Didactic material for the MaThCryst schools

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Classification of reflection conditions

- **General**: apply to all Wyckoff positions.
- **Special**: apply to special Wyckoff positions. In particular, in presence of non-characteristic and extraordinary orbits one gets additional special reflection conditions.
- **Integral**: appear when a non-primitive unit cell is selected.
- **Zonal**: appear in presence of glide planes.
- **Serial**: appear in presence of screw axes.

**Warning!**

- Systematic extinctions
- Systematic absences (actually, presences!)
- Reflection conditions
Integral conditions
They affect the whole reciprocal space and show up when a non-primitive cell is chosen
Integral reflection condition: depend on the choice of the unit cell, not on the structure

When you choose a primitive unit cell you do not see integral reflection conditions.
Change of coordinate system

**Covariant quantities**

\[(abc)P = (a'b'c')\]
\[(hkl)P = (h'k'l')\]

Row vectors

**Contravariant quantities**

\[P^{-1}\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} = \begin{pmatrix} a'^* \\ b'^* \\ c'^* \end{pmatrix}\]
\[P^{-1}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}\]
\[P^{-1}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u' \\ v' \\ w' \end{pmatrix}\]

Column vectors
Integral reflection conditions: $C$ type of unit cell

Direct space

Change of coordinate system in direct space (covariant vectors)

\[ a_P = (a_C + b_C)/2 \; ; \; a_C = a_P - b_P \]
\[ b_P = (-a_C + b_C)/2 \; ; \; b_C = a_P + b_P \]

\[
\begin{pmatrix}
\frac{1}{2} & 1 & 1 & 0 \\
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 2 & 1
\end{pmatrix}
\begin{pmatrix}
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

Change of coordinate system in reciprocal space (contravariant vectors)

\[ a^*_C = (a^*_P - b^*_P)/2 \; ; \; a^*_P = a^*_C + b^*_C \]
\[ b^*_C = (a^*_P + b^*_P)/2 \; ; \; a^*_P = -a^*_C + b^*_C \]

\[
\begin{pmatrix}
1 & 1 & 0 \\
1 & 1 & 0 \\
0 & 0 & 2
\end{pmatrix}
\begin{pmatrix}
1 & 1 & 0 \\
1 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

In both direct and reciprocal space, the conventional unit cell is $C$-centred.

Reflection conditions: $hkl : h+k = 2n$
Reminder: \( I \) vs. \( F \) cell

**\( I \)-centred cell**

\[ t(\frac{1}{2}\frac{1}{2}\frac{1}{2}) \]

**\( F \)-centred cell**

\[ t(\frac{1}{2}\frac{1}{2}0), t(\frac{1}{2}0\frac{1}{2}), t(0\frac{1}{2}\frac{1}{2}) \]
Transformation of an $I$-centred cell to a primitive cell

\begin{align*}
\mathbf{a}_p &= (-\mathbf{a}_I + \mathbf{b}_I + \mathbf{c}_I)/2 \\
\mathbf{b}_p &= (\mathbf{a}_I - \mathbf{b}_I + \mathbf{c}_I)/2 \\
\mathbf{c}_p &= (\mathbf{a}_I + \mathbf{b}_I - \mathbf{c}_I)/2
\end{align*}

\begin{align*}
\mathbf{a}_I &= \mathbf{b}_p + \mathbf{c}_p \\
\mathbf{b}_I &= \mathbf{a}_p + \mathbf{c}_p \\
\mathbf{c}_I &= \mathbf{a}_p + \mathbf{b}_p
\end{align*}

\begin{align*}
\frac{1}{2} \begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{pmatrix} & \begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix} \\
I \rightarrow P & \quad P \rightarrow I
\end{align*}
Transformation of an $F$-centred cell to a primitive cell

\[ a_F = (b_F + c_F)/2 \]  \hspace{1cm}  \[ a_P = -a_p + b_p + c_p \]
\[ b_F = (a_F + c_F)/2 \]  \hspace{1cm}  \[ b_F = a_p - b_p + c_p \]
\[ c_F = (a_F + b_F)/2 \]  \hspace{1cm}  \[ c_F = a_p + b_p - c_p \]

\[
\begin{pmatrix}
1 & 0 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0 \\
\end{pmatrix}
\]
\[ F \rightarrow P \]

\[
\begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\
\end{pmatrix}
\]
\[ P \rightarrow F \]
Reciprocal of an $I$-centred cell

In the reciprocal space, the conventional cell is $F$-centred

Reflection conditions

$hkl : h+k+l = 2n$

$h'+k'+l' = 2h+2k+2l$ even
Reciprocal of an $F$-centred cell

\[
\begin{pmatrix}
1 & 0 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}
\xrightarrow{F \rightarrow P}
\begin{pmatrix}
\bar{1} & 1 & 1 \\
1 & \bar{1} & 1 \\
1 & 1 & \bar{1}
\end{pmatrix}
\]

\[
\begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}
\xrightarrow{P \rightarrow F}
\begin{pmatrix}
1 & 0 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}
\]

\[
\begin{pmatrix}
1 & 0 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0
\end{pmatrix}
\xrightarrow{P \rightarrow I}
\begin{pmatrix}
0 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{pmatrix}
\]

In the reciprocal space, the conventional cell is $I$-centred

\[
(hkl)_P \begin{pmatrix}
\bar{1} & 1 & 1 \\
1 & \bar{1} & 1 \\
1 & 1 & \bar{1}
\end{pmatrix} = (h'k'l')_F
\]

Reflection conditions
\[
hkl : h+k = 2n ; h+l = 2n ; k+l = 2n
\]

\[
h'+k' = 2l \text{ even} \\
h'+l' = 2k \text{ even} \\
k'+l' = 2h \text{ even}
\]
Zonal reflection conditions
They affect one plane of the reciprocal space and show up in presence of a glide plane
Zonal reflection conditions: witness of glide planes
Zonal reflection conditions: witness of glide planes

Direct space
In projection along the $a$ axis the period along $b$ seems halved.

Reciprocal space
On the $(0kl)^*$ plane the period along the $b^*$ axis appears doubled.

Reflection conditions: $0kl : k = 2n$
Glide plane with a glide component along a diagonal

Primitive cell, $n_{[100]}$ glide
Glide plane with a glide component along a diagonal

In this projection, the unit cell looks like $A$-centred

Reflection conditions: $0kl : k+l = 2n$
Same as for an $A$-centred cell but valid only on the $(0kl)^*$ plane (zonal instead of integral conditions)
Serial reflection conditions
They affect one row of the reciprocal space and show up in presence of a screw axis
Serial reflection conditions: witness of screw axes

Direct space
In the projection on the c axis the period appear reduced to $\frac{1}{4}$.

Reciprocal space
In the [001]* direction the period appears multiplied by four.

Reflection conditions:

00l : $l = 4n$
From reflections conditions to space groups (absence of metric specialisation is assumed hereafter)
Example 1: $a, b, c; \alpha = \beta = \gamma = 90^\circ$

Integral reflection conditions: centred cell

\[
\begin{align*}
    hkl: k+l &= 2n \\
    0kl: k+l &= 2n \\
    h0l: l &= 2n \\
    h00: h &= 2n \\
    h02: k &= 2n \\
    0k0: h &= 2n \\
    00l: l &= 2n
\end{align*}
\]

Zonal reflection conditions: glide plane

\[
\begin{align*}
    0A \\
    h even: a \text{ glide} \\
    \text{hk0: perpendicular to } [001] \\
    a_{[001]}
\end{align*}
\]

Extinction symbol: $A--a$

Possible space-group types: $Am2a, A2_1ma, Amma$
Example 2: $a = b, c; \alpha = \beta = \gamma = 90^\circ$

No integral reflection condition $\rightarrow tP$

- $hk0: h+k = 2n$
- $0k0: k = 2n$
- $hhl: l = 2n$
- $00l: l = 2n$

Zonal reflection conditions: glide plane

- $hk0: \text{perpendicular to } [001]$
- $h+k \text{ even: } n \text{ glide}$
- $hhl: \text{perpendicular to } [1\bar{1}0]$
- $l \text{ even: } c \text{ glide}$

Non-independent

Extinction symbol: $Pn-c$

Possible space-group type: $P4_2/nmc$
Example 3: $a = b = c; \alpha = \beta = \gamma = 90^\circ$

\[ hkl : h + k + l = 2n \quad \text{Integral reflection condition} \]

\[ 0kl : k = 2n \quad \text{Zonal reflection condition} \]
\[ 0kl : l = 2n \]
\[ h0l : h = 2n \]
\[ h0l : l = 2n \quad \text{Zonal reflection condition} \]
\[ hk0 : h = 2n \]
\[ hk0 : k = 2n \]
\[ hhl : 2h + l = 4n \quad \text{Zonal reflection condition} \]
\[ hhl : l = 2n \]
\[ 00l : l = 4n \]

\[ 0kl : \text{perpendicular to [100], } k \text{ even} \quad b_{[100]} \]
\[ 0kl : \text{perpendicular to [100], } l \text{ even} \quad c_{[100]} \]
\[ h0l : \text{perpendicular to [010], } h \text{ even} \quad a_{[010]} \]
\[ h0l : \text{perpendicular to [010], } l \text{ even} \quad c_{[010]} \]
\[ hk0 : \text{perpendicular to [001], } h \text{ even} \quad a_{[001]} \]
\[ hk0 : \text{perpendicular to [001], } k \text{ even} \quad b_{[001]} \]
\[ hhl : \text{perpendicular to [1\bar{1}0], } 2h + l = 4n \quad ?? \]
Example 3: $a = b = c; \alpha = \beta = \gamma = 90^\circ$

Direct lattice: $(a+b+c)/4$  
Reciprocal lattice: $h+k+l = 4n$  
$(110) \Rightarrow h = k \quad h+h+l = 4n$

$hhl: 2h+l = 4n \quad d_{[1\bar{1}0]}$
Example 3: $a = b = c; \alpha = \beta = \gamma = 90^\circ$

- Integral reflection condition: $cI$
  - $0kl: k = 2n$ (perpendicular to [100], $k$ even)
  - $0kl: l = 2n$ (perpendicular to [100], $l$ even)
  - $h0l: h = 2n$ (perpendicular to [010], $h$ even)
  - $h0l: l = 2n$ (perpendicular to [010], $l$ even)
  - $hk0: h = 2n$ (perpendicular to [001], $h$ even)
  - $hk0: k = 2n$ (perpendicular to [001], $k$ even)

- Zonal reflection condition:
  - $hkl: h+k+l = 2n$ (perpendicular to [110], $2h+l = 4n$)
  - $hhl: 2h+l = 4n$ (perpendicular to [110], $2h+l = 4n$)
  - $hhl: l = 2n$
  - $00l: l = 4n$

Extinction symbol: $Ia-d$

Possible space-group type: $Ia\bar{3}d$
Example 3: $a = b = c; \alpha = \beta = \gamma = 90^\circ$

Reflection conditions

$h, k, l$ permutable

General:

$hkl : h + k + l = 2n$

$0kl : k, l = 2n$

$hhl : 2h + l = 4n$

$h00 : h = 4n$
Symmorphic space groups (1)

$C \ m \ m \ m$

$hk0: h+k = 2n$

$h0l: h = 2n$

$0kl: k = 2n$
Symmorphic space groups (2)

However, \( h + h = 2h \) always true!