AIC Commission on Crystallographic Teaching
AIC International Crystallography School 2019

CRYSTALLOGRAPHIC INFORMATION

FIESTA

www.cristallografia.org/aicschool2019

30 August
3 September
2019
Naples, Italy
Mois I. Aroyo
Universidad del País Vasco, Bilbao, Spain
Crystallographic Databases

International Tables for Crystallography
Crystallographic databases

Group-subgroup relations

Structural utilities

Representations of point and space groups

Solid-state applications
Extensive tabulations and illustrations of the 17 plane groups and of the 230 space groups

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

\[ \text{P4}_2/mbc \quad D_{4h}^{13} \quad 4/mmm \quad \text{Tetragonal} \]

No. 135

\[ P \ 4_2/m \ 2_1/b \ 2/c \]

Patterson symmetry \( P4/mmm \)

**Origin** at centre \((2/m)\) at \(4_{2}/m\ 1n\)

**Asymmetric unit** \(0 \leq x \leq \frac{1}{2}; \ 0 \leq y \leq \frac{1}{2}; \ 0 \leq z \leq \frac{1}{4}\)

**Symmetry operations**

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \ 0,0,z \\
(3) & \quad 4^+ \ (0,0,\frac{1}{2}) \ 0,0,z \\
(4) & \quad 4^- \ (0,0,\frac{1}{2}) \ 0,0,z \\
(5) & \quad 2(0,\frac{1}{2},0) \ \frac{1}{2},y,0 \\
(6) & \quad 2(\frac{1}{2},0,0) \ x,\frac{1}{2},0 \\
(7) & \quad 2(\frac{1}{2},\frac{1}{2},0) \ x,x,\frac{1}{2} \\
(8) & \quad 2 \ x,\bar{x}+\frac{1}{2},\frac{1}{4} \\
(9) & \quad 1 \ 0,0,0 \\
(10) & \quad m \ x,y,0 \\
(11) & \quad 4^+ \ 0,0,z; \ 0,0,\frac{1}{4} \\
(12) & \quad 4^- \ 0,0,z; \ 0,0,\frac{1}{4} \\
(13) & \quad a \ x,\frac{1}{2},z \\
(14) & \quad b \ \frac{1}{2},y,z \\
(15) & \quad c \ x+\frac{1}{2},\bar{x},z \\
(16) & \quad n(\frac{1}{2},\frac{1}{2},\frac{1}{2}) \ x,x,z
\end{align*}
\]
### Generators selected

(1); \( t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ (2); \ (3); \ (5); \ (9)\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16  ( i \ 1 )</td>
<td></td>
</tr>
<tr>
<td>(1) ( x,y,z )</td>
<td></td>
</tr>
<tr>
<td>(2) ( \tilde{x},\tilde{y},z )</td>
<td></td>
</tr>
<tr>
<td>(3) ( \tilde{y},x,z+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(4) ( y,\tilde{x},z+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(5) ( \tilde{x}+\frac{1}{2},y+\frac{1}{2},\tilde{z} )</td>
<td></td>
</tr>
<tr>
<td>(6) ( x+\frac{1}{2},\tilde{y}+\frac{1}{2},\tilde{z} )</td>
<td></td>
</tr>
<tr>
<td>(7) ( y+\frac{1}{2},x+\frac{1}{2},\tilde{z}+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(8) ( \tilde{y}+\frac{1}{2},\tilde{x}+\frac{1}{2},\tilde{z}+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(9) ( \tilde{x},\tilde{y},\tilde{z} )</td>
<td></td>
</tr>
<tr>
<td>(10) ( x,y,\tilde{z} )</td>
<td></td>
</tr>
<tr>
<td>(11) ( y,\tilde{x},\tilde{z}+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(12) ( \tilde{y},x,\tilde{z}+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(13) ( x+\frac{1}{2},\tilde{y}+\frac{1}{2},z )</td>
<td></td>
</tr>
<tr>
<td>(14) ( \tilde{x}+\frac{1}{2},y+\frac{1}{2},z )</td>
<td></td>
</tr>
<tr>
<td>(15) ( \tilde{y}+\frac{1}{2},\tilde{x}+\frac{1}{2},z+\frac{1}{2} )</td>
<td></td>
</tr>
<tr>
<td>(16) ( y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2} )</td>
<td></td>
</tr>
</tbody>
</table>

### Reflection conditions

**General:**
- \( 0kl : \ k = 2n \)
- \( hhl : \ l = 2n \)
- \( 00l : \ l = 2n \)
- \( h00 : \ h = 2n \)

**Special:** as above, plus no extra conditions
- \( hkl : \ l = 2n \)
- \( hkl : \ h+k,l = 2n \)
- \( hkl : \ h+k,l = 2n \)
- \( hkl : \ h+k,l = 2n \)
- \( hkl : \ h+k,l = 2n \)
### Space-group symmetry

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>GENPOS</td>
<td>Generators and General Positions of Space Groups</td>
</tr>
<tr>
<td>WYCKPOS</td>
<td>Wyckoff Positions of Space Groups</td>
</tr>
<tr>
<td>HKLCOND</td>
<td>Reflection conditions of Space Groups</td>
</tr>
<tr>
<td>MAXSUB</td>
<td>Maximal Subgroups of Space Groups</td>
</tr>
<tr>
<td>SERIES</td>
<td>Series of Maximal Isomorphic Subgroups of Space Groups</td>
</tr>
<tr>
<td>WYCKSETS</td>
<td>Equivalent Sets of Wyckoff Positions</td>
</tr>
<tr>
<td>NORMALIZER</td>
<td>Normalizers of Space Groups</td>
</tr>
<tr>
<td>KVEC</td>
<td>The k-vector types and Brillouin zones of Space Groups</td>
</tr>
<tr>
<td>SYMMETRY OPERATIONS</td>
<td>Geometric interpretation of matrix column representations of symmetry operations</td>
</tr>
<tr>
<td>IDENTIFY GROUP</td>
<td>Identification of a Space Group from a set of generators in an arbitrary setting</td>
</tr>
</tbody>
</table>
Problem: Matrix-column presentation
Geometrical interpretation

Generators and General Positions

How to select the group

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

To see the data in a non conventional setting click on [Non conventional Setting] or [ITA Settings] for checking the non

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

Choose it 14

Show:

- Generators only
- All General Positions

Standard/Default Setting

Non Conventional Setting

ITA Settings
Example GENPOS: Space group \( P2_1/c \) (14)

**Space-group \( P2_1/c \) symmetry operations**

- **Short-hand notation**
  \[
  \begin{pmatrix}
  W_{11} & W_{12} & W_{13} \\
  W_{21} & W_{22} & W_{23} \\
  W_{31} & W_{32} & W_{33}
  \end{pmatrix}
  \begin{pmatrix}
  w_1 \\
  w_2 \\
  w_3
  \end{pmatrix}
  \]

- **Matrix-column presentation**

**Geometric interpretation**

**Seitz symbols**

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

<table>
<thead>
<tr>
<th>No.</th>
<th>((x,y,z)) form</th>
<th>Matrix form</th>
<th>Symmetry operation</th>
</tr>
</thead>
</table>
| 1   | \(x,y,z\)        | \[
  \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 1 & 0
  \end{pmatrix}
  \] | ITA: 1 \{1 | 0\} |
| 2   | \(-x,y+1/2,-z+1/2\) | \[
  \begin{pmatrix}
  -1 & 0 & 0 & 0 \\
  0 & 0 & 1 & 1/2 \\
  0 & -1 & 0 & 1/2
  \end{pmatrix}
  \] | ITA: 2 \(0,1/2,0\) \(0,y,1/4\) \{200 | 0 1/2 1/2\} |
| 3   | \(-x,-y,-z\)     | \[
  \begin{pmatrix}
  -1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & -1 & 0
  \end{pmatrix}
  \] | ITA: -1 0,0,0 \{-1 | 0\} |
| 4   | \(-x,-y+1/2,z+1/2\) | \[
  \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & -1 & 0 & 1/2 \\
  0 & 0 & 1 & 1/2
  \end{pmatrix}
  \] | ITA: \(c,x,1/4,z\) \{m010 | 0 1/2 1/2\} |

**ITA data**

- **General positions**
  
  \[
  \begin{pmatrix}
  4 & e & 1 \\
  \end{pmatrix}
  \]

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

**Symmetry operations**

- (1) 1
- (2) \(2(0,\frac{1}{2},0)\) \(0,y,\frac{1}{4}\)
- (3) \(\bar{1}\) \(0,0,0\)
- (4) \(c\) \(x,\frac{1}{4},z\)
Problem: Wyckoff positions Site-symmetry groups

Wyckoff Positions

How to select the group

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

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

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

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

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

### Space Group: 68 (Ccce) [origin choice 1]
- Point: (0,1/4,1/4)
- Wyckoff Position: 4a

#### Site Symmetry Group 222

<table>
<thead>
<tr>
<th>x,y,z</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-x,y,-z+1/2</td>
<td>-1</td>
</tr>
<tr>
<td>-x,-y+1/2,z</td>
<td>-1</td>
</tr>
<tr>
<td>x,-y+1/2,z</td>
<td>-1</td>
</tr>
</tbody>
</table>

#### Bilbao Crystallographic Server

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**Bilbao Crystallographic Server**
Example **WYCKPOS**: Wyckoff Positions Ccce (68)

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)

Variable parameters \((x,y,z)\) are also accepted

\[
\begin{align*}
x &= \frac{1}{2} \\
y &= \frac{1}{4} \\
z &= \frac{1}{4}
\end{align*}
\]

Show

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

Site Symmetry Group 222

<table>
<thead>
<tr>
<th>(x,y,z)</th>
<th>(\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix})</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-x+1,y,-z+1/2)</td>
<td>(\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix})</td>
<td>2 1/2,y,1/4</td>
</tr>
<tr>
<td>(-x+1,-y+1/2,z)</td>
<td>(\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1/2 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix})</td>
<td>2 1/2,1/4,z</td>
</tr>
<tr>
<td>(x,-y+1/2,-z+1/2)</td>
<td>(\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix})</td>
<td>2 x,1/4,1/4</td>
</tr>
</tbody>
</table>
### Geometric Interpretation of Matrix Column Representation of Symmetry Operation

**Symmetry Operation**

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

**Input:**

- i) The crystal system or the space group number.
- ii) The matrix column representation of symmetry operation.

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

**Output:**

We obtain the geometric interpretation of the symmetry operation.

**Bilbao Crystallographic Server**

**Problem:** Geometric Interpretation of \((W,w)\)

**Symmetry Operation of the Space Group 35 (Cmm2)**

<table>
<thead>
<tr>
<th>In matrix form</th>
<th>Rotational part</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(-1 0 0)</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(0 1 0)</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(0 0 1)</td>
<td>0</td>
</tr>
</tbody>
</table>

- \(-x+1/2, y+1/2, z\)

- \(b/4, y, z\)
1. Characterize geometrically the matrix-column pairs listed under General position of the space group P4mm in ITA.

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

3. Compare your results with the results of the program SYMMETRY OPERATIONS
Consider the special Wyckoff positions of the space group $P4mm$.

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

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

Compare your results with the results of the program WYCKPOS.
Co-ordinate transformations in crystallography

3-dimensional space

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

\((a', b', c'), \text{ origin } O': \text{ point } X(x', y', z')\)

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

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

\[
(a', b', c') = (a, b, c)P = \begin{pmatrix}
P_{11} & P_{12} & P_{13} \\
P_{21} & P_{22} & P_{23} \\
P_{31} & P_{32} & P_{33}
\end{pmatrix} = (P_{11}a + P_{21}b + P_{31}c, P_{12}a + P_{22}b + P_{32}c, P_{13}a + P_{23}b + P_{33}c).
\]

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

\(O' = O + p\)  
the origin \(O'\) has coordinates \((p_1, p_2, p_3)\) in the old coordinate system
Co-ordinate transformations in crystallography

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

\[
(W',w') = (P,p)^{-1} (W,w) (P,p)
\]

Structure-description transformation transformation by \((P,p)\)

unit cell parameters: metric tensor \(G\):

\[
G' = P^t G P
\]

atomic coordinates \(X(x,y,z)\):

\[
\begin{pmatrix}
x' \\
y' \\
z
\end{pmatrix} = (P,p)^{-1} \begin{pmatrix}
P_{11} & P_{12} & P_{13} & p_1 \\
P_{21} & P_{22} & P_{23} & p_2 \\
P_{31} & P_{32} & P_{33} & p_3 \\
p_1 & p_2 & p_3
\end{pmatrix}^{-1} \begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
\]
### Problem: ITA SETTINGS

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

#### Monoclinic descriptions

<table>
<thead>
<tr>
<th>HM</th>
<th>Transf.</th>
<th>abc</th>
<th>cba</th>
<th>abc</th>
<th>bač</th>
<th>abc</th>
<th>ācb</th>
</tr>
</thead>
<tbody>
<tr>
<td>HM</td>
<td>C2/c</td>
<td>C12/c1</td>
<td>A12/a1</td>
<td>A112/a</td>
<td>B112/b</td>
<td>B2/b11</td>
<td>C2/c11</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A12/n1</td>
<td>C12/n1</td>
<td>B112/n</td>
<td>A112/n</td>
<td>C2/n11</td>
<td>B2/n11</td>
</tr>
<tr>
<td></td>
<td></td>
<td>I12/a1</td>
<td>I12/c1</td>
<td>I112/b</td>
<td>I112/a</td>
<td>I2/c11</td>
<td>I2/b11</td>
</tr>
</tbody>
</table>

**Monoclinic axis b**

**Monoclinic axis c**

**Monoclinic axis a**

Cell type 1

Cell type 2

Cell type 3

#### Orthorhombic descriptions

<table>
<thead>
<tr>
<th>No.</th>
<th>HM</th>
<th>abc</th>
<th>bač</th>
<th>cab</th>
<th>āba</th>
<th>bca</th>
<th>aćb</th>
</tr>
</thead>
<tbody>
<tr>
<td>33</td>
<td>Pna2</td>
<td>Pna2</td>
<td>Pbn2</td>
<td>P2_1nb</td>
<td>P2_1cn</td>
<td>P2_1cn</td>
<td>Pn2_1a</td>
</tr>
</tbody>
</table>
Problem: Co-ordinate transformations in crystallography

Generators
General positions

Bilbao Crystallographic Server

Generators and General Positions

How to select the group

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

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

choose it 15

Show:

Generators only
All General Positions

Conventional Setting
Non Conventional Setting
ITA Settings

[ Bilbao Crystallographic Server Main Menu ]

Bilbao Crystallographic Server
http://www.cryst.ehu.es

Transformation of the basis
ITA-settings
symmetry data

space group
Example **GENPOS:**

default setting $C12/c1$

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

final setting $A112/a$

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>$P$</th>
<th>$P^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>$C12/c1$</td>
<td>$a,b,c$</td>
<td>$a,b,c$</td>
</tr>
<tr>
<td>15</td>
<td>$A12/n1$</td>
<td>$-a-c,b,a$</td>
<td>$c,b,-a-c$</td>
</tr>
<tr>
<td>15</td>
<td>$I12/a1$</td>
<td>$c,b,-a-c$</td>
<td>$-a-c,b,a$</td>
</tr>
<tr>
<td>15</td>
<td>$A12/a1$</td>
<td>$c,-b,a$</td>
<td>$c,-b,a$</td>
</tr>
<tr>
<td>15</td>
<td>$C12/n1$</td>
<td>$a,-b,a-c$</td>
<td>$a,-b,a-c$</td>
</tr>
<tr>
<td>15</td>
<td>$I12/c1$</td>
<td>$-a-c,-b,c$</td>
<td>$-a-c,-b,c$</td>
</tr>
<tr>
<td>15</td>
<td>$A112/a$</td>
<td>$c,a,b$</td>
<td>$b,c,a$</td>
</tr>
<tr>
<td>15</td>
<td>$B112/n$</td>
<td>$a,-a-c,b$</td>
<td>$a,c,-a-b$</td>
</tr>
<tr>
<td>15</td>
<td>$I122/b$</td>
<td>$-a-c,c,b$</td>
<td>$-a-c,c,b$</td>
</tr>
<tr>
<td>15</td>
<td>$B112/b$</td>
<td>$a,c,-b$</td>
<td>$a,-c,b$</td>
</tr>
<tr>
<td>15</td>
<td>$A112/n$</td>
<td>$a,-c,a,b$</td>
<td>$b,-c,a-b$</td>
</tr>
<tr>
<td>15</td>
<td>$I122/a$</td>
<td>$c,-a-c,b$</td>
<td>$-a-c,-b,c$</td>
</tr>
<tr>
<td>15</td>
<td>$B2/b11$</td>
<td>$b,c,a$</td>
<td>$c,a,b$</td>
</tr>
<tr>
<td>15</td>
<td>$C2/n11$</td>
<td>$b,a,-a-c$</td>
<td>$b,a,-b-c$</td>
</tr>
<tr>
<td>15</td>
<td>$I2/c11$</td>
<td>$b,-a-c,c$</td>
<td>$b,-c,a,c$</td>
</tr>
<tr>
<td>15</td>
<td>$C2/c11$</td>
<td>$-b,a,c$</td>
<td>$b,-a,c$</td>
</tr>
<tr>
<td>15</td>
<td>$B2/n11$</td>
<td>$-b,-a-c,a$</td>
<td>$c,-a,b-c$</td>
</tr>
<tr>
<td>15</td>
<td>$I2/b11$</td>
<td>$b,-c,a-c$</td>
<td>$b,-c,-a,b$</td>
</tr>
</tbody>
</table>
**Example GENPOS: ITA settings of C2/c(15)**

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

<table>
<thead>
<tr>
<th>N</th>
<th>Standard/Default Setting C2/c</th>
<th>ITA-Setting A 1 1 2/a</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(x,y,z) form</td>
<td>matrix form</td>
</tr>
</tbody>
</table>
| 1 | x, y, z | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | 1 | x, y, z | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | 1 |
| 2 | -x, y, -z+1/2 | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\] | 2, 0, 1/4 | -x+1/2, -y, z | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | 2, 1/4, 0, z |
| 3 | -x, -y, -z | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | -1, 0, 0, 0 | -x, -y, -z | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | -1, 0, 0, 0 |
| 4 | x, -y, z+1/2 | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 1/2 \\
\end{pmatrix}
\] | c, x, 0, z | x+1/2, y, -z | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | a, x, y, 0 |
| 5 | x+1/2, y+1/2, z | \[
\begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & 1 & 0 & 1/2 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}
\] | t (1/2, 1/2, 0) | x, y+1/2, z+1/2 | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 1/2 \\
0 & 0 & 1 & 1/2 \\
\end{pmatrix}
\] | t (0, 1/2, 1/2) |
| 6 | -x+1/2, y+1/2, -z+1/2 | \[
\begin{pmatrix}
-1 & 0 & 0 & 1/2 \\
0 & 1 & 0 & 1/2 \\
0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\] | 2, (0, 1/2, 0) 1/4, y, 1/4 | -x+1/2, -y+1/2, z+1/2 | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\] | 2, (0, 0, 1/2) 1/4, 1/4, z |
| 7 | -x+1/2, -y+1/2, -z | \[
\begin{pmatrix}
-1 & 0 & 0 & 1/2 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
\end{pmatrix}
\] | -1, 1/4, 1/4, 0 | -x, -y+1/2, -z+1/2 | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\] | -1, 0, 1/4, 1/4 |
| 8 | x+1/2, -y+1/2, z+1/2 | \[
\begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 1/2 \\
\end{pmatrix}
\] | n (1/2, 0, 1/2) x, 1/4, z | x+1/2, y+1/2, -z+1/2 | \[
\begin{pmatrix}
1 & 0 & 0 & 1/2 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\] | n (1/2, 1/2, 0) x, y, 1/4 |
Problem: Coordinate transformations

Wyckoff positions

How to select the group

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

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


ITA-Settings for the Space Group 68

The settings must be read by columns. P is the transformation

\[(a, b, c)_n = (a, b, c) \cdot P\]

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>P</th>
<th>P⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>C c c e [origin 1]</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>68</td>
<td>A e a a [origin 1]</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
<tr>
<td>68</td>
<td>B b e b [origin 1]</td>
<td>b,c,a</td>
<td>c,a,b</td>
</tr>
<tr>
<td>68</td>
<td>C c e [origin 2]</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>68</td>
<td>A e a a [origin 2]</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
<tr>
<td>68</td>
<td>B b e b [origin 2]</td>
<td>b,c,a</td>
<td>c,a,b</td>
</tr>
</tbody>
</table>
Problem: Space-group identification by a set of generators in arbitrary basis

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

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

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

\(x + 1/2, y + 1/2, z\)
\(-y + 1/3, x + 1/4, z + 1/4\)

Assumed lattice translations:
\(x + 1, y, z\)
\(x, y + 1, z\)
\(x, y, z + 1\)

\(x, y, z\)
Consider the space group $P2_1/c$ (No. 14). Show that the relation between the General and Special position data of $P112_1/a$ (setting unique axis $c$) can be obtained from the data $P12_1/c1$ (setting unique axis $b$) applying the transformation $(a',b',c')_c = (a,b,c)_bP$, with $P = c,a,b$.

Use the retrieval tools GENPOS (generators and general positions) and WYCKPOS (Wyckoff positions) for accessing the space-group data. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in ITA.
Use the retrieval tools GENPOS or Generators and General positions, WYCKPOS (or Wyckoff positions) for accessing the space-group data on the Bilbao Crystallographic Server or Symmetry Database server. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in ITA.

Consider the General position data of the space group \( \text{Im}-3\text{m} \) (No. 229). Using the option Non-conventional setting obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation \((a',b',c') = 1/2(-a+b+c,a-b+c,a+b-c)\)
A body-centred cubic lattice (bc) has as its conventional basis the conventional basis \((a_P, b_P, c_P)\) of a primitive cubic lattice, but the lattice also contains the centring vector \(1/2a_P + 1/2b_P + 1/2c_P\) which points to the centre of the conventional cell.

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

(i) for the conventional basis \((a_P, b_P, c_P)\);

(ii) for the primitive basis:

\[ a_I = 1/2(-a_P + b_P + c_P), \quad b_I = 1/2(a_P - b_P + c_P), \quad c_I = 1/2(a_P + b_P - c_P) \]

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

\[ G' = P^t \, G \, P \]

Hint: metric tensor transformation
Problem 1.6

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

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

(i) for the conventional basis ($a_P, b_P, c_P$);

(ii) for the primitive basis:

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

(iii) determine the lattice parameters of the primitive cell if $a_P = 4 \text{ Å}$
Group-Subgroup Relations of Space Groups

- Lattice of Maximal Subgroups
- Distribution of subgroups in conjugated classes
- Coset decomposition for a group-subgroup pair
- The splitting of the Wyckoff Positions
- Minimal Supergroups of Space Groups
- Supergroups of Space Groups
- List of subgroups for a given k-index.
- List of supergroups for a given k-index.
- Non Characteristic orbits.
- Common Subgroups of Space Groups
- Common Supergroups of Two Space Groups
- Index of a group subgroup pair
- Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)
Maximal subgroups of space groups

### I Maximal \textit{translationengleiche} subgroups

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>(P411) ((75, P4))</td>
<td>1; 2; 3; 4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(P21m) ((35, Cmm2))</td>
<td>1; 2; 7; 8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(P2m1) ((25, Pmm2))</td>
<td>1; 2; 5; 6</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(a-b, a+b, c)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### II Maximal \textit{klassengleiche} subgroups

#### Enlarged unit cell

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>(P4_{1}mc) ((105))</td>
<td>(2; 5; 3+ (0,0,1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(P4_{1}cc) ((103))</td>
<td>(2; 3; 5+ (0,0,1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(P4_{2}cm) ((101))</td>
<td>(2; (3; 5) + (0,0,1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>(P4_{4}mm) ((99))</td>
<td>(2; 3; 5)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(a, b, 2c\)

#### Series of maximal isomorphic subgroups

- \([p]\) \(c' = pc\)
  - \(P4_{1}mm\) \((99)\)
    - \(2; 3; 5\)
    - \(a, b, pc\)
    - \(p > 1\)
    - No conjugate subgroups

- \([p^2]\) \(a' = pa, b' = pb\)
  - \(P4_{1}mm\) \((99)\)
    - \(2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (0, 2v, 0)\)
    - \(pa, pb, c\)
    - \(u, v, 0\)
    - \(p > 2; 0 \leq u < p; 0 \leq v < p\)
    - \(p^2\) conjugate subgroups for the prime \(p\)
Problem: SUBGROUPS OF SPACE GROUPS

Group-Subgroup Lattice and Chains of Maximal Subgroups

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

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

subgroup index \([i] = [i_P] \cdot [i_L]\)
General graph for $P4_{1212} > P2_1$

Graph for $P4_{1212} > P2_1$

Maximal subgroup graph

Three $P2_1$ subgroups in two conjugacy classes

Index $[i]=4$
PROBLEM: Domain-structure analysis

\[ \mathbf{G} \overset{[i]}{\rightarrow} \mathbf{H} \]

twins and antiphase domains

twinning operation

symmetry groups of the domain states; multiplicity and degeneracy

Hermann, 1929:

\[
\begin{align*}
\mathbf{G} & \quad \overset{\mathbf{M}}{\rightarrow} \quad \mathbf{H} \\
\mathbf{M} & \quad \overset{\mathbf{H}}{\rightarrow} \quad \mathbf{P} \\
\mathbf{H} & \quad \overset{\mathbf{L}}{\rightarrow} \quad \mathbf{G}
\end{align*}
\]

subgroup index
\[ [i] = [i_p] \cdot [i_L] \]

- twins: \[ i_p = P_G / P_H \]
- antiphase: \[ i_L = Z_{H,p} / Z_{G,p} = V_{H,p} / V_{G,p} \]
Problem: SPLITTING OF WYCKOFF POSITIONS

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

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

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

$\star$ 1/2 0 z 1c mm2
$\star$ 0 1/2 z' 1b mm2

<table>
<thead>
<tr>
<th>Axes Coordinates</th>
<th>Wyckoff positions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1a</td>
</tr>
<tr>
<td>I Maximal <em>translationengleiche</em> subgroups</td>
<td></td>
</tr>
<tr>
<td>[2] <em>P</em>4 (75)</td>
<td>1a</td>
</tr>
<tr>
<td>[2] <em>Pmm2</em> (25)</td>
<td>1a</td>
</tr>
<tr>
<td>[2] <em>Cmm2</em> (35) a−b, ( \frac{1}{2} (x−y), \frac{1}{2} (x+y), z ) a+b, c</td>
<td>2a</td>
</tr>
</tbody>
</table>

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

<table>
<thead>
<tr>
<th>Axes Coordinates</th>
<th>Wyckoff positions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4a</td>
</tr>
<tr>
<td>[2] <em>I4cm</em> (108) a−b, ( \frac{1}{2} (x−y), \frac{1}{2} (x+y), \frac{1}{2} z ); a+b, 2c ( +(0, 0, \frac{1}{2}) )</td>
<td>4b</td>
</tr>
<tr>
<td>[2] <em>I4cm</em> (108) a−b, ( \frac{1}{2} (x−y) + \frac{1}{2} (x+y), \frac{1}{2} z ); a+b, 2c ( +(0, 0, \frac{1}{2}) )</td>
<td>2×4a</td>
</tr>
<tr>
<td>[2] <em>I4mm</em> (107) a−b, ( \frac{1}{2} (x−y), \frac{1}{2} (x+y), \frac{1}{2} z ); a+b, 2c ( +(0, 0, \frac{1}{2}) )</td>
<td>4b</td>
</tr>
<tr>
<td>[2] <em>I4mm</em> (107) a−b, ( \frac{1}{2} (x−y) + \frac{1}{2} (x+y), \frac{1}{2} z ); a+b, 2c ( +(0, 0, \frac{1}{2}) )</td>
<td>4b</td>
</tr>
<tr>
<td>[2] <em>P4_2mc</em> (105) a, b, 2c ( x, y, \frac{1}{2} z; +(0, 0, \frac{1}{2}) )</td>
<td>2a</td>
</tr>
<tr>
<td>[2] <em>P4cc</em> (103) a, b, 2c ( x, y, \frac{1}{2} z; +(0, 0, \frac{1}{2}) )</td>
<td>2a</td>
</tr>
<tr>
<td>[2] <em>P4_2cm</em> (101) a, b, 2c ( x, y, \frac{1}{2} z; +(0, 0, \frac{1}{2}) )</td>
<td>2a</td>
</tr>
<tr>
<td>[2] <em>P4bm</em> (100) a−b, ( \frac{1}{2} (x−y), \frac{1}{2} (x+y), \frac{1}{2} z ); a+b, c ( +(1, \frac{1}{2}, 0) )</td>
<td>2a</td>
</tr>
</tbody>
</table>
Wyckoff Positions Splitting

Conventional Settings

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:

Enter supergroup or **choose it**

Enter subgroup or **choose it**

Please, define the transformation relating the group and the subgroup bases.
(Note: If you don't know the transformation click here for possible workarounds)

Transformation matrix: (P_p)

<table>
<thead>
<tr>
<th>rotational matrix</th>
<th>1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

origin shift:

| 0 | 0 | 0 |

Show group–subgroup data.

Wyckoff Positions Splitting

136 (P4_2/mnm) > 65 (Cmmm)

Group Data

- 16r (x, y, z)
- 8q (x, y, 1/2)
- 8p (x, y, 0)

Subgroup Data

- 8o (x, 0, z)
- 16k (x, y, z)
- 8n (0, y, z)
- 8j (x, x, z)
- 8m (1/4, 1/4, z)
- 8i (x, y, 0)
- 8h (0, 1/2, z)
- 8k (0, 0, z)
- 4g (x, -x, 0)
- 4l (0, 0, z)
- 4f (x, 0, 0)
- 4e (0, 0, z)
- 4d (0, 1/2, 1/4, 4g (x, 0, 0))

Two-level input:
Choice of the Wyckoff positions
## Wyckoff Positions Splitting

### Two-level output:

**Relations between coordinate triplets**

### Result from splitting

<table>
<thead>
<tr>
<th>No</th>
<th>Group</th>
<th>Subgroup</th>
<th>More...</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8g</td>
<td>4b 4b 4b 4b</td>
<td>Relations</td>
</tr>
<tr>
<td>2</td>
<td>4f</td>
<td>4b 4b</td>
<td>Relations</td>
</tr>
<tr>
<td>3</td>
<td>4e</td>
<td>4b 4b</td>
<td>Relations</td>
</tr>
<tr>
<td>4</td>
<td>4d</td>
<td>4b 2a 2a</td>
<td>Relations</td>
</tr>
<tr>
<td>5</td>
<td>2c</td>
<td>4b</td>
<td>Relations</td>
</tr>
<tr>
<td>6</td>
<td>1b</td>
<td>2a</td>
<td>Relations</td>
</tr>
<tr>
<td>7</td>
<td>1a</td>
<td>2a</td>
<td>Relations</td>
</tr>
</tbody>
</table>

### Splitting of Wyckoff position 4d

<table>
<thead>
<tr>
<th>Representative</th>
<th>Subgroup Wyckoff position</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>group basis</td>
</tr>
<tr>
<td>----</td>
<td>-------------</td>
</tr>
<tr>
<td>1</td>
<td>(x, x, z)</td>
</tr>
<tr>
<td>2</td>
<td>(-x, -x, z)</td>
</tr>
<tr>
<td>3</td>
<td>(x+1, x, z)</td>
</tr>
<tr>
<td>4</td>
<td>(-x+1, -x, z)</td>
</tr>
<tr>
<td>5</td>
<td>(-x, x, z)</td>
</tr>
<tr>
<td>6</td>
<td>(-x+1, x, z)</td>
</tr>
<tr>
<td>7</td>
<td>(x, -x, z)</td>
</tr>
<tr>
<td>8</td>
<td>(x+1, -x, z)</td>
</tr>
</tbody>
</table>
MAGNETIC SYMMETRY AND APPLICATIONS

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

D.B. Litvin  *Magnetic Space Groups v. V3.02*  
http://www.bk.psu.edu/faculty/litvin/Download.html
<table>
<thead>
<tr>
<th>Representations and Applications</th>
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Databases of Representations

Representations of space and point groups

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

- POINT
  - character tables
  - multiplication tables
  - symmetrized products

Retrieval tools

Bilbao Crystallographic Server
Database on Representations of Point Groups

### Bilbao Crystallographic Server

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

<table>
<thead>
<tr>
<th>Character Table</th>
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<tbody>
<tr>
<td>$C_{6v}(6mm)$</td>
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<tr>
<td>-----------------</td>
</tr>
<tr>
<td>Mult.</td>
</tr>
<tr>
<td>$A_1$</td>
</tr>
<tr>
<td>$A_2$</td>
</tr>
<tr>
<td>$B_1$</td>
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<tr>
<td>$B_2$</td>
</tr>
<tr>
<td>$E_2$</td>
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<td>$E_1$</td>
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#### Group-subgroup relations

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</tr>
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</tr>
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</tr>
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</tr>
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#### The Rotation Group D(L)

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<tr>
<td>4</td>
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<td>1</td>
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[List of irreducible representations in matrix form]

character tables
matrix representations
basis functions
Reciprocal space groups
Brillouin zones
Representation domain
Wave-vector symmetry

Symmorphic space groups
IT unit cells
Asymmetric unit
Wyckoff positions

The k-vector Types of Group 22 [F222]

<table>
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<tr>
<th>k-vector description</th>
<th>Wyckoff Position</th>
<th>ITA description</th>
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<td>Conventional-ITA</td>
<td>ITA</td>
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<td>Label</td>
<td>Primitive</td>
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<tr>
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<td>0,0,0</td>
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<td>0,1,1</td>
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<td>T~T2</td>
<td>b</td>
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<td>1/2,0,1/2</td>
<td>0,1,0</td>
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<tr>
<td>Y~Y2</td>
<td>d</td>
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</tr>
<tr>
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<td>0,u,u ex</td>
<td>2u,0,0</td>
</tr>
<tr>
<td>U</td>
<td>1,1/2+u,1/2+u ex</td>
<td>2u,1,1</td>
</tr>
<tr>
<td>U=SM1=[SM0 T2]</td>
<td>e</td>
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<td>SM+SM1=[GM T2]</td>
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c^2 > a^2 + b^2
The k-vector Types of Group 22 [F222]

Brillouin zone

( Diagram for arithmetic crystal class 222F )

$c^2 < a^2 + b^2$

$c^2 > a^2 + b^2$
SUBPERIODIC GROUPS: LAYER, ROD AND FRIEZE GROUPS

ECM31-Oviedo Satellite

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

29-31 August 2018

Subperiodic Groups: Layer, Rod and Frieze Groups

<table>
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<td>Wyckoff Positions of Subperiodic Groups</td>
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<tr>
<td>MAXSUB</td>
<td>Maximal Subgroups of Subperiodic Groups</td>
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<tr>
<td>KVEC</td>
<td>The k-vector types and Brillouin zones of Layers Groups</td>
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<tr>
<td>SECTIONS</td>
<td>Identification of Layer Symmetry of Periodic Sections</td>
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Point-group symmetry