Group definition and properties

A group \((G, \ast)\) is a nonempty set \(G\) together with a binary operation \(\ast\) satisfying the group axioms below. \(a \ast b\) represents the result of applying the operation \(\ast\) to the ordered pair \((a, b)\) of elements of \(G\). The group axioms are the following:

- **Associativity:** For all \(a, b, c\) in \(G\), \((a \ast b) \ast c = a \ast (b \ast c)\).
- **Identity element:** There is an element \(e\) in \(G\) such that for all \(a\) in \(G\), \(e \ast a = a \ast e = a\).
- **Inverse element:** For all \(a\) in \(G\), there is an element \(b\) in \(G\) such that \(a \ast b = b \ast a = e\), where \(e\) is the identity element from the previous axiom.

You will often also see the axiom:

- **Closure:** For all \(a\) and \(b\) in \(G\), \(a \ast b\) belongs to \(G\).

**Example:** Proper point group 4

\[
4 = \{1, 4, 2, 4^{-1}\}
\]

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
0 & 1 & 0 \\
-1 & 0 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\]

Bicolor Symmetry Groups

1929 Heesch, introduces the antiidentity operation properties: \(u^2 = 1, \; ut = tu\) for all \(t\in T\)

aka time reversal group = \(\{1,1'\}\)

1945 Shubnikov, re-introduces concept

1951 Shubnikov, describes and illustrates all of the bicolor point groups

1955 Belov et al., first complete listing of the bicolor space groups

1957 Zamorzaev, group theoretical derivation of bicolor space groups

1965 Opechowski and Guccione, first complete derivation and enumeration of the bicolor space groups

2001 Litvin, corrected Opechowski-Guccione symbols

Alexey Vasilyevich Shubnikov 1887-1970

Heesch, introduces the antiidentity operation properties: \(u^2 = 1, ut = tu\) for all \(t\in T\)

aka time reversal group = \(\{1,1'\}\)

1945 Shubnikov, re-introduces concept

1951 Shubnikov, describes and illustrates all of the bicolor point groups

1955 Belov et al., first complete listing of the bicolor space groups

1957 Zamorzaev, group theoretical derivation of bicolor space groups

1965 Opechowski and Guccione, first complete derivation and enumeration of the bicolor space groups

2001 Litvin, corrected Opechowski-Guccione symbols
Derivation of Antisymmetry Point Groups

If $M$ is an antisymmetry group, and $1'$ an antiidentity operation

Type I, $M = G$ for some crystallographic point group $G$

Type II, $M = G \cup G1'$ for some crystallographic point group $G$

Type III, $M = H \cup (G\mid H)1'$ for some crystallographic point group $G$, where $H$ is a halving group of $G$.

example: $G = 2/m = \{1,2,i,m\}$

$H = \{2\}$

$21' = \{1,2,1',2'\}$

$2' = \{1,2'\}$

$M = 2/m' \cup 2'/m \cup 2'/m'$

Example Magnetic Point Groups

<table>
<thead>
<tr>
<th>Point group</th>
<th>nontrivial</th>
<th>magnetic</th>
<th>point groups</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1</td>
<td>-1'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m</td>
<td>m</td>
<td>m</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2/m</td>
<td>2/m</td>
<td>2/m'</td>
<td>2'/m'</td>
</tr>
<tr>
<td>222</td>
<td>2'2'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>mm2</td>
<td>m'm2'</td>
<td>m'm2'</td>
<td></td>
</tr>
<tr>
<td>mmm</td>
<td>m'm'm</td>
<td>m'm'm</td>
<td>m'm'm'm</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-4</td>
<td>-4'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/m</td>
<td>4/m</td>
<td>4/m'</td>
<td>4'/m'</td>
</tr>
<tr>
<td>422</td>
<td>4'2'2'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4mm</td>
<td>4'm'm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-42m</td>
<td>-4'2'm</td>
<td>-4'2'm'</td>
<td>-42'm'</td>
</tr>
<tr>
<td>4/mmm</td>
<td>4/m'm</td>
<td>4'/m'm</td>
<td>4'/m'm'</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

122 crystallographic magnetic point groups
### Derivation of Antisymmetry Space Groups

If M is an antisymmetry group, and 1' an antiidentity operation

- **Type I, M = F** for some crystallographic space group F
- **Type II, M = F ∪ F1'** for some crystallographic space group F
- **Type III, M = D ∪ (F\D)1'** for some crystallographic space group F, where D is a subgroup of index two of F.

#### 674 a. $M_T$, where D is an equi-translation subgroup of F
   (D has the same lattice type as F and M)

#### 517 b. $M_R$, where D is an equi-class subgroup of F
   ($M_R$ contains anti-translations and is doubled with respect to F)

#### 1651 Total

### Cosets

Let G denote a group, H a subgroup of G and $a ∈ G$. Then the right coset of H in G determined by a, denoted $Ha$, is

$$Ha = \{ha | h ∈ H\}$$

The left coset of H in G determined by a, denoted aH, is

$$aH = \{ah | h ∈ H\}$$

A subgroup H of a group G is said to be normal if $gH = Hg$ for all $g ∈ G$, i.e., left and right cosets are the same.
Cosets

Example: Let \( G = 4 = \{1,4,2,4^{-1}\} \), \( H = 2 = \{1,2\} \). Find the right cosets \( 2g \) and the left cosets \( g2 \) for each \( g \in 4 \).

\[
\begin{align*}
2*1 &= 1, 2*1 = 1, 2 \quad &1*2 &= 1, 2 = 1, 2 \\
2*4 &= 1, 2, 4 = \{4, 4^{-1}\} \quad &4*2 &= 4, 1, 2 = \{4, 4^{-1}\} \\
2*2 &= 1, 2, 2 = \{2, 1\} \quad &2*2 &= 2, 1, 2 = \{2, 1\} \\
2*4^{-1} &= 1, 2, 4^{-1} = \{4^{-1}, 4\} \quad &4^{-1}*2 &= 1, 2, 4^{-1} = \{4^{-1}, 4\}
\end{align*}
\]

Two unique cosets of 2 in 4. The right and left cosets are the same, so 2 is a normal subgroup.

Cosets

Of great interest is the coset decomposition of the space groups with respect to their translational subgroups.

Let \( T = (\Omega|\tau) \) be a translational group defining a lattice, and \( W \) be an arbitrary symmetry operation \( (W|w) \) of space group \( G \).

Then for all of the products \( (\Omega|\tau)(W|w) = (W|w+\tau) \), for every \( j \) the matrix part \( W \) is the same.

Thus, \( TW \) denotes the right coset decomposition of \( T \) in \( G \). The left cosets \( WT \) are the same, so translational subgroups are normal subgroups.

The decomposition of the space groups into cosets is the basis of description of the space groups in the International Tables.

Derivation of Antisymmetry Space Groups

If \( M \) is an antisymmetry group, and \( 1' \) an antiidentity operation

Type I, \( M = F \) for some crystallographic space group \( F \)

Type II, \( M = F \cup F 1' \) for some crystallographic space group \( F \)

Type III, \( M = D \cup (F\setminus D)1' \) for some crystallographic space group \( F \), where \( D \) is a subgroup of index two of \( F \).

a. \( M_T \), where \( D \) is an equi-translation subgroup of \( F \)  
(D has the same lattice type as \( F \) and \( M \))

b. \( M_R \), where \( D \) is an equi-class subgroup of \( F \)  
(\( M_R \) contains anti-translations and is doubled with respect to \( F \))

Magnetic Space Group

Type IIIa, \( M_T \), Example \( P2'/m \) (No. 11.3.61)

\[
\begin{align*}
F &= P2/m = T(1|0,0,0) + T(2|0,0,0) + T(m|0,0,0) + T(i|0,0,0) \\
D &= Pm = T(1|0,0,0) + T(m|0,0,0) \\
M_T &= D + (F\setminus D)1' \\
(F\setminus D) &= T(2|0,0,0) + T(i|0,0,0) \\
(F\setminus D)1' &= T(2|0,0,0)' + T(i|0,0,0)' \\
M_T &= T(1|0,0,0) + T(m|0,0,0) + T(2|0,0,0)' + T(i|0,0,0)'
\end{align*}
\]
MAGNETIC SPACE GROUP LATTICES

triclinic system

\[ P = P_{a,b,c} \]
\[ P_{2\alpha} = P_{a,b,2c} \]
\[ T_\alpha = c = (0,0,1) \]

anti-translations join open and full circles
regular translations join open-open and full-full circles

\( T_\alpha = \) anti-translation

Taken from Litvin (2001) after Opechowski & Guccione (1965)

monoclinic system (y is the unique axis)

\[ P = P_{a,b,y} \]
\[ P_{2\alpha} = P_{a,b,y} \]
\[ T_\alpha = a = (1,0,0) \]
\[ T_y = b = (0,1,0) \]
\[ T_\alpha = c = (0,0,1) \]
\[ T_y = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \]

MAGNETIC SPACE GROUP LATTICES

orthorhombic system

\[ P = P_{a,b,c} \]
\[ P_{2\alpha} = P_{a,b,2c} \]
\[ T_\alpha = a = (1,0,0) \]
\[ T_y = b = (0,1,0) \]

\[ T_\alpha = c = (0,0,1) \]

\[ P_z = P_{d,2\alpha,0} \]
\[ T_z = a = (1,0,0) \]
\[ T_y = b = (0,1,0) \]

\[ T_\alpha = c = (0,0,1) \]

MAGNETIC SPACE GROUP LATTICES

orthorhombic system, continued

\[ A = A_{a,b,1/2c} \]
\[ A_{2\alpha} = A_{a,b,1/2c} \]
\[ T_\alpha = a = (1,0,0) \]
\[ T_y = b = (0,1,0) \]
\[ T_\alpha = c = (0,0,1) \]

\[ T_x = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \]

\[ A_1 = A_{a,b,1/2c} \]
\[ T_\alpha = a = (1,0,0) \]
\[ T_y = b = (0,1,0) \]
\[ T_\alpha = c = (0,0,1) \]

\[ T_x = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \]
MAGNETIC SPACE GROUP LATTICES

orthorhombic system, continued

F = F_{16(a+b+c)}
\begin{align*}
T_a &= \frac{1}{2}(a+c) = (\frac{1}{2},0,0) \\
T_b &= \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \\
T_c &= \frac{1}{2}(a+b+c) = (0,0,1)
\end{align*}

MAGNETIC SPACE GROUP LATTICES
tetragonal system

P = P_{a,b,c}
\begin{align*}
P_{a,b,c} &= P_{a,b,c} \\
T_a &= a = (1,0,0)
\end{align*}

MAGNETIC SPACE GROUP LATTICES
trigonal system

R = R_{a,b,c}
\begin{align*}
R_{a,b,c} &= R_{a,b,c} \\
T_a &= a = (1,0,0)
\end{align*}

MAGNETIC SPACE GROUP LATTICES
cubic system

P = P_{a,b,c}
\begin{align*}
P_{a,b,c} &= P_{a,b,c} \\
T_a &= a = (1,0,0)
\end{align*}

hexagonal system

P = P_{a,b,c}
\begin{align*}
P_{a,b,c} &= P_{a,b,c} \\
T_a &= c = (0,0,1)
\end{align*}
Magnetic Space Group
Type IIIb, $M_R$, Example $P_{2b}c'a'2_1$ (No. 29.7.204)

\[ F = Pca_2_1 = T + T(m_x|1/2,0,1/2) + T(m_y|1/2,2,0,0) + T(2z|0,0,1/2) \]

\[ P_{2b} = P_{a,2b,c} \]

\[ t_x = b = (0,1,0) \]

\[ D = Pca_2_1 = T^0 + T^0(m_x|1/2,1,1/2) + T^0(m_y|1/2,2,1,0) + T^0(2z|0,0,1/2) \]

If it is primed in the Opechowski-Guccione symbol then it appears in $D$ coupled with $t_x$, and primed in $(F\backslash D)^1$.

If it is unprimed in the Opechowski-Guccione symbol then it appears unchanged in $D$, and coupled with $t_x$ and primed in $(F\backslash D)^1$.

\[ M_R = T_D(1|0,0,0) + T_D(m_x|1/2,1,1/2) + T_D(m_y|1/2,2,0,0) + T_D(2z|0,0,1/2) \]

\[ + T_D(1|0,0,0)' + T_D(m_x|1/2,0,1/2)' + T_D(m_y|1/2,0,0)' + T_D(2z|0,1,1/2)' \]

\[ N_1.N_2.N_3, \text{ where } N_1 \text{ is a sequence number for the group type to which } F \text{ belongs, numbered the same as given in the International Tables. } N_2 \text{ is a sequence number of the magnetic space group types of the superfamily of } F. \text{ Group types } F \text{ always have the assigned number } N_1.1.N_3, \text{ and group types } F^1 \text{ the assigned number } N_1.2.N_3. \text{ } N_3 \text{ is a global sequential numbering of the magnetic space group types.} \]
Recognizing the different space group types, Type I, uncolored space groups

Recognizing the different space group types, Type II, grey groups

Coset representatives of the decomposition of the magnetic space group with respect to its translational subgroup.
Recognizing the different space group types, Type IIIa, $M_I$ (no anti-translations)

Entries with primed coset representatives

Recognizing the different space group types, Type IIIb, $M_R$ (with anti-translations)

Entries with unprimed coset representatives (and colored lattices)

Typos in Opechowski & Guccione (1965) corrected by Opechowski (1986), given in Litvin (2001)

<table>
<thead>
<tr>
<th>Numbering In Table 1</th>
<th>Opechowski &amp; Guccione (1965)</th>
<th>Opechowski (1986)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.4.102</td>
<td>$P_{2a} 222$</td>
<td>$P_{2a} 222$</td>
</tr>
<tr>
<td>43.4.323</td>
<td>$Fdd'2$</td>
<td>$Fdd'2$</td>
</tr>
<tr>
<td>47.6.352</td>
<td>$P_{2a} mmm$</td>
<td>$P_{2a} mmm$</td>
</tr>
<tr>
<td>67.17.593</td>
<td>$C_{11} m'm'a'$</td>
<td>$C_{11} m'm'a'$</td>
</tr>
<tr>
<td>108.8.899</td>
<td>$I4'm'$</td>
<td>$I4'm'$</td>
</tr>
<tr>
<td>108.9.900</td>
<td>$I4c'm'$</td>
<td>$I4c'm'$</td>
</tr>
<tr>
<td>124.1.1018</td>
<td>$P4/mcr$</td>
<td>$P4/mcc$</td>
</tr>
<tr>
<td>132.4.1113</td>
<td>$P4_{1}/mcm'$</td>
<td>$P4_{1}/mcm'$</td>
</tr>
</tbody>
</table>

Other changes to Opechowski-Guccione symbols given by Litvin (2001)

In both Opechowski & Guccione (1965) Opechowski (1986) the symbol $P_{2a} c'ca$ is listed twice, in the numbering of Table 1, at entries 54.11.438 and 54.13.440. The second has been changed to $P_{2a} c'ca'$, a magnetic group which has a non-magnetic subgroup of the type $Pnna$.

<table>
<thead>
<tr>
<th>Numbering In Table 1</th>
<th>Opechowski &amp; Guccione (1965)</th>
<th>Opechowski (1986)</th>
<th>Table 1 Litvin (2001)</th>
</tr>
</thead>
<tbody>
<tr>
<td>131.13.1109</td>
<td>$P_{2} 4'2/m'm'c'$</td>
<td>$P_{2} 4'2/m'm'c'$</td>
<td></td>
</tr>
<tr>
<td>177.7.1385</td>
<td>$P_{2c} 6'22'$</td>
<td>$P_{2c} 6'22'$</td>
<td></td>
</tr>
<tr>
<td>180.7.1402</td>
<td>$P_{2c} 6'22'$</td>
<td>$P_{2c} 6'22'$</td>
<td></td>
</tr>
</tbody>
</table>
References
Boisen, M.B. Jr. (1977) The adjunction of antiidentity operations to point groups, including a derivation of the magnetic point groups. Z. Krist. 145, S. 197-215.

Colored lattice types that cannot be setup with color group option in GSAS
Triclinic: \( P_{2a} \)
Monoclinic: \( P_{2a}, P_{2ba}, P_{2ca}, P_{C2}, C_{2a} \)
Orthorhombic: \( P_{2a}, P_{2ba}, P_{2ca}, P_{C2}, P_{F}, P_{T}, P_{A}, A_{2a}, A_{T}, C_{2ca}, C_{i} \)
Tetragonal: \( P_{2a}, P_{C2}, P_{I} \)
Trigonal: \( R_{R} \)
Hexagonal: \( P_{2c} \)
Cubic: \( P_{F} \)

Colored lattice types that can be setup with color group option in GSAS
Monoclinic: \( C_{p} \)
Orthorhombic: \( A_{p}, C_{p}, F_{C}, F_{A}, I_{p} \)
Tetragonal: \( I_{p} \)
Cubic: \( I_{p} \)