Lecture course on crystallography, 2015

Lecture 9: Space groups and International Tables for Crystallography
Consider a crystal lattice. According to its Bravais type we chose the conventional pair (triple) of basis vectors: \textit{a}, \textit{b} and \textit{c}. The crystallographic unit cell is defined by putting atoms, molecules, etc to the sites, \(R_1\), \(R_2\), ..., \(R_n\) \textit{inside the parallelogram based on the vectors} \textit{a}, \textit{b} and \textit{c}. The site of each and every atom in the unit cell is given by the \textit{fraction atomic positions}, \(x\), \(y\) and \(z\).

\[
R = xa + yb + zc,
\]
with \(0 \leq x < 1, 0 \leq y < 1, 0 \leq z < 1\)

The lattice translations are applied to each atomic positions, i.e. if there is an atom with the coordinate \([x,y,z]\) then there is also an atom with the coordinates \([x+u, y+v, z+w]\). Translation \([uvw]\) is regarded as symmetry operation.
CRYSTALLOGRAPHIC SPACE GROUP IS THE COMPLETE DESCRIPTION OF THE SYMMETRY OF CRYSTAL STRUCTURES. THE **GROUPS** ARE COMPILED FROM THE FOLLOWING SYMMETRY OPERATIONS:

1. **Lattice translation** \( A_{uvw} = u \ a + v \ b + w \ c \). Defines crystal system and type of the Bravais lattice

2. **Further point symmetry and space symmetry operations accepted by the chosen crystal systems.**
   - Rotation
   - Reflection
   - Inversion
   - Rotoinversion
   - Glide planes
   - Screw axes
Any symmetry operation can be presented by the rotation matrix and displacement vector. Suppose the lattice is built on the basis vectors \( a, b \) and \( c \) and the position of atoms are given by the fractional coordinates \([xyz]\) so that \( R = xa+yb+zc \). If we apply the movement related to the particular symmetry operation, the vectors \( a, b \) and \( c \) are transformed into \( a', b' \) and \( c' \) and the origin is displaced by the vector \( d \). The position of symmetry equivalent atom is

\[
R' = x \ a' + y \ b' + z \ c' + d = x_1 \ a + y_1 \ b + z_1 \ c
\]

\[
\begin{align*}
\begin{cases}
a' = S_{11}a + S_{21}b + S_{31}c \\
b' = S_{12}a + S_{22}b + S_{32}c \\
c' = S_{13}a + S_{23}b + S_{33}c \\
d = d_1 \ a + d_2 \ b + d_3 \ c
\end{cases}
\end{align*}
\]

\[
\begin{pmatrix}
x_1 \\
y_1 \\
z_1
\end{pmatrix} =
\begin{pmatrix}
S_{11} & S_{12} & S_{13} \\
S_{21} & S_{22} & S_{23} \\
S_{31} & S_{32} & S_{33}
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix} +
\begin{pmatrix}
d_1 \\
d_2 \\
d_3
\end{pmatrix}
\]

\text{Rotation matrix} \quad \text{Displacement vector}
Combination of symmetry operations in terms of matrices

Symmetry operation 1: \( \{S_1, d_1\} \) \[ R_1 = S_1 R_0 + d_1 \]

Symmetry operation 2: \( \{S_2, d_2\} \) \[ R_2 = S_2 R_0 + d_2 \]

Symmetry operation 3: \( \{S_1, d_1\} \rightarrow \{S_2, d_2\} \)

\[ R_2 = S_2 R_1 + d_2 = S_2 S_1 R_0 + S_2 d_1 + d_2 \]

The combination of symmetry operation is represented by the rotation matrix \( S_2 S_1 \) and displacement vector \( S_2 d_1 + d_2 \)
THE PRINCIPLE OF SPACE GROUP FORMATION IS SIMILAR TO THAT FOR THE POINT GROUP.

CRYSTAL LATTICE (THE SPACE SYMMETRY GROUP OF A CRYSTAL LATTICE)

TAKING OUT A SYMMETRY ELEMENT

Making sure that this symmetry element is not restored by the combination of the remaining symmetry elements

Getting a space symmetry group for a crystal
Space groups in 2D and 3D space

There are 17 2D (planar) space groups and 230 3D space groups. For the first time the space groups were described by Russian crystallographer E.S Fedorov

E.S. Fedorov (1853-1919)

Each of the space groups has the own name (space group symbol). As an example

P2₁, Fd3m, Cm, Cc, C2, I4bm, ...

We will start with the planar space groups.
OBLIQUE: p2

1) x, y; 2) -x, -y
OBLIQUE p1

1) $x,y$
RECTANGULAR p2mm

1) x y  
2) x -y  
3) -x y  
4) -x -y
RECTANGULAR pm

1) $x y$
2) $x - y$
1) x y
2) x + 1/2  -y
1) \(x\ y\)  
2) \(-x\ -y\)  
3) \(-x+1/2\ y+1/2\)  
4) \(x+1/2\ -y+1/2\)
RECTANGULAR c22mm

1) $x \ y$
2) $x \ -y$
3) $-x \ y$
4) $-x \ -y$
5) $x+1/2 \ y+1/2$
6) $x+1/2 \ -y+1/2$
7) $-x+1/2 \ y+1/2$
8) $-x+1/2 \ -y+1/2$
1) $x$ $y$
2) $-x$ $-y$
3) $-y$ $x$
4) $y$ $-x$
5) $-x + 1/2$ $y + 1/2$
6) $x + 1/2$ $-y + 1/2$
7) $y + 1/2$ $x + 1/2$
8) $-y + 1/2$ $-x + 1/2$
HEXAGONAL: p3

1) $x \ y$
2) $-y \ x-y$
3) $-x+y \ -x$
HEXAGONAL  p3m1

1) $x \ y$  2) $-y \ x-y$  3) $-x+y \ -x$  4) $-y \ -x$  5) $-x \ +y \ y$  6) $x \ x-y$
HEXAGONAL p31m

1) $x \ y$
2) $-y \ x-y$
3) $-x+y \ -x$
4) $y \ x$
5) $x \ -y \ -y$
6) $-x \ -x+y$
HEXAGONAL p6mm

1) x y      2) -y x-y
3) -x+y -x    4) -x -y
5) y -x+y    6) x-y x
7) -y -x    8) -x+y -y
9) x x-y 10) y x 11) x-y -y 12) -x -x+y
Escher Web Sketch

By: Nicolas Schoeni, Wes Hardaker and Gervais Chapuis
At: The Swiss Federal Institute of Technology (EPFL), Switzerland

http://escher.epfl.ch/escher/

NB! I recommend you to download Escher.jar file and run it locally from your computer
SPACE GROUPS IN 3D

International tables for crystallography VOLUME A
**P2₁/c**  

**No. 14**  
**P2₁/c**  
**Monoclinic**  
**Patterson symmetry P2/m1**  
**UNIQUE AXIS b, CELL CHOICE I**

### Generators selected

1. \( (1,0,0); (0,1,0); (0,0,1); (2); (3) \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>General:</td>
<td></td>
<td>( H ): ( f = 2n )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( 0 ): ( f = 2n )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( 0 ): ( f = 2n )</td>
</tr>
<tr>
<td>Special:</td>
<td></td>
<td>( k + l = 2n )</td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [001] \( P2_1/m \)
  
  \( a = a, b = b, c = c \)  
  Origin at \( 0,0,0 \)

### Maximal non-isomorphic subgroups

- \( \{ \} \)  
  \( P2_1/m \)  
  \( 1; 4 \)
- \( \{ \} \)  
  \( P2_1/2 \)  
  \( 1; 3 \)
- \( \{ \} \)  
  \( P1 \)  
  \( 1 \)

### Maximal isomorphic subgroups of lowest index

- \( \{ \} \)  
  \( P2_1/1 \)  
  \( \{ \} \)  
  \( 1 \)

### Minimal non-isomorphic supergroups

- \( \{ \} \)  
  \( P1 \)  
  \( 1 \)
- \( \{ \} \)  
  \( P2_1/c \)  
  \( 1 \)

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SG symbol and number
No. 14

Crystal system
Monoclinic

Point group
$P 2_1/c$

Patterson symmetry $P12/m$

Unit cell in different projections

Symmetry elements and their positions in the unit cell

Asymmetric unit of the unit cell
Positions inside a unit cell

General positions

Point symmetry group of the position

Special positions

Reflection conditions

General:

$\{h0l : l = 2n\}$

$\{0k0 : k = 2n\}$

$\{00l : l = 2n\}$

Special: as above, plus

$\{hkl : k + l = 2n\}$

$\{hkl : k + l = 2n\}$

$\{hkl : k + l = 2n\}$

$\{hkl : k + l = 2n\}$

Point symmetry group of the position

Maximal non-isomorphic subgroups

Maximal isomorphic subgroups of lowest index

Minimal non-isomorphic supergroups
Another source of information about space groups:

**Bilbao crystallographic server**

http://www.cryst.ehu.es/