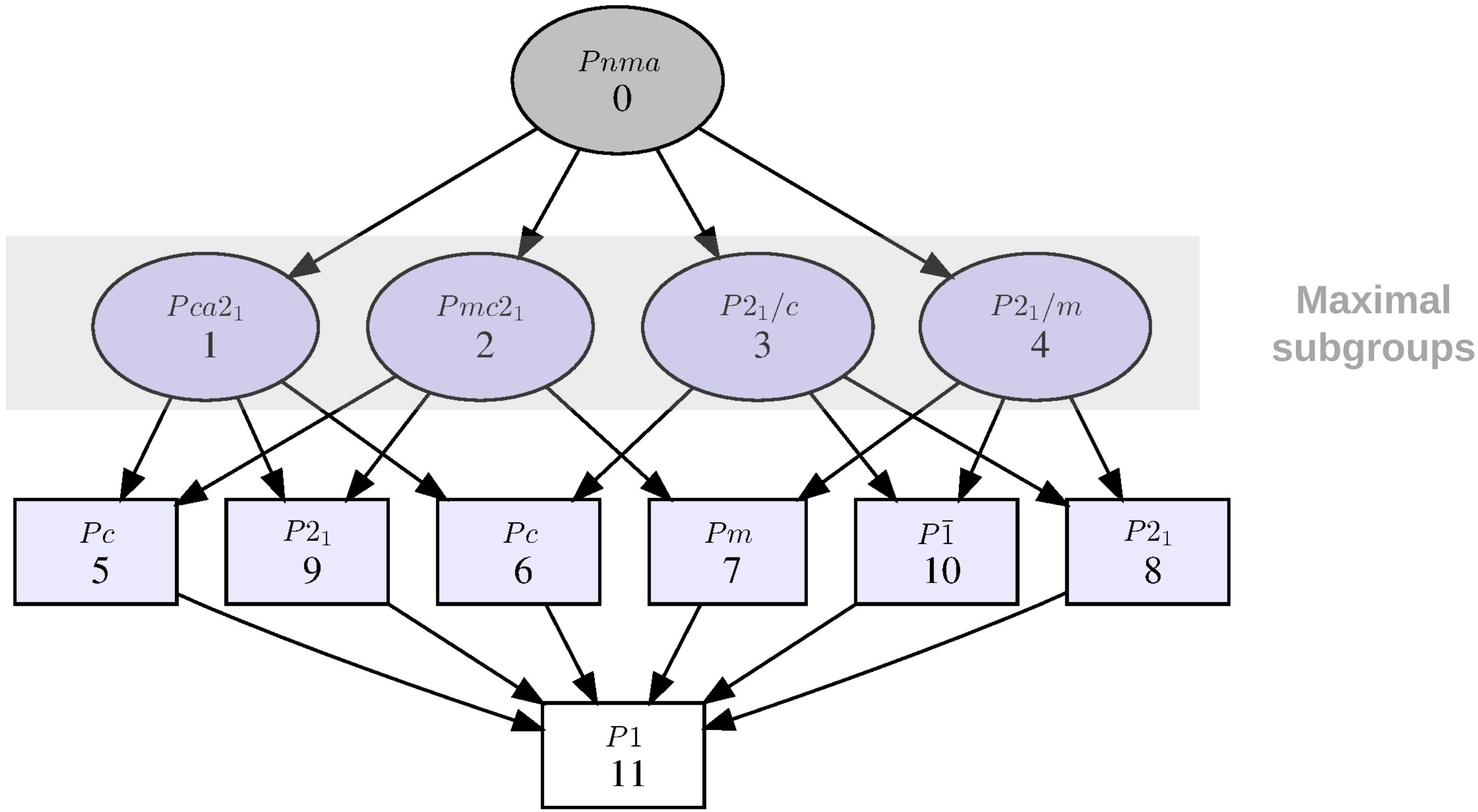
List of subgroups that fulfill the given conditions

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
5	Pc (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
7	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
8	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
9	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
10	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
11	$P1$ (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps

Without any additional restriction the program lists 11 possible space group symmetries

Example 2: Parent space group $Pnma$ (b)



Example 2: Parent space group *Pnma* (b)

Go back to the input page

Possible limitations of the subgroup list.

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

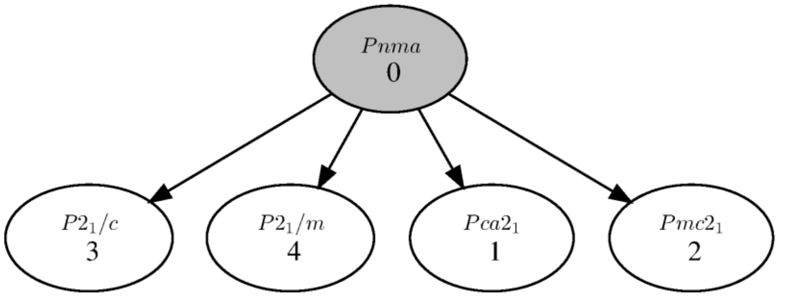
(Check only one option on the left and the specific value on the right)

- ○ Lowest space group to consider — choose it — 1
- ○ Lowest point group to consider — -------
- ○ Lowest crystal system to consider — -------
- ◉ 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	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps



Example 2: Parent space group *Pnma* (c)

Go back to the input page

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)

- (selected) Lowest space group to consider — [choose it] [1]
- Lowest point group to consider — [--------]
- Lowest crystal system to consider — [--------]
- Only maximal subgroups

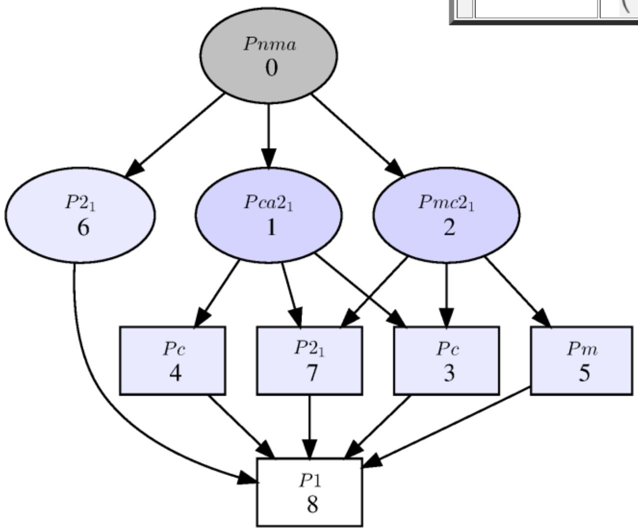
Further limitations considering physical properties of the point groups

- Only centrosymmetric/non centrosymmetric groups — [all]
- Only polar/non polar groups — [Polar]
- Only proper ferroelastic phase transitions — [no]

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	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	Pc (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
4	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
5	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
7	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
8	$P1$ (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps



Example 2: Parent space group *Pnma* (d)

Go back to the input page

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)

- (selected) Lowest space group to consider — choose it — 1
- Lowest point group to consider — --------
- Lowest crystal system to consider — --------
- Only maximal subgroups

Further limitations considering physical properties of the point groups

- Only centrosymmetric/non centrosymmetric groups — all
- Only polar/non polar groups — all
- Only proper ferroelastic phase transitions — no

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
5	Pc (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
7	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
8	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
9	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
10	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
11	$P1$ (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*Pnma* (No. 62) a,b,c;0,0,0	matrices of the irreps
	GM_3^-: (a)	$Pmc2_1$ (No. 26) b,-c,-a;0,1/4,1/4	
Z: **(0,0,1/2)**	Z_2: (a,a)	$Pca2_1$ (No. 29) -2c,b,a;0,1/4,-1/4	matrices of the irreps

Example 2: Parent space group *Pnma* (e)

Go back to the input page

☑ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

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 [-------]
- ○ Only maximal subgroups

Further limitations considering physical properties of the point groups

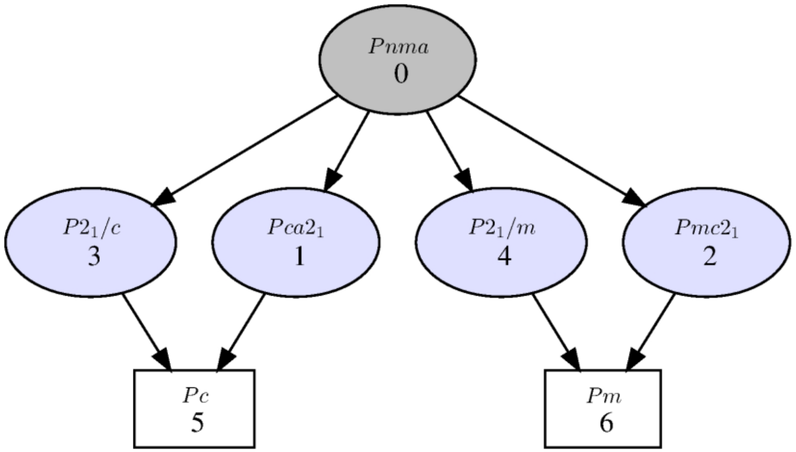
- Only centrosymmetric/non centrosymmetric groups [all]
- Only polar/non polar groups [all]
- Only proper ferroelastic phase transitions [no]

◉ List of subgroups ○ Graph of subgroups

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
1	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
5	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps



Example 2: Parent space group *Pnma* (f)

Go back to the input page

Enter the serial number of the space group: 62 [choose it]

Introduce the supercell

[Alternatively give the modulation wave-vectors]

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

The supercell is centred: P

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.

Enter the serial number of the space group: 62 [choose it]

Introduce the wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 0 k_{1y} 0 k_{1z} 1/2

Show the independent vectors of the star

☐ Choose the whole star of the propagation vector

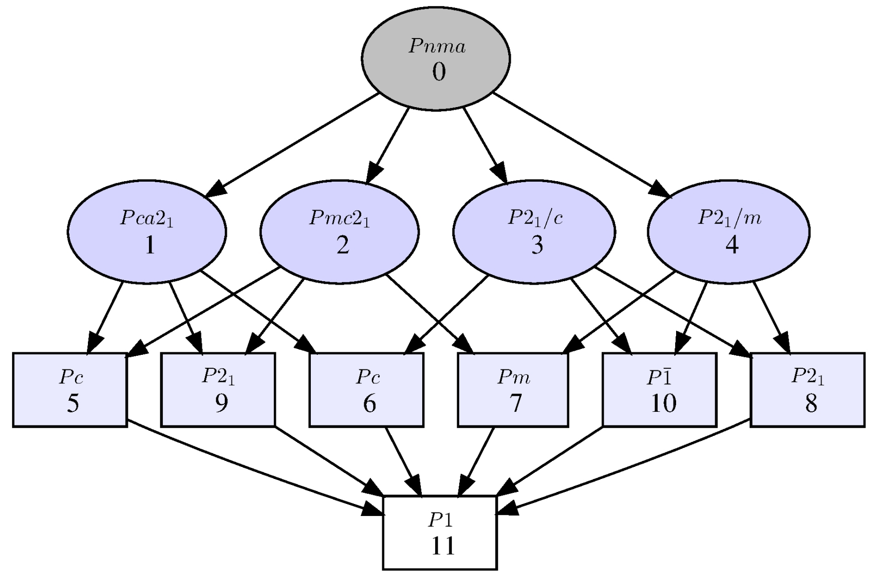
[More wave-vectors needed]

Example 2: Parent space group $Pnma$ (g)

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	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
5	Pc (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
7	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
8	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
9	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
10	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
11	$P1$ (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps



Example 2: Parent space group $Pnma$ (h)

Go back to the input page

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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be included.
- When a set of wave-vectors is used as input, the output can be further refined introducing the Wyckoff positions of the atoms and/or a set of irreducible representations.

Enter the serial number of the space group: [62] [choose it]

Introduce the wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} [0] k_{1y} [0] k_{1z} [1/2]

Show the independent vectors of the star

☐ Choose the whole star of the propagation vector

[More wave-vectors needed]

☐ Include the subgroups compatible with intermediate cells.

(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms

Give the Wyckoff positions [Wyckoff]

☐ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Optional: refine further the subgroups of the output giving a set of irreps

Choose the irreps [Representations]

Example 2: Parent space group *Pnma* (h)

The possible irreps that can describe such type of distortion

Space group: (No. 62)
Choose the irreducible representation(s) for each modulation vector

If no Wyckoff position has been given, a general position will be assumed

Possible irreducible representations

Wave-vectors of the star (1 vector):
Z:(0,0,1/2)
Descomposition of the mechanical representation(s) into irreps.
8d:(x,y,z) → 6×Z1(2) ⊕ 6×Z2(2)
Choose the representation(s)

irreps:	☐ Z1(2) ☐ Z2(2)

(In parentheses, the dimensions of the irreducible representations of the little group of k)

Submit

Example 2: Parent space group $Pnma$ (i)

Space group: (No. 62)
Choose the irreducible representation(s) for each modulation vector

If no Wyckoff position has been given, a general position will be assumed

Possible irreducible representations

Wave-vectors of the star (1 vector):

Z:(0,0,1/2)

Descomposition of the mechanical representation(s) into irreps.

8d:(x,y,z) → 6×Z1(2) ⊕ 6×Z2(2)

Choose the representation(s)

irreps:	☑ Z1(2) ☐ Z2(2)

(In parentheses, the dimensions of the irreducible representations of the little group of k)

Submit

Example 2: Parent space group *Pnma* (i)

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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be included.
- When a set of wave-vectors is used as input, the output can be further refined introducing the Wyckoff positions of the atoms and/or a set of irreducible representations.

Tutorial_SUBGROUPS: download

See the Help for details.

Space group: (No. 62)

Set of chosen modulation wave-vectors

k_1=(0,0,1/2)

☐ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Chosen representations

Z:(0,0,1/2) Z1(2)

Optional: 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)

choose it

- ◉ Lowest space group to consider [1]
- ○ Lowest point group to consider [-------]
- ○ Lowest crystal system to consider [-------]
- ○ Only maximal subgroups

Optional: further limitations considering physical properties of the point groups

- Only centrosymmetric / non-centrosymmetric groups [all]
- Only polar / non-polar groups [all]
- Only proper ferroelastic phase transitions [no]
  (This option is incompatible with the previous two options and with the selection of representations)

◉ List of subgroups ○ Graph of subgroups

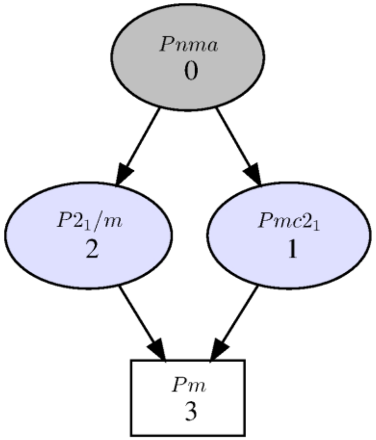
Submit

List of subgroups compatible which have as primary irreps all the irreps given

Get the subgroup-graph More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps

The list of possible symmetries is now reduced to three



The other three possible symmetries correspond to the other possible irreps Z2

Example 2: Parent space group $Pnma$ (i)

Space group: (No. 62)
Choose the irreducible representation(s) for each modulation vector

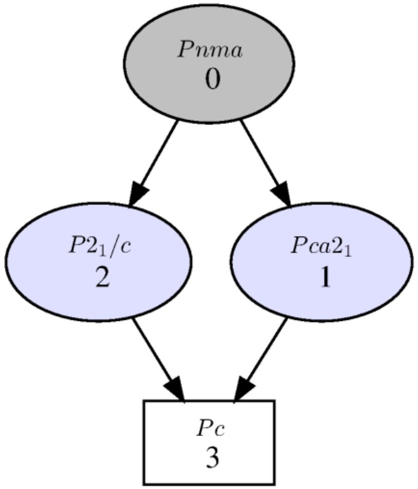
If no Wyckoff position has been given, a general position will be assumed

Possible irreducible representations

Wave-vectors of the star (1 vector):
Z:(0,0,1/2)
Descomposition of the mechanical representation(s) into irreps.
8d:(x,y,z) → 6×Z1(2) ⊕ 6×Z2(2)
Choose the representation(s)
irreps: ☐ Z1(2) ☑ Z2(2)
(In parentheses, the dimensions of the irreducible representations of the little group of k)

Submit

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps



Example 2: Parent space group $Pnma$ (j)

Space group: (No. 62)
Choose the irreducible representation(s) for each modulation vector

If no Wyckoff position has been given, a general position will be assumed

Possible irreducible representations

Wave-vectors of the star (1 vector):
Z:(0,0,1/2)
Descomposition of the mechanical representation(s) into irreps.
8d:(x,y,z) → 6×Z1(2) ⊕ 6×Z2(2)
Choose the representation(s)

irreps:	☑ Z1(2) ☑ Z2(2)

(In parentheses, the dimensions of the irreducible representations of the little group of k)

Submit

Example 2: Parent space group $Pnma$ (j)

Input data

Subgroups of the space group :	*Pnma* (N. 62)
Lowest space group to consider:	*P*1 (N. 1)
Modulation wave-vectors	(0,0,1/2)
Irreducible representations	
Z:(0,0,1/2)	Z1,Z2

List of subgroups compatible which have as primary irreps all the irreps given

Get the subgroup-graph More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	*Pc* (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
2	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
3	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
4	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
5	*P*1 (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps

The list is reduced to 5 subgroups that were not listed when choosing separately Z1 and Z2 as single active irreps

Example 2: Parent space group *Pnma* (j)

○	**All** irreps should be active to reach the subgroup.
◉	**At least one** irrep should be active to reach the subgroup.

Submit

List of subgroups compatible which have as primary irreps some of the given irreps

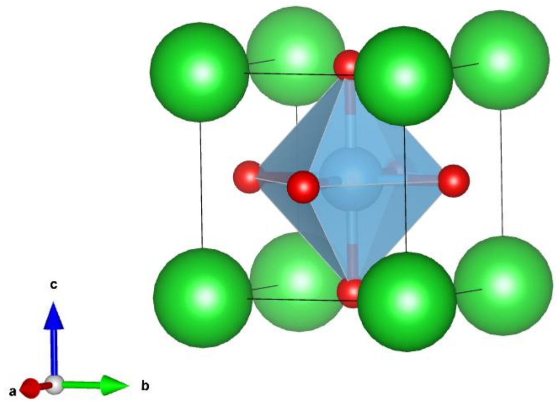
Get the subgroup-graph | More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$Pca2_1$ (No. 29)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1/4 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
2	$Pmc2_1$ (No. 26)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
3	$P2_1/c$ (No. 14)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
4	$P2_1/m$ (No. 11)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	4=2x2	Conjugacy Class	Get irreps
5	Pc (No. 7)	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -2 & 0 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
6	Pc (No. 7)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
7	Pm (No. 6)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
8	$P2_1$ (No. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
9	$P2_1$ (No. 4)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
10	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
11	$P1$ (No. 1)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	16=2x8	Conjugacy Class	Get irreps

Example 3: Perovskite

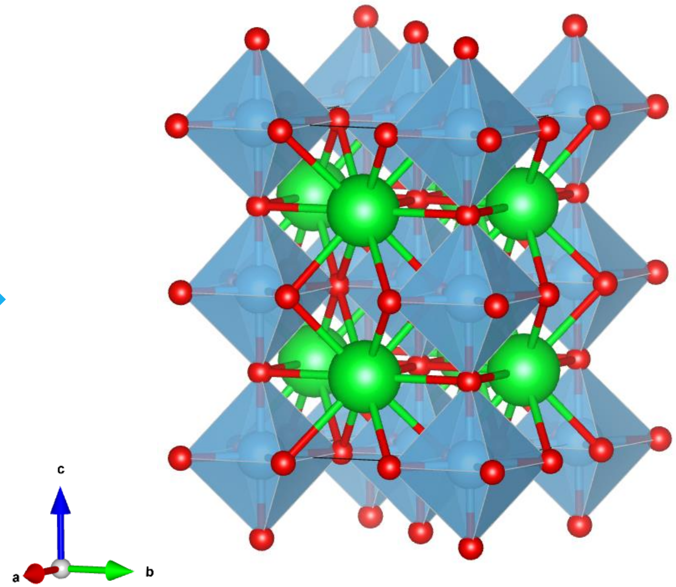
$SrTiO_3$

$Pm\bar{3}m$ (No. 221)



105 K

$I4/mcm$ (No. 140)



$$(\boldsymbol{a}_P + \boldsymbol{b}_P, -\boldsymbol{a}_P + \boldsymbol{b}_P, 2\boldsymbol{c}_P; 0, 0, 0)$$

All possible symmetries that can occur in a perovskite duet to unstable rigid-unit modes

Example 3: Perovskite(a)

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.

Enter the serial number of the space group: 221 [choose it]

Introduce the supercell

[Alternatively give the modulation wave-vectors]

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

The supercell is centred: I

98 subgroups are possible

◉ List of subgroups ○ Graph of subgroups

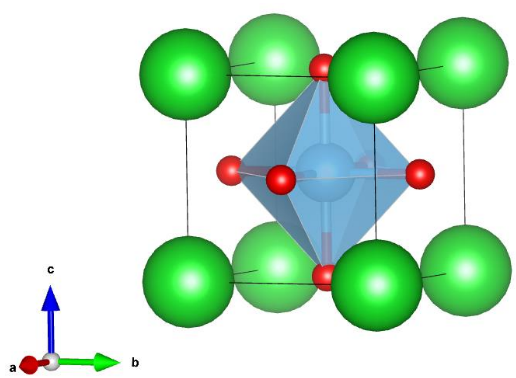
[Submit]

Example 3: Perovskite (b)

Go back to the input page

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms

Give the Wyckoff positions [Wyckoff]



221
3.9064 3.9064 3.9064 90. 90. 90.
3
Sr 1 1a 0 0 0
Ti 1 1b 0.5 0.5 0.5
O 1 3c 0.5 0.5 0

Space group $Pm\bar{3}m$ (No. 221)
Check the type of Wyckoff positions of the atoms

	Multiplicity	Wyckoff Letter	Coordinates
☐	48	n	(x,y,z),(x,-z,y),(x,z,-y),(z,y,-x) (-z,y,x),(-y,x,z),(y,-x,z),(x,-y,-z) (-x,y,-z),(-x,-y,z),(y,x,-z),(-y,-x,-z) (-x,z,y),(-x,-z,-y),(z,-y,x),(-z,-y,-x) (z,x,y),(y,z,x),(-y,z,-x),(-z,-x,y) (-y,-z,x),(z,-x,-y),(y,-z,-x),(-z,x,-y) (-x,-y,-z),(-x,z,-y),(-x,-z,y),(-z,-y,x) (z,-y,-x),(y,-x,-z),(-y,x,-z),(-x,y,z) (x,-y,z),(x,y,-z),(-y,-x,z),(y,x,z) (x,-z,-y),(x,z,y),(-z,y,-x),(z,y,x) (-z,-x,-y),(-y,-z,-x),(y,-z,x),(z,x,-y) (y,z,-x),(-z,x,y),(-y,z,x),(z,-x,y)
☐	24	m	(x,x,z),(x,-z,x),(x,z,-x),(z,x,-x) (-z,x,x),(-x,x,z),(x,-x,z),(x,-x,-z) (-x,x,-z),(-x,-x,z),(x,x,-z),(-x,-x,-z) (-x,z,x),(-x,-z,-x),(z,-x,x),(-z,-x,-x) (z,x,x),(x,z,x),(-x,z,-x),(-z,-x,x) (-x,-z,x),(z,-x,-x),(x,-z,-x),(-z,x,-x)
☐	24	l	(1/2,y,z),(1/2,-z,y),(1/2,z,-y),(z,y,1/2) (-z,y,1/2),(-y,1/2,z),(y,1/2,z),(1/2,-y,-z) (1/2,y,-z),(1/2,-y,z),(y,1/2,-z),(-y,1/2,-z) (1/2,z,y),(1/2,-z,-y),(z,-y,1/2),(-z,-y,1/2) (z,1/2,y),(y,z,1/2),(-y,z,1/2),(-z,1/2,y) (-y,-z,1/2),(z,1/2,-y),(y,-z,1/2),(-z,1/2,-y)
☐	24	k	(0,y,z),(0,-z,y),(0,z,-y),(z,y,0) (-z,y,0),(-y,0,z),(y,0,z),(0,-y,-z) (0,y,-z),(0,-y,z),(y,0,-z),(-y,0,-z) (0,z,y),(0,-z,-y),(z,-y,0),(-z,-y,0) (z,0,y),(y,z,0),(-y,z,0),(-z,0,y) (-y,-z,0),(z,0,-y),(y,-z,0),(-z,0,-y)
☐	12	j	(1/2,y,y),(1/2,-y,y),(1/2,y,-y),(y,y,1/2) (-y,y,1/2),(-y,1/2,y),(y,1/2,y),(1/2,-y,-y) (y,1/2,-y),(-y,1/2,-y),(y,-y,1/2),(-y,-y,1/2)
☐	12	i	(0,y,y),(0,-y,y),(0,y,-y),(y,y,0) (-y,y,0),(-y,0,y),(y,0,y),(0,-y,-y) (y,0,-y),(-y,0,-y),(y,-y,0),(-y,-y,0)
☐	12	h	(x,1/2,0),(x,0,1/2),(0,1/2,-x),(0,1/2,x) (1/2,x,0),(1/2,-x,0),(-x,1/2,0),(-x,0,1/2) (0,x,1/2),(1/2,0,x),(1/2,0,-x),(0,-x,1/2)
☐	8	g	(x,x,x),(x,-x,x),(x,x,-x),(-x,x,x) (x,-x,-x),(-x,x,-x),(-x,-x,x),(-x,-x,-x)
☐	6	f	(x,1/2,1/2),(1/2,1/2,-x),(1/2,1/2,x) (1/2,x,1/2),(1/2,-x,1/2),(-x,1/2,1/2)
☐	6	e	(x,0,0),(0,0,-x),(0,0,x) (0,x,0),(0,-x,0),(-x,0,0)
☑	3	d	(1/2,0,0),(0,0,1/2),(0,1/2,0)
☐	3	c	(0,1/2,1/2),(1/2,1/2,0),(1/2,0,1/2)
☑	1	b	(1/2,1/2,1/2)
☑	1	a	(0,0,0)

☐ Do not consider subgroups attainable only through strain-like distortions

[Submit]

The list is reduced to 68

Example 3: Perovskite (c)

Enter the serial number of the space group: [choose it] 221

Introduce the supercell

[Alternatively give the modulation wave-vectors]

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

The supercell is centred: I

☐ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

☐ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Wyckoff positions of the atoms
3d:(1/2,0,0)
1b:(1/2,1/2,1/2)
1a:(0,0,0)

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 --------
◉ Only maximal subgroups

List of possible subgroups assuming the given wyckoff positions

[Get the subgroup-graph] [More options]

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	*Fm*$\bar{3}$*c* (No. 226)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps
2	*Fm*$\bar{3}$*c* (No. 226)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 2 & 0 & 1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps
3	*Fm*$\bar{3}$*m* (No. 225)	$\begin{pmatrix} 2 & 0 & 0 & 1/2 \\ 0 & 2 & 0 & 1/2 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps
4	*Fm*$\bar{3}$*m* (No. 225)	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	2=2x1	Conjugacy Class	Get irreps
5	*I4/mcm* (No. 140)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
6	*I4/mcm* (No. 140)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 0 & 0 & -2 & 1/2 \\ 1 & 1 & 0 & 1/2 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
7	*I4/mmm* (No. 139)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 1/2 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
8	*I4/mmm* (No. 139)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 1/2 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
9	*Imma* (No. 74)	$\begin{pmatrix} 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 1/2 \\ 2 & 0 & 0 & 0 \end{pmatrix}$	12=2x6	Conjugacy Class	Get irreps
10	*Imma* (No. 74)	$\begin{pmatrix} 0 & 1 & -1 & 1/2 \\ 0 & 1 & 1 & 0 \\ 2 & 0 & 0 & 1/2 \end{pmatrix}$	12=2x6	Conjugacy Class	Get irreps

Example 3: Perovskite (d)

Subgroups that belong to the same conjugacy class, limited to those compatible with the given supercell or the supercell determined by the given wave vector(s).

N	Group Symbol	Transformation matrix	Group-Subgroup index	Symmetry operations	Set of subgroups*	irreps
5.1	*I*4/*mcm* (No. 140)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Plain text format Matrix form	List of subgroups Graph of subgroups	Get irreps
5.2	*I*4/*mcm* (No. 140)	$\begin{pmatrix} 0 & 0 & 2 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Plain text format Matrix form	List of subgroups Graph of subgroups	Get irreps
5.3	*I*4/*mcm* (No. 140)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	6=2x3	Plain text format Matrix form	List of subgroups Graph of subgroups	Get irreps

* List or graph of subgroups that are related with the chosen group through group-subgroup relation.

Example 3: Perovskite (e)

Group→subgroup	Transformation matrix
$Pm\bar{3}m$ (N. 221)→$I4/mcm$ (N. 140)	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$

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)	$Pm\bar{3}m$ (No. 221) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,0)	$P4/mmm$ (No. 123) a,b,c;0,0,0	
R: **(1/2,1/2,1/2)**	R_4^+: (a,0,0)	$I4/mcm$ (No. 140) a-b,a+b,2c;0,0,0	matrices of the irreps

Example 3: Perovskite (f)

Group→subgroup	Transformation matrix
$Pm\bar{3}m$ (N. 221)→$I4/mcm$ (N. 140)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$

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)	$Pm\bar{3}m$ (No. 221) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,-($\sqrt{3}$ a))	$P4/mmm$ (No. 123) a,-c,b;0,0,0	
R: **(1/2,1/2,1/2)**	R_4^+: (0,0,a)	$I4/mcm$ (No. 140) a+c,-a+c,-2b;0,0,0	matrices of the irreps

Group→subgroup	Transformation matrix
$Pm\bar{3}m$ (N. 221)→$I4/mcm$ (N. 140)	$\begin{pmatrix} 0 & 0 & 2 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}$

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)	$Pm\bar{3}m$ (No. 221) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,$\sqrt{3}$ a)	$P4/mmm$ (No. 123) -c,b,a;0,0,0	
R: **(1/2,1/2,1/2)**	R_4^+: (0,a,0)	$I4/mcm$ (No. 140) b-c,b+c,2a;0,0,0	matrices of the irreps

The direction changed for the R_4^+

Example 3: Perovskite (g)

Go back to the input page

Enter the serial number of the space group: [choose it] 221

Introduce the supercell

[Alternatively give the modulation wave-vectors]

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

The supercell is centred: I

☐	6	f	(1/2,x,1/2),(1/2,-x,1/2),(-x,1/2,1/2)
☐	6	e	(x,0,0),(0,0,-x),(0,0,x) (0,x,0),(0,-x,0),(-x,0,0)
☑	3	d	(1/2,0,0),(0,0,1/2),(0,1/2,0)
☐	3	c	(0,1/2,1/2),(1/2,1/2,0),(1/2,0,1/2)
☑	1	b	(1/2,1/2,1/2)
☑	1	a	(0,0,0)

☐ Do not consider subgroups attainable only through strain-like distortions

[Submit]

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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be

Enter the serial number of the space group: [choose it] 221

Introduce the wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 1/2 k_{1y} 1/2 k_{1z} 1/2

Show the independent vectors of the star

☐ Choose the whole star of the propagation vector

[More wave-vectors needed]

☐ Include the subgroups compatible with intermediate cells.

(It is not applied when only the maximal subgroups are calculated)

Optional: refine further the subgroups of the output giving the Wyckoff positions of the atoms

Give the Wyckoff positions [Wyckoff]

Example 3: Perovskite (g)

Go back to the input page

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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be included.
- When a set of wave-vectors is used as input, the output can be further refined introducing the Wyckoff positions of the atoms and/or a set of irreducible representations.

Tutorial_SUBGROUPS: download

See the Help for details.

Space group: $Pm\bar{3}m$ (No. 221)

Set of chosen modulation wave-vectors

k_1=(1/2,1/2,1/2)

☐ Include the subgroups compatible with intermediate cells.

(It is not applied when only the maximal subgroups are calculated)

Wyckoff positions of the atoms

3d:(1/2,0,0)

1b:(1/2,1/2,1/2)

1a:(0,0,0)

☐ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Optional: refine further the subgroups of the output giving a set of irreps

Choose the irreps [Representations]

Optional: 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 --------

○ Only maximal subgroups

Example 3: Perovskite (g)

Space group: *Pm*$\bar{3}$*m* (No. 221)
Choose the irreducible representation(s) for each modulation vector

If no Wyckoff position has been given, a general position will be assumed

Non bolded irreps are incompatible with the given Wyckoff positions
Bolded irreps are compatible with at least one given Wyckoff position
Red colored irreps are compatible with all the Wyckoff positions given

Possible irreducible representations

Wave-vectors of the star (1 vector):
R:(1/2,1/2,1/2)
Descomposition of the mechanical representation(s) into irreps.

3d:(1/2,0,0)	→	1×**R1+(1)** ⊕ 1×**R3+(2)** ⊕ 1×**R4+(3)** ⊕ 1×**R5+(3)**
1b:(1/2,1/2,1/2)	→	1×**R5+(3)**
1a:(0,0,0)	→	1×**R4-(3)**

Choose the representation(s)

irreps:	☐ **R1+(1)**	R1-(1)	R2+(1)	R2-(1)	☐ **R3+(2)**	R3-(2)	☑ **R4+(3)**	☐ **R4-(3)**	☐ **R5+(3)**	R5-(3)

(In parentheses, the dimensions of the irreducible representations of the little group of k)

Submit

Only 4 of the 10 possible irreps are relevant

Example 3: Perovskite (g)

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 wave-vectors stars.
- The subgroups compatible with intermediate unit cells between the unit cell of the parent space group and the given supercell (or the supercell determined by the given wave vector(s) when the previous option is used) can be included.
- When a set of wave-vectors is used as input, the output can be further refined introducing the Wyckoff positions of the atoms and/or a set of irreducible representations.

Tutorial_SUBGROUPS: download

See the Help for details.

Space group: $Pm\bar{3}m$ (No. 221)

Set of chosen modulation wave-vectors

k_1=(1/2,1/2,1/2)

☐ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Wyckoff positions of the atoms

3d:(1/2,0,0)
1b:(1/2,1/2,1/2)
1a:(0,0,0)

Chosen representations

R:(1/2,1/2,1/2) R4+(3)

Optional: 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 [-------]
- ○ Only maximal subgroups

Optional: further limitations considering physical properties of the point groups

- Only centrosymmetric / non-centrosymmetric groups [all]
- Only polar / non-polar groups [all]
- Only proper ferroelastic phase transitions [no]

(This option is incompatible with the previous two options and with the selection of representations)

◉ List of subgroups ○ Graph of subgroups

[Submit]

Example 3: Perovskite (g)

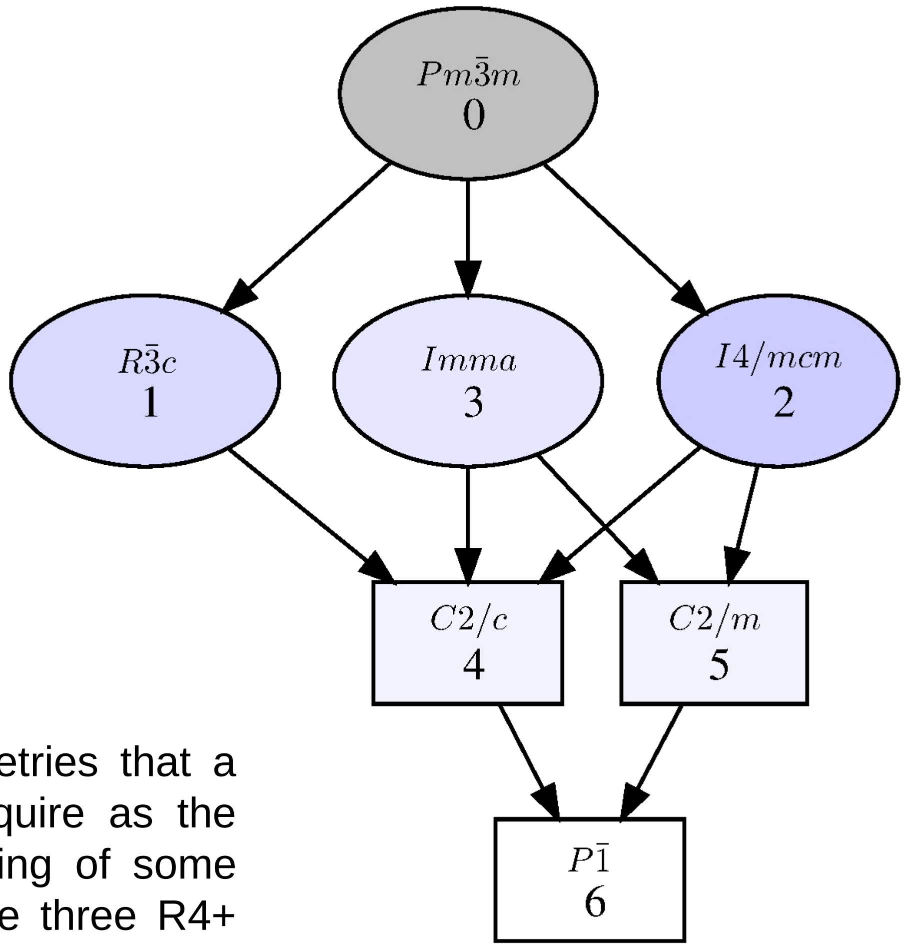
List of possible subgroups assuming the given wyckoff positions and that have as primary irreps all the irreps given

Get the subgroup-graph   More options

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$R\bar{3}c$ (No. 167)	$\begin{pmatrix} -1 & 0 & 2 & 0 \\ 0 & -1 & -2 & 0 \\ 1 & -1 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
2	$I4/mcm$ (No. 140)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
3	$Imma$ (No. 74)	$\begin{pmatrix} 0 & 1 & -1 & 1/2 \\ 0 & 1 & 1 & 0 \\ 2 & 0 & 0 & 1/2 \end{pmatrix}$	12=2x6	Conjugacy Class	Get irreps
4	$C2/c$ (No. 15)	$\begin{pmatrix} 1 & 1 & -1 & 1/2 \\ -2 & 0 & 0 & 1/2 \\ -1 & 1 & 1 & 0 \end{pmatrix}$	24=2x12	Conjugacy Class	Get irreps
5	$C2/m$ (No. 12)	$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1/2 \\ 0 & -2 & 0 & 1/2 \end{pmatrix}$	24=2x12	Conjugacy Class	Get irreps
6	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 1 & 0 \end{pmatrix}$	48=2x24	Conjugacy Class	Get irreps

All possible distinct space group symmetries (subgroups of the parent $Pm\bar{3}m$) that can result from an order parameter with R4+ symmetry.

Example 3: Perovskite (h)



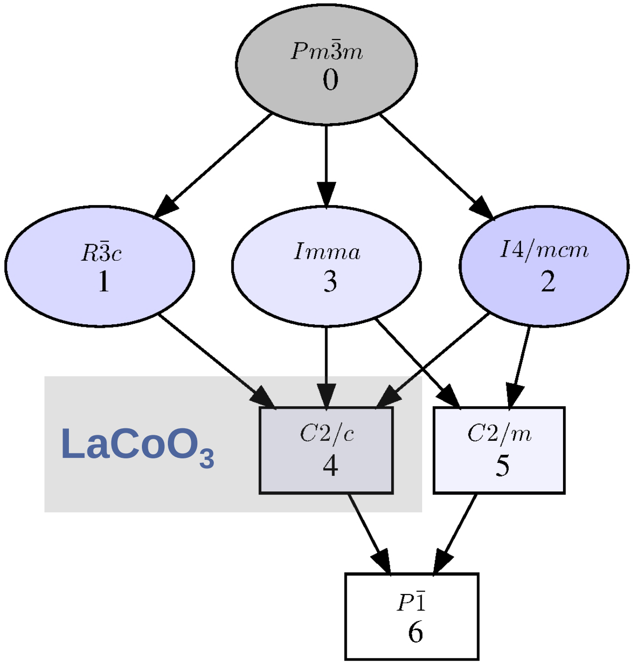
All possible symmetries that a perovskite can acquire as the result of the freezing of some combinations of the three R4+ distortions

Example 3: Perovskite (k)

SUBGROUPS can be combined with the program TRANSTRU to create an initial structural model of a distorted structure under one or more of the symmetries obtained with SUBGROUPS.

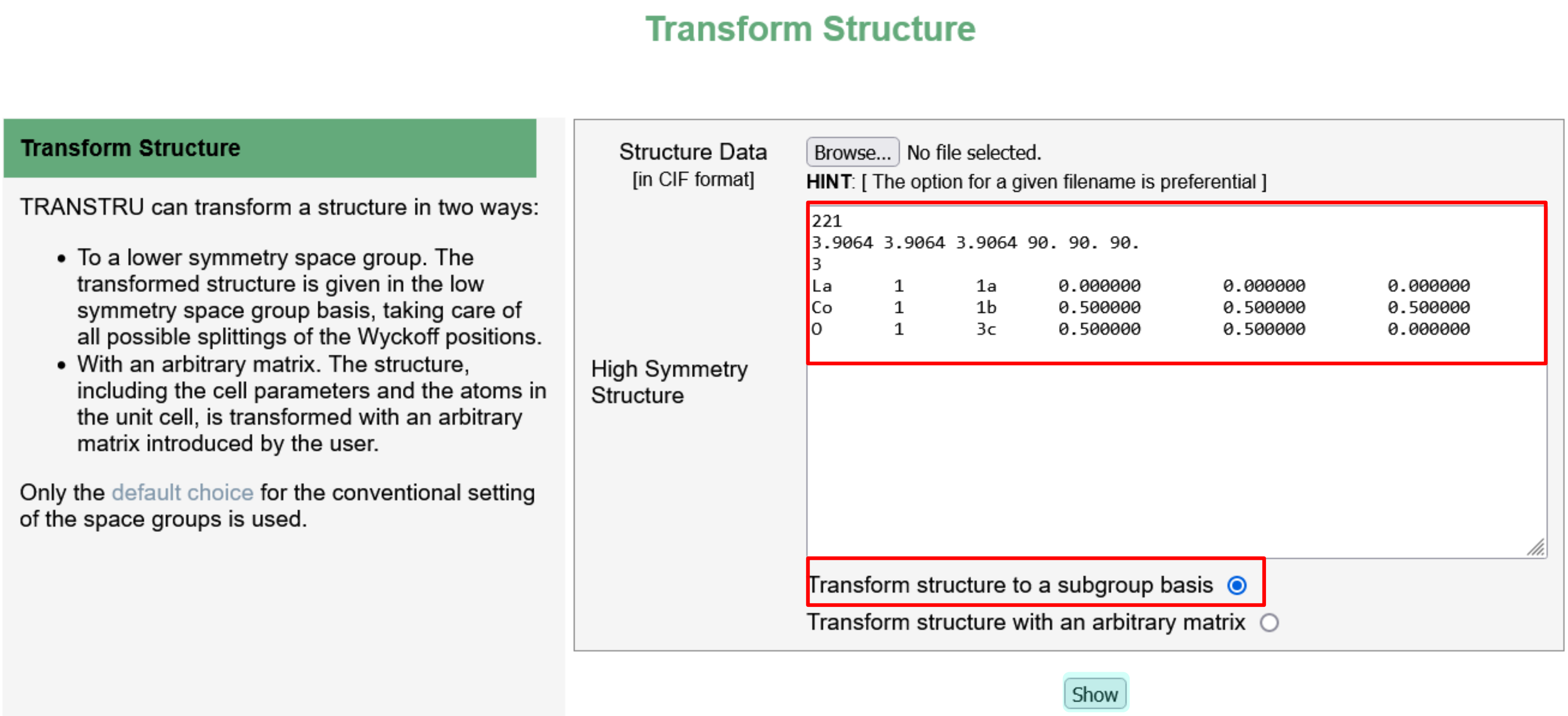
Create the CIF file for the $C2/c$ structure observed in $LaCoO_3$.

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps
1	$R\bar{3}c$ (No. 167)	$\begin{pmatrix} -1 & 0 & 2 & 0 \\ 0 & -1 & -2 & 0 \\ 1 & -1 & 2 & 0 \end{pmatrix}$	8=2x4	Conjugacy Class	Get irreps
2	$I4/mcm$ (No. 140)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$	6=2x3	Conjugacy Class	Get irreps
3	$Imma$ (No. 74)	$\begin{pmatrix} 0 & 1 & -1 & 1/2 \\ 0 & 1 & 1 & 0 \\ 2 & 0 & 0 & 1/2 \end{pmatrix}$	12=2x6	Conjugacy Class	Get irreps
4	$C2/c$ (No. 15)	$\begin{pmatrix} 1 & 1 & -1 & 1/2 \\ -2 & 0 & 0 & 1/2 \\ -1 & 1 & 1 & 0 \end{pmatrix}$	24=2x12	Conjugacy Class	Get irreps
5	$C2/m$ (No. 12)	$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1/2 \\ 0 & -2 & 0 & 1/2 \end{pmatrix}$	24=2x12	Conjugacy Class	Get irreps
6	$P\bar{1}$ (No. 2)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 1 & 0 \end{pmatrix}$	48=2x24	Conjugacy Class	Get irreps



Example 3: Perovskite (k)

https://www.cryst.ehu.es/cryst/transtru.html



Transform Structure

Transform Structure

TRANSTRU can transform a structure in two ways:

- To a lower symmetry space group. The transformed structure is given in the low symmetry space group basis, taking care of all possible splittings of the Wyckoff positions.
- With an arbitrary matrix. The structure, including the cell parameters and the atoms in the unit cell, is transformed with an arbitrary matrix introduced by the user.

Only the default choice for the conventional setting of the space groups is used.

Structure Data [in CIF format] — Browse... No file selected.

HINT: [The option for a given filename is preferential]

High Symmetry 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
```

Transform structure to a subgroup basis ◉

Transform structure with an arbitrary matrix ○

Show

Example 3: Perovskite (k)

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

Example 3: Perovskite (k)

Transform structure

Transformation matrix: a+2b-c,-a-c+1/2,-a+c+1/2

High symmetry 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
```

Visualize this structure | CIF File | Cartesian Coordinates

Low symmetry structure

```
015
9.568686 5.524484 5.524484 90.000000 125.264397 90.000000
5
La       1        4c       0.750000        0.250000        0.500000
Co       1        4e       0.000000        0.750000        0.750000
O        1        4a       0.000000        0.000000        0.500000
O        1_2      4b       0.000000        0.500000        0.000000
O        1_3      4d       0.250000        0.250000        0.500000
```

Visualize this structure | CIF File | Cartesian Coordinates

You can download directly the CIF file with the atomic positions corresponding to the ideal perovskite structure